



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 02:40 PM UTC

PDB ID : 8Y7E / pdb_00008y7e
EMDB ID : EMD-39013
Title : Cryo-EM Structure of the human minor pre-B complex (pre-precatalytic spliceosome) U12 snRNP part
Authors : Bai, R.; Yuan, M.; Zhang, P.; Luo, T.; Shi, Y.; Wan, R.
Deposited on : 2024-02-04
Resolution : 4.66 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:

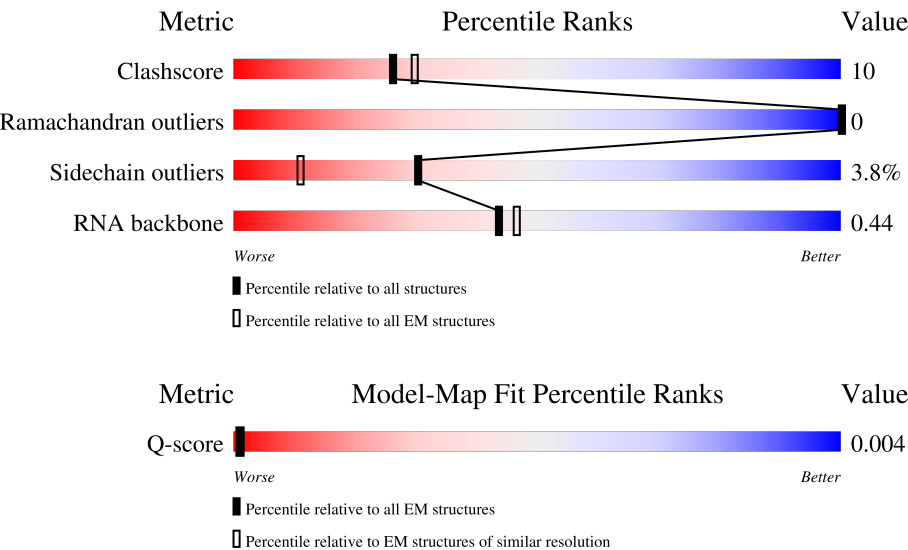
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 4.66 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	2028 (4.16 - 5.16)

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	A	280	5% . . 89%
2	1	1304	26% 61% 12% 26%
3	2	895	12% 20% 76%

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Mol	Chain	Length	Quality of chain
4	3	1217	
5	4	424	
6	5	125	
7	6	110	
8	7	86	
9	H	150	
10	h	126	
11	i	240	
12	j	119	
13	k	118	
14	l	92	
15	m	86	
16	n	76	
17	v	230	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 26949 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	30	Total	C	N	O	P	0	0
			613	276	86	221	30		

- Molecule 2 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1	971	Total	C	N	O	P	S	0	0
			7766	4961	1342	1415	1	47		

- Molecule 3 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	216	Total	C	N	O	S	0	0
			1674	1067	296	305	6		

- Molecule 4 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	3	1193	Total	C	N	O	P	S	0	0
			9352	5932	1590	1784	1	45		

- Molecule 5 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	4	78	Total	C	N	O	0	0
			383	227	78	78		

- Molecule 6 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	109	Total	C	N	O	S	0	0
			906	582	157	163	4		

- Molecule 7 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	105	Total	C	N	O	S	0	0
			811	502	145	151	13		

- Molecule 8 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	81	Total	C	N	O	S	0	0
			669	422	117	124	6		

- Molecule 9 is a RNA chain called U12 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	50	Total	C	N	O	P	0	0
			1079	482	203	344	50		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	h	80	Total	C	N	O	0	0
			393	233	80	80		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	i	86	Total	C	N	O	0	0
			422	250	86	86		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	j	82	Total	C	N	O	0	0
			406	242	82	82		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	k	85	Total	C	N	O	0	0
			422	252	85	85		

- Molecule 14 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	l	79	Total	C	N	O	0	0
			391	233	79	79		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
15	m	74	Total	C	N	O	0	0
			361	213	74	74		

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

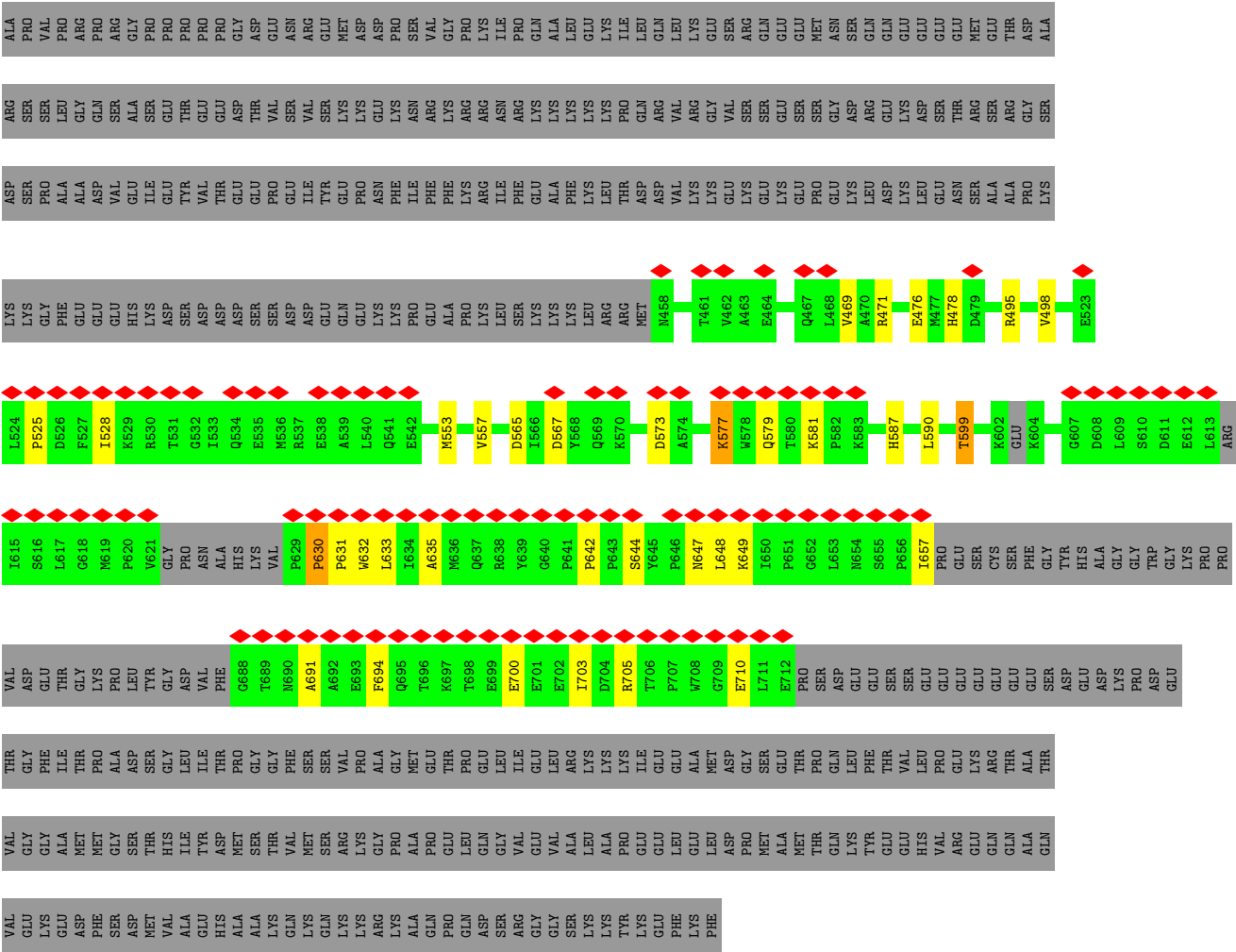
Mol	Chain	Residues	Atoms				AltConf	Trace
16	n	68	Total	C	N	O	0	0
			334	198	68	68		

- Molecule 17 is a protein called Sodium channel modifier 1.

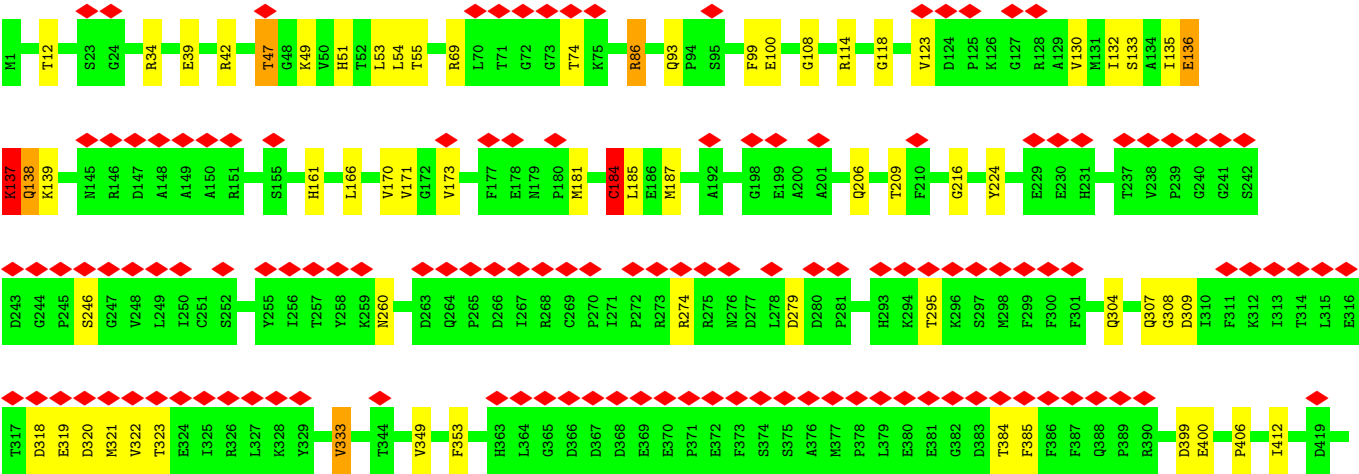
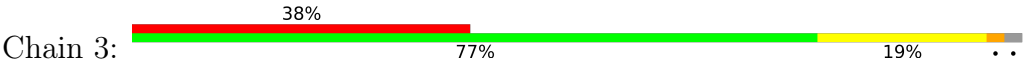
Mol	Chain	Residues	Atoms					AltConf	Trace
17	v	119	Total	C	N	O	S	0	0
			963	601	179	178	5		

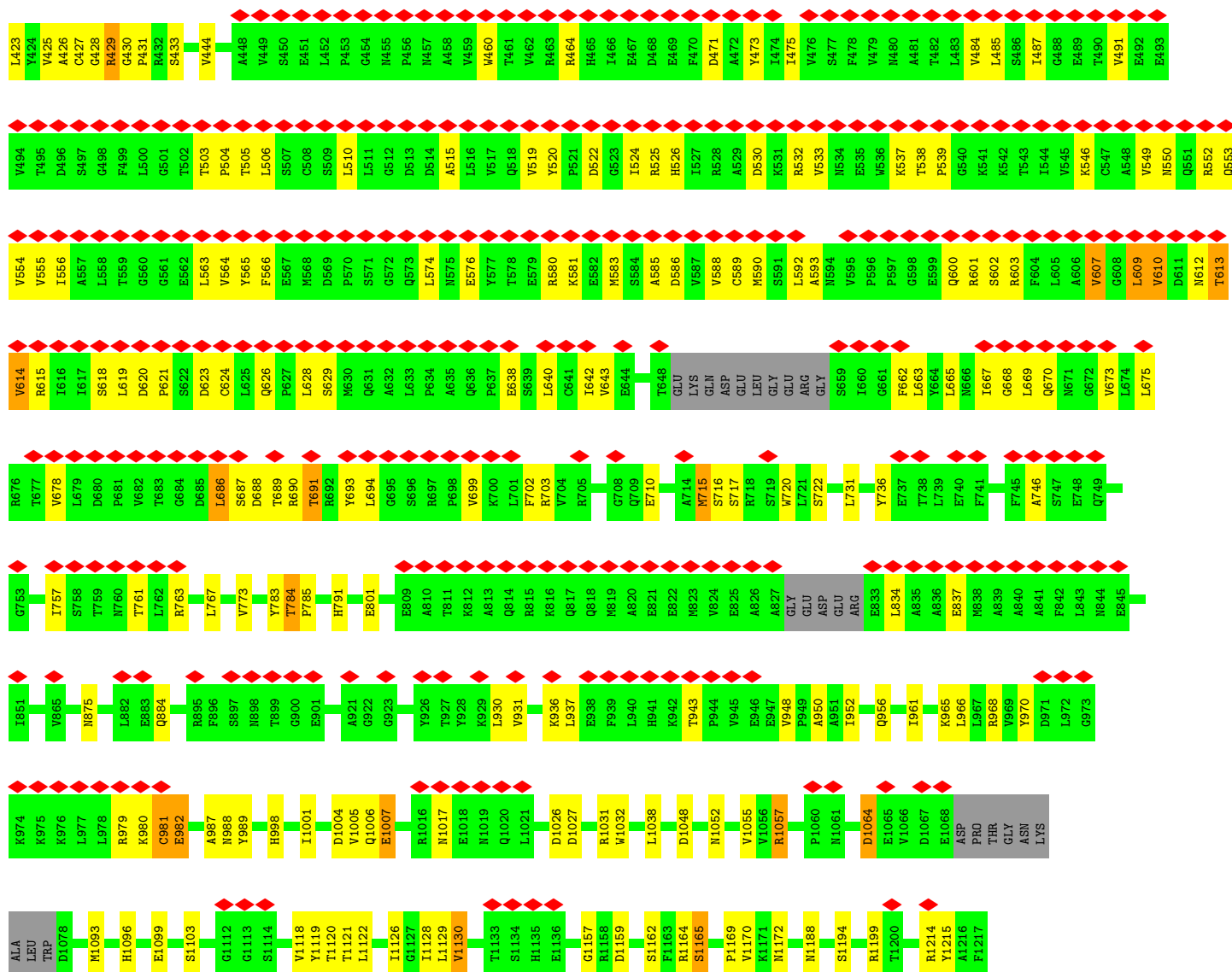
- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
18	6	3	Total	Zn	0
			3	3	
18	v	1	Total	Zn	0
			1	1	

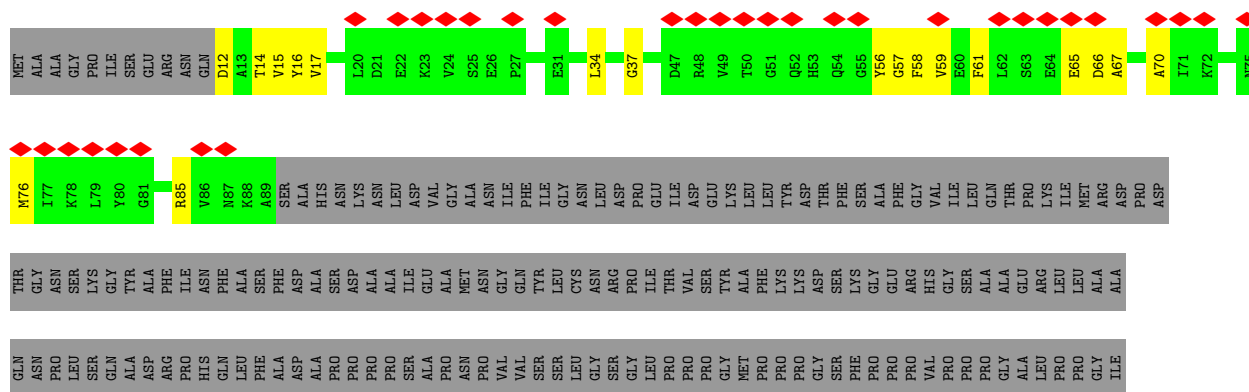


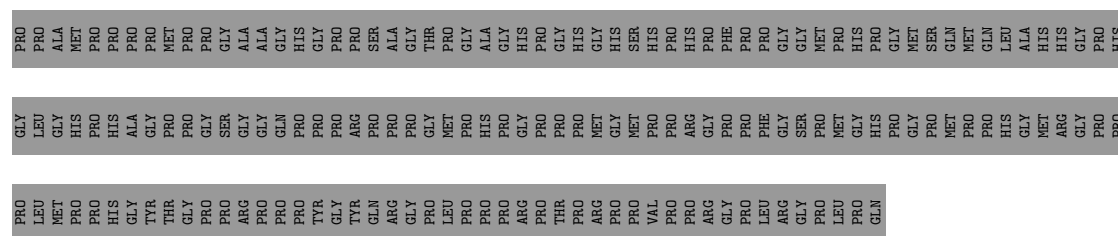
● Molecule 4: Splicing factor 3B subunit 3



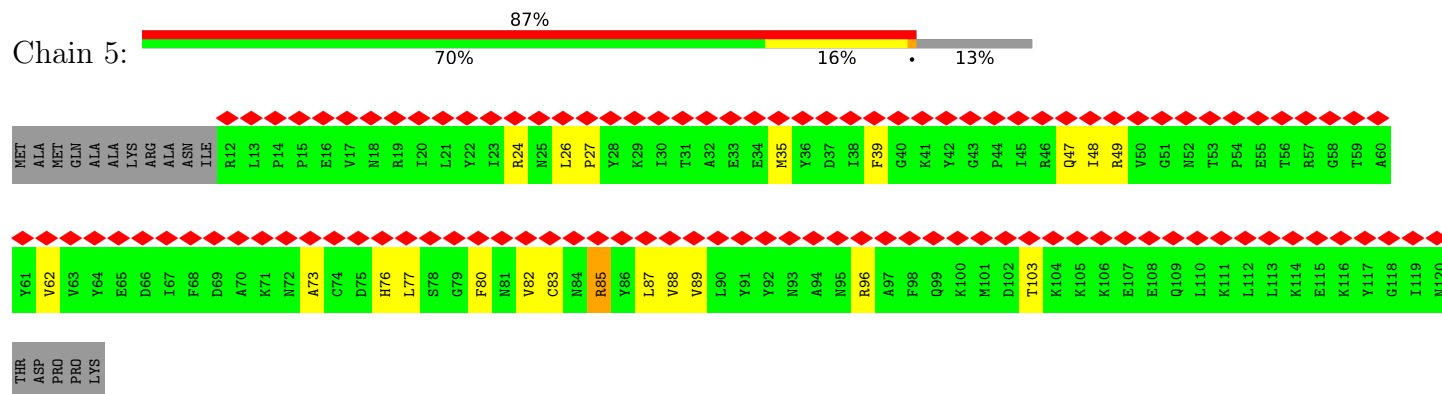


• Molecule 5: Splicing factor 3B subunit 4

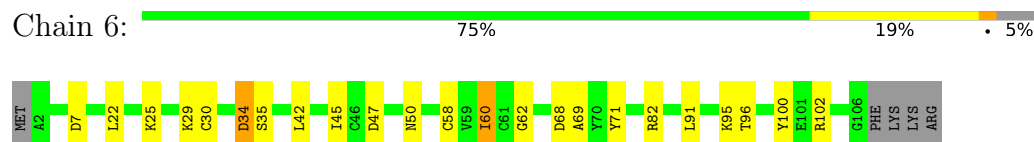




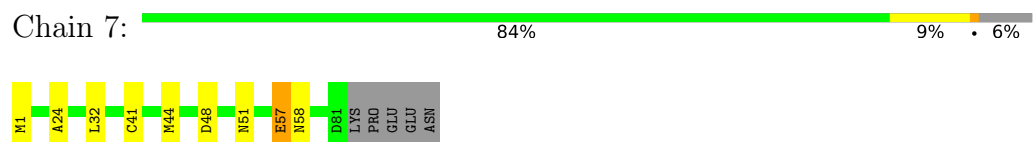
- Molecule 6: Splicing factor 3B subunit 6



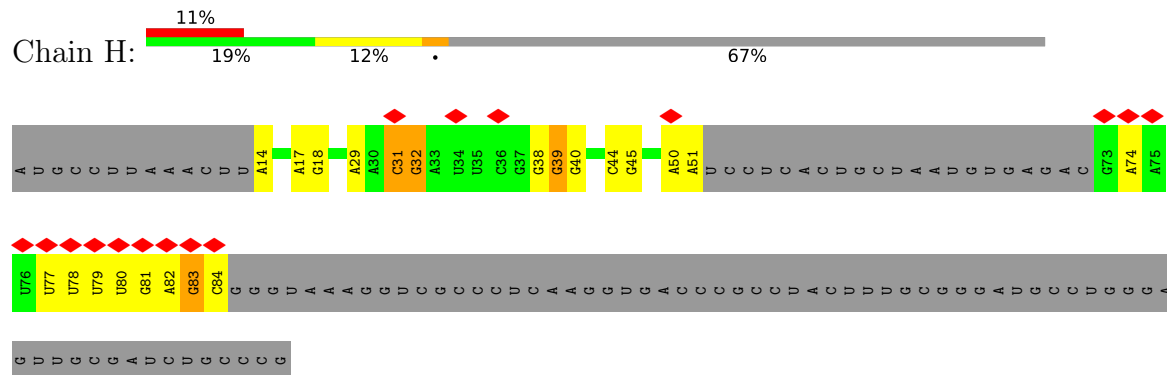
- Molecule 7: PHD finger-like domain-containing protein 5A



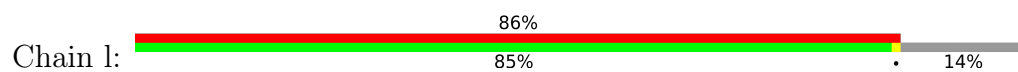
- Molecule 8: Splicing factor 3B subunit 5



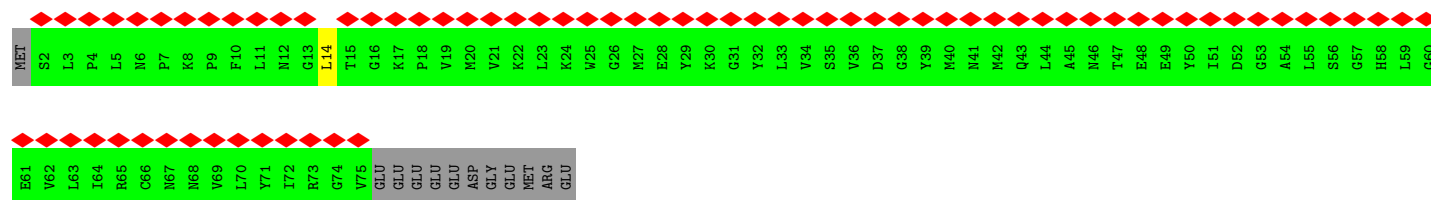
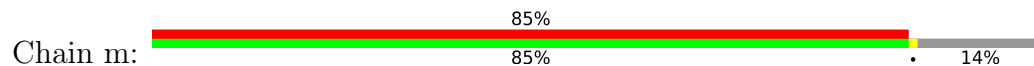
- Molecule 9: U12 snRNA



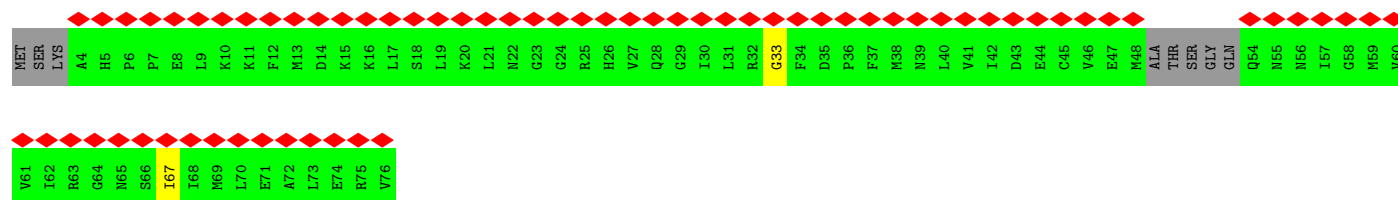
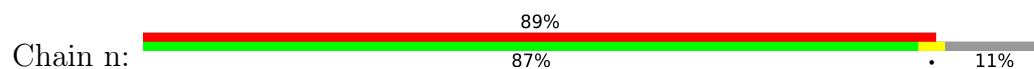
- Molecule 10: Small nuclear ribonucleoprotein Sm D3



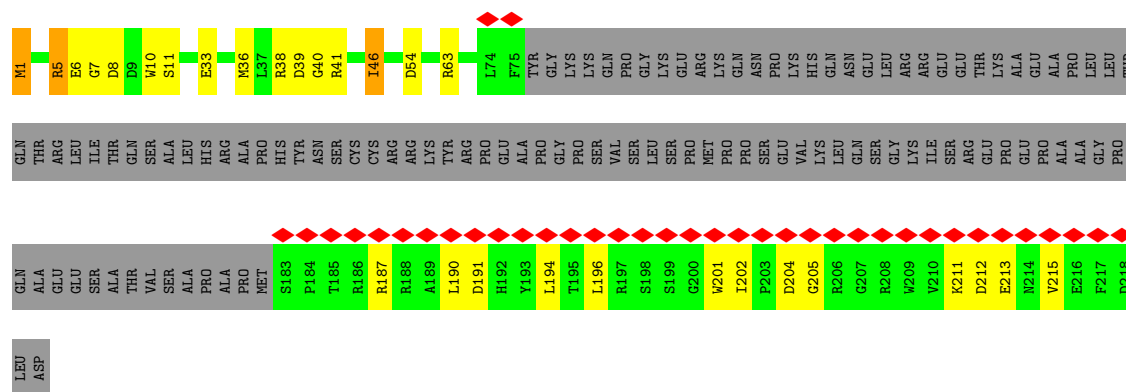
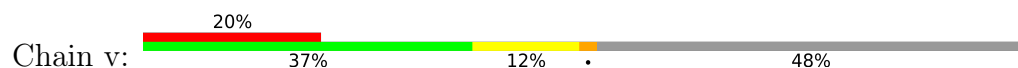
• Molecule 15: Small nuclear ribonucleoprotein F



• Molecule 16: Small nuclear ribonucleoprotein G



• Molecule 17: Sodium channel modifier 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	107724	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.029	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size ($\text{\AA}$)	549.9904, 549.9904, 549.9904	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, ZN, TPO

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	A	0.28	0/678	0.40	0/1048
2	1	1.13	0/7908	0.87	10/10698 (0.1%)
3	2	0.98	0/1710	0.88	5/2306 (0.2%)
4	3	1.00	1/9531 (0.0%)	0.81	12/12931 (0.1%)
5	4	0.95	0/382	1.12	0/529
6	5	0.77	0/925	0.80	0/1247
7	6	1.09	0/825	1.01	4/1106 (0.4%)
8	7	1.27	0/688	0.92	2/930 (0.2%)
9	H	0.32	0/1209	0.39	0/1882
10	h	0.79	0/391	0.99	0/540
11	i	0.85	0/421	1.14	3/583 (0.5%)
12	j	0.87	0/405	1.11	0/563
13	k	1.11	0/420	1.20	1/583 (0.2%)
14	l	1.02	0/390	1.24	0/542
15	m	1.21	1/360 (0.3%)	1.24	0/497
16	n	0.85	0/332	1.09	1/458 (0.2%)
17	v	0.95	0/984	0.76	3/1326 (0.2%)
All	All	1.01	2/27559 (0.0%)	0.86	41/37769 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	784	THR	C-N	-5.23	1.28	1.33
15	m	14	LEU	CA-C	5.11	1.59	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	6	60	ILE	N-CA-C	8.66	119.45	110.62
3	2	642	PRO	CA-C-N	8.25	128.21	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	642	PRO	C-N-CA	8.25	128.21	119.05
2	1	1262	ARG	N-CA-C	7.36	118.95	111.07
4	3	981	CYS	N-CA-C	6.94	120.96	111.39
4	3	137	LYS	N-CA-C	6.58	120.88	112.86
2	1	1250	CYS	N-CA-C	6.53	118.40	111.28
2	1	844	VAL	N-CA-C	6.42	118.00	111.00
4	3	979	ARG	N-CA-C	6.26	119.86	109.46
2	1	1003	VAL	N-CA-C	6.03	116.81	110.72
16	n	67	ILE	CB-CA-C	-5.96	104.80	111.23
4	3	1172	ASN	N-CA-C	5.80	119.55	111.90
4	3	184	CYS	N-CA-C	5.74	118.12	109.23
7	6	47	ASP	N-CA-C	5.74	117.99	111.11
11	i	52	LYS	CA-C-N	-5.56	114.20	119.76
11	i	52	LYS	C-N-CA	-5.56	114.20	119.76
4	3	320	ASP	N-CA-C	5.54	117.32	111.28
7	6	71	TYR	N-CA-C	-5.50	101.90	110.42
3	2	647	ASN	N-CA-C	5.46	120.06	113.17
11	i	5	LYS	N-CA-C	5.46	118.16	111.82
3	2	630	PRO	CA-C-N	5.42	125.06	119.05
3	2	630	PRO	C-N-CA	5.42	125.06	119.05
2	1	556	ILE	CA-C-N	-5.36	111.14	121.58
2	1	556	ILE	C-N-CA	-5.36	111.14	121.58
4	3	1130	VAL	N-CA-C	5.33	113.71	107.89
7	6	34	ASP	N-CA-C	5.29	118.93	111.52
17	v	224	PRO	CA-C-N	5.28	125.18	119.85
17	v	224	PRO	C-N-CA	5.28	125.18	119.85
4	3	884	GLN	CA-C-N	-5.26	114.36	123.25
4	3	884	GLN	C-N-CA	-5.26	114.36	123.25
2	1	941	ASN	CA-C-N	-5.24	113.57	123.27
2	1	941	ASN	C-N-CA	-5.24	113.57	123.27
8	7	57	GLU	CA-C-N	-5.21	114.20	122.23
8	7	57	GLU	C-N-CA	-5.21	114.20	122.23
2	1	567	VAL	N-CA-CB	-5.20	105.36	112.28
2	1	1251	LEU	N-CA-C	5.09	121.65	110.80
13	k	99	MET	N-CA-C	5.09	116.80	108.76
17	v	219	SER	N-CA-C	5.07	116.81	111.28
4	3	333	VAL	N-CA-C	-5.07	103.29	109.01
4	3	715	MET	CA-C-N	5.01	128.77	122.16
4	3	715	MET	C-N-CA	5.01	128.77	122.16

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	A	613	0	315	24	0
2	1	7766	0	7934	146	0
3	2	1674	0	1580	44	0
4	3	9352	0	9273	210	0
5	4	383	0	173	25	0
6	5	906	0	913	27	0
7	6	811	0	788	17	0
8	7	669	0	631	8	0
9	H	1079	0	541	15	0
10	h	393	0	170	1	0
11	i	422	0	177	1	0
12	j	406	0	170	0	0
13	k	422	0	175	1	0
14	l	391	0	163	1	0
15	m	361	0	158	0	0
16	n	334	0	143	1	0
17	v	963	0	945	51	0
18	6	3	0	0	0	0
18	v	1	0	0	0	0
All	All	26949	0	24249	516	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 (516) 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)
2:1:641:ILE:HD11	2:1:675:MET:CE	1.58	1.31
5:4:14:THR:HA	5:4:59:VAL:O	1.32	1.23
5:4:12:ASP:CB	5:4:67:ALA:HB1	1.80	1.11
2:1:641:ILE:CD1	2:1:675:MET:CE	2.27	1.10
3:2:691:ALA:HB1	17:v:190:LEU:HD21	1.27	1.10
17:v:223:GLU:CG	17:v:224:PRO:HD2	1.81	1.10
3:2:694:PHE:HE2	17:v:191:ASP:OD1	1.32	1.09
3:2:694:PHE:HE1	17:v:187:ARG:CZ	1.66	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:950:ALA:HB2	4:3:989:TYR:OH	1.53	1.07
17:v:223:GLU:HG3	17:v:224:PRO:CD	1.85	1.07
5:4:17:VAL:HA	5:4:85:ARG:O	1.53	1.06
2:1:641:ILE:HD11	2:1:675:MET:HE3	1.09	1.05
4:3:968:ARG:HG2	4:3:982:GLU:HB2	1.35	1.05
2:1:971:MET:HE1	2:1:1003:VAL:HG11	1.40	1.03
2:1:641:ILE:HG13	2:1:675:MET:HE1	1.43	1.00
4:3:1130:VAL:CG1	4:3:1215:TYR:CE1	2.46	0.98
6:5:39:PHE:HE1	6:5:77:LEU:HD21	1.28	0.98
2:1:613:MET:HE1	2:1:635:VAL:HG11	1.45	0.97
2:1:641:ILE:CD1	2:1:675:MET:HE3	1.93	0.95
4:3:54:LEU:HD23	4:3:99:PHE:CE2	2.00	0.95
4:3:47:THR:CG2	4:3:49:LYS:HG2	1.96	0.94
2:1:641:ILE:CG1	2:1:675:MET:CE	2.45	0.94
5:4:12:ASP:CB	5:4:67:ALA:CB	2.47	0.92
4:3:1130:VAL:CG1	4:3:1215:TYR:CZ	2.53	0.92
3:2:694:PHE:CD2	17:v:190:LEU:HD22	2.04	0.92
3:2:694:PHE:CE2	17:v:191:ASP:OD1	2.22	0.92
4:3:429:ARG:HH21	4:3:429:ARG:HG2	1.35	0.90
4:3:170:VAL:HG22	4:3:184:CYS:SG	2.11	0.90
4:3:586:ASP:OD1	4:3:610:VAL:HG11	1.71	0.90
4:3:1004:ASP:OD2	4:3:1007:GLU:HB2	1.70	0.90
2:1:1004:ILE:HD11	2:1:1009:MET:SD	2.12	0.89
17:v:223:GLU:HG3	17:v:224:PRO:HD2	0.94	0.88
4:3:1130:VAL:HG11	4:3:1215:TYR:CE2	2.09	0.88
2:1:614:ARG:HD2	2:1:614:ARG:O	1.74	0.87
3:2:694:PHE:CE1	17:v:187:ARG:CZ	2.55	0.87
4:3:49:LYS:HG3	4:3:51:HIS:CE1	2.10	0.87
3:2:657:ILE:O	3:2:657:ILE:HG22	1.73	0.86
3:2:691:ALA:HB1	17:v:190:LEU:CD2	2.06	0.86
4:3:1130:VAL:HG11	4:3:1215:TYR:CD2	2.11	0.86
4:3:1057:ARG:HG3	4:3:1057:ARG:HH11	1.38	0.86
6:5:73:ALA:O	6:5:77:LEU:HB3	1.77	0.85
5:4:61:PHE:CB	5:4:66:ASP:CB	2.54	0.84
6:5:39:PHE:HE1	6:5:77:LEU:CD2	1.90	0.84
4:3:1130:VAL:HG13	4:3:1215:TYR:CE1	2.10	0.84
6:5:27:PRO:HG2	6:5:83:CYS:HB3	1.60	0.84
4:3:47:THR:HG22	4:3:49:LYS:HG2	1.59	0.83
2:1:1058:ILE:HD13	2:1:1058:ILE:O	1.81	0.81
17:v:201:TRP:CE2	17:v:224:PRO:HB3	2.15	0.81
2:1:641:ILE:CG1	2:1:675:MET:HE1	2.08	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:1260:LYS:O	2:1:1264:VAL:HG12	1.82	0.80
2:1:971:MET:HE1	2:1:1003:VAL:CG1	2.12	0.80
4:3:585:ALA:HB3	4:3:609:LEU:CD2	2.11	0.80
17:v:201:TRP:NE1	17:v:224:PRO:HB3	1.96	0.79
9:H:77:U:H5''	9:H:78:U:H5'	1.64	0.79
4:3:699:VAL:HG12	4:3:716:SER:HB2	1.63	0.79
2:1:641:ILE:HG13	2:1:675:MET:CE	2.12	0.79
4:3:1130:VAL:HG11	4:3:1215:TYR:CZ	2.16	0.79
2:1:614:ARG:HD2	2:1:614:ARG:C	2.07	0.78
6:5:27:PRO:HG3	6:5:85:ARG:HD2	1.65	0.78
2:1:641:ILE:HD11	2:1:675:MET:HE2	1.62	0.78
5:4:12:ASP:C	5:4:67:ALA:CB	2.56	0.78
5:4:17:VAL:O	5:4:56:TYR:HA	1.83	0.77
6:5:39:PHE:CE1	6:5:77:LEU:HD21	2.18	0.77
4:3:539:PRO:HG2	4:3:580:ARG:HH22	1.48	0.77
4:3:1130:VAL:HG11	4:3:1215:TYR:CG	2.20	0.77
4:3:675:LEU:CD2	4:3:691:THR:HG22	2.15	0.76
4:3:47:THR:HG21	4:3:49:LYS:HG2	1.67	0.76
3:2:557:VAL:HG11	17:v:1:MET:HB3	1.67	0.76
4:3:1057:ARG:HG3	4:3:1057:ARG:NH1	1.97	0.76
5:4:12:ASP:C	5:4:67:ALA:HB2	2.12	0.74
2:1:721:ILE:HD12	2:1:721:ILE:O	1.88	0.74
6:5:73:ALA:O	6:5:77:LEU:CB	2.37	0.73
4:3:429:ARG:HG2	4:3:429:ARG:NH2	1.97	0.73
4:3:662:PHE:CE2	4:3:678:VAL:HG13	2.23	0.73
4:3:1130:VAL:CG1	4:3:1215:TYR:CD1	2.71	0.73
2:1:1075:ARG:HA	2:1:1078:VAL:HG22	1.72	0.72
4:3:550:ASN:HB2	4:3:592:LEU:HD23	1.71	0.72
1:A:213:C:C4'	1:A:214:C:OP2	2.37	0.71
4:3:47:THR:CG2	4:3:49:LYS:HE3	2.20	0.71
4:3:1130:VAL:HG11	4:3:1215:TYR:CE1	2.25	0.71
2:1:968:GLU:HA	2:1:971:MET:HG2	1.71	0.71
4:3:662:PHE:HE2	4:3:678:VAL:HG13	1.53	0.71
4:3:1165:SER:OG	4:3:1170:VAL:HG23	1.90	0.71
1:A:206:C:O2'	1:A:207:A:OP2	2.07	0.71
3:2:644:SER:CB	5:4:65:GLU:CB	2.69	0.71
1:A:213:C:H4'	1:A:214:C:H5'	1.71	0.70
4:3:1055:VAL:HG23	4:3:1093:MET:HE3	1.73	0.70
2:1:1109:ARG:HA	2:1:1112:THR:CG2	2.21	0.70
4:3:138:GLN:HG3	4:3:161:HIS:CE1	2.27	0.70
2:1:641:ILE:CG1	2:1:675:MET:HE2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:585:ALA:HB3	4:3:609:LEU:HD23	1.73	0.69
2:1:1100:ASN:O	2:1:1103:VAL:HG23	1.92	0.69
4:3:961:ILE:HB	4:3:970:TYR:CE2	2.26	0.69
4:3:1130:VAL:HG11	4:3:1215:TYR:CD1	2.27	0.69
2:1:394:GLU:HG3	2:1:396:ASN:H	1.58	0.69
17:v:5:ARG:NH1	17:v:7:GLY:O	2.25	0.69
4:3:586:ASP:OD1	4:3:610:VAL:CG1	2.41	0.69
4:3:54:LEU:HD23	4:3:99:PHE:CD2	2.28	0.69
17:v:41:ARG:NH2	17:v:54:ASP:OD1	2.26	0.68
7:6:29:LYS:HD3	7:6:34:ASP:OD1	1.94	0.67
4:3:114:ARG:HG3	8:7:41:CYS:SG	2.34	0.67
4:3:487:ILE:HA	4:3:491:VAL:HG22	1.76	0.67
4:3:783:TYR:HB2	4:3:801:GLU:HB3	1.77	0.67
4:3:1006:GLN:O	4:3:1006:GLN:HG2	1.95	0.67
3:2:691:ALA:CB	17:v:190:LEU:HD21	2.16	0.66
4:3:930:LEU:HD12	4:3:937:LEU:HD23	1.77	0.66
3:2:694:PHE:HE1	17:v:187:ARG:NH1	1.93	0.66
9:H:84:C:H6	9:H:84:C:O5'	1.78	0.66
4:3:736:TYR:OH	4:3:763:ARG:NH1	2.28	0.66
4:3:761:THR:HG21	4:3:763:ARG:HH21	1.59	0.66
1:A:210:G:N3	1:A:210:G:H3'	2.11	0.65
1:A:217:U:H6	1:A:217:U:H5'	1.61	0.65
2:1:632:PHE:HA	2:1:635:VAL:HG13	1.77	0.65
3:2:657:ILE:O	3:2:657:ILE:CG2	2.45	0.65
17:v:33:GLU:HG3	17:v:46:ILE:HD11	1.79	0.64
2:1:550:HIS:CE1	7:6:96:THR:HG22	2.33	0.64
2:1:661:ARG:NH1	2:1:696:ASP:OD2	2.30	0.64
6:5:76:HIS:O	6:5:76:HIS:ND1	2.27	0.64
2:1:1115:ALA:O	2:1:1119:VAL:HG12	1.97	0.64
4:3:586:ASP:O	4:3:610:VAL:HG13	1.97	0.64
2:1:1180:ARG:HB2	2:1:1180:ARG:HH21	1.62	0.64
5:4:12:ASP:C	5:4:67:ALA:HB1	2.22	0.63
5:4:15:VAL:O	5:4:58:PHE:HA	1.98	0.63
2:1:696:ASP:O	2:1:702:ARG:NH1	2.29	0.63
4:3:950:ALA:HB2	4:3:989:TYR:HH	1.63	0.63
4:3:1130:VAL:HG13	4:3:1215:TYR:CD1	2.33	0.63
2:1:1108:ASN:O	2:1:1112:THR:HG22	1.98	0.63
4:3:47:THR:HG22	4:3:49:LYS:H	1.62	0.63
1:A:219:U:OP1	1:A:219:U:H6	1.80	0.63
2:1:404:LEU:HD23	6:5:47:GLN:OE1	1.97	0.63
4:3:791:HIS:CE1	4:3:930:LEU:HD23	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:1164:ARG:O	4:3:1170:VAL:HG22	1.98	0.63
2:1:1055:TRP:HA	2:1:1058:ILE:HG22	1.81	0.62
3:2:644:SER:HA	5:4:65:GLU:CB	2.29	0.62
4:3:47:THR:HG21	4:3:49:LYS:HE3	1.81	0.62
4:3:669:LEU:HD12	4:3:673:VAL:HG23	1.82	0.62
6:5:77:LEU:CD2	6:5:89:VAL:HG11	2.29	0.62
2:1:1261:VAL:O	2:1:1264:VAL:HG13	1.98	0.62
2:1:1224:PRO:HA	2:1:1227:ILE:HG22	1.82	0.62
2:1:588:TYR:CZ	7:6:91:LEU:HD21	2.35	0.61
4:3:412:ILE:HG12	4:3:423:LEU:HG	1.82	0.61
5:4:12:ASP:O	5:4:67:ALA:CB	2.48	0.61
2:1:719:TYR:HB3	4:3:216:GLY:O	2.00	0.61
2:1:1109:ARG:O	2:1:1112:THR:HG23	2.00	0.61
2:1:971:MET:CE	2:1:1003:VAL:HG11	2.23	0.61
2:1:621:ASP:HB2	2:1:624:VAL:HG22	1.82	0.61
4:3:1130:VAL:HG12	4:3:1215:TYR:CZ	2.36	0.61
2:1:665:ILE:HG23	2:1:690:ILE:HD12	1.82	0.61
4:3:968:ARG:HB2	4:3:970:TYR:CE2	2.35	0.61
9:H:31:C:H2'	9:H:32:G:H5''	1.83	0.61
4:3:93:GLN:NE2	4:3:100:GLU:OE1	2.34	0.61
3:2:599:THR:HG23	3:2:599:THR:O	2.00	0.60
17:v:204:ASP:OD1	17:v:205:GLY:N	2.34	0.60
2:1:546:ASP:OD1	2:1:546:ASP:N	2.32	0.60
2:1:1179:ASP:OD1	17:v:38:ARG:NH1	2.33	0.60
3:2:557:VAL:HG11	17:v:1:MET:CB	2.31	0.60
7:6:22:LEU:HD22	7:6:60:ILE:HD12	1.83	0.60
2:1:549:ARG:NH2	2:1:584:ASP:OD2	2.34	0.60
4:3:86:ARG:HD2	4:3:1157:GLY:O	2.01	0.60
4:3:406:PRO:HA	4:3:1122:LEU:O	2.00	0.60
5:4:14:THR:CA	5:4:59:VAL:O	2.28	0.60
1:A:206:C:O2'	1:A:207:A:P	2.60	0.60
3:2:703:ILE:HG21	3:2:705:ARG:HE	1.66	0.60
1:A:213:C:H4'	1:A:214:C:OP2	2.00	0.60
2:1:405:ASP:OD1	6:5:49:ARG:NH2	2.34	0.60
2:1:1109:ARG:HA	2:1:1112:THR:HG22	1.83	0.59
6:5:77:LEU:HD23	6:5:89:VAL:HG11	1.84	0.59
4:3:1004:ASP:CG	4:3:1007:GLU:HB2	2.27	0.59
2:1:631:ALA:O	2:1:635:VAL:HG13	2.03	0.59
7:6:58:CYS:HB3	7:6:62:GLY:H	1.67	0.59
17:v:202:ILE:HG22	17:v:204:ASP:H	1.68	0.59
2:1:774:ILE:HD11	2:1:810:ILE:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:1000:ILE:O	2:1:1004:ILE:HG12	2.03	0.59
6:5:39:PHE:CE1	6:5:77:LEU:CD2	2.80	0.58
4:3:675:LEU:HD21	4:3:691:THR:HG22	1.85	0.58
4:3:585:ALA:HB3	4:3:609:LEU:HD22	1.84	0.58
4:3:1017:ASN:HB3	17:v:194:LEU:CD2	2.34	0.58
6:5:24:ARG:HB2	6:5:88:VAL:HB	1.85	0.58
2:1:1058:ILE:HD13	2:1:1058:ILE:C	2.28	0.58
4:3:1064:ASP:OD1	4:3:1064:ASP:N	2.27	0.58
4:3:429:ARG:HD2	8:7:58:ASN:OD1	2.04	0.58
2:1:855:ASP:N	2:1:855:ASP:OD1	2.34	0.58
17:v:36:MET:HE3	17:v:40:GLY:HA2	1.86	0.57
4:3:47:THR:HG23	4:3:49:LYS:HE3	1.84	0.57
4:3:613:TPO:O2P	4:3:613:TPO:HG21	2.04	0.57
4:3:471:ASP:OD2	4:3:746:ALA:N	2.34	0.57
2:1:1044:ASP:OD1	2:1:1044:ASP:N	2.28	0.57
6:5:76:HIS:HD1	6:5:76:HIS:C	2.12	0.56
1:A:217:U:H5'	1:A:217:U:C6	2.39	0.56
4:3:524:ILE:HD11	4:3:556:ILE:HG21	1.87	0.56
17:v:8:ASP:N	17:v:8:ASP:OD1	2.36	0.56
4:3:638:GLU:OE2	4:3:670:GLN:HG3	2.05	0.56
4:3:1188:ASN:N	4:3:1188:ASN:OD1	2.38	0.56
9:H:38:G:H2'	9:H:39:G:H5'	1.86	0.56
2:1:1258:ALA:HB3	2:1:1261:VAL:CG1	2.35	0.56
4:3:1027:ASP:OD2	4:3:1031:ARG:NH1	2.39	0.56
10:h:4:GLY:N	11:i:35:ASP:CB	2.69	0.56
9:H:81:G:H2'	9:H:82:A:H5''	1.87	0.55
4:3:549:VAL:HG13	4:3:554:VAL:HG22	1.87	0.55
2:1:129:SEP:O2P	2:1:572:HIS:ND1	2.29	0.55
3:2:694:PHE:CD2	17:v:190:LEU:CD2	2.86	0.55
4:3:279:ASP:OD2	4:3:307:GLN:NE2	2.40	0.55
4:3:565:TYR:OH	4:3:624:CYS:SG	2.62	0.55
1:A:213:C:H4'	1:A:214:C:C5'	2.37	0.54
2:1:1128:VAL:HG23	2:1:1128:VAL:O	2.07	0.54
4:3:108:GLY:O	7:6:82:ARG:NH1	2.35	0.54
2:1:1174:GLU:OE1	2:1:1210:HIS:NE2	2.36	0.54
2:1:508:THR:H	2:1:511:MET:HE3	1.72	0.54
6:5:26:LEU:HD21	6:5:35:MET:HE1	1.89	0.54
4:3:185:LEU:HB3	4:3:206:GLN:HE21	1.73	0.54
2:1:550:HIS:CE1	7:6:96:THR:CG2	2.91	0.54
2:1:1223:SER:HB3	2:1:1226:VAL:CG1	2.37	0.54
4:3:525:ARG:HE	4:3:533:VAL:HG21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:1276:SER:O	2:1:1276:SER:OG	2.19	0.54
3:2:525:PRO:HG2	3:2:528:ILE:HD12	1.89	0.54
9:H:38:G:H2'	9:H:39:G:C5'	2.36	0.54
1:A:222:U:H4'	1:A:222:U:OP1	2.08	0.54
4:3:1165:SER:HB3	4:3:1169:PRO:HA	1.90	0.54
1:A:196:A:H5''	1:A:196:A:N3	2.23	0.53
4:3:555:VAL:HG22	4:3:565:TYR:HB3	1.90	0.53
4:3:304:GLN:HE21	4:3:308:GLY:HA2	1.73	0.53
1:A:213:C:O4'	1:A:214:C:OP2	2.26	0.53
3:2:567:ASP:OD1	3:2:567:ASP:N	2.40	0.53
4:3:678:VAL:O	4:3:686:LEU:HA	2.07	0.53
4:3:1103:SER:O	4:3:1119:TYR:HA	2.08	0.53
17:v:220:ASP:N	17:v:220:ASP:OD1	2.40	0.53
2:1:1054:GLU:OE1	2:1:1057:ARG:NH1	2.42	0.53
3:2:694:PHE:CE1	17:v:187:ARG:NH2	2.77	0.53
4:3:1055:VAL:HB	4:3:1093:MET:HB3	1.91	0.53
2:1:631:ALA:O	2:1:635:VAL:CG1	2.57	0.53
4:3:426:ALA:HB1	4:3:785:PRO:CG	2.39	0.53
5:4:12:ASP:O	5:4:67:ALA:HB1	2.08	0.53
8:7:48:ASP:OD1	8:7:51:ASN:ND2	2.41	0.53
3:2:469:VAL:HG12	3:2:471:ARG:H	1.74	0.52
2:1:1103:VAL:HG13	17:v:11:SER:HB3	1.90	0.52
4:3:618:SER:HB2	4:3:628:LEU:HD11	1.89	0.52
3:2:633:LEU:C	3:2:635:ALA:H	2.17	0.52
4:3:675:LEU:HD21	4:3:691:THR:CG2	2.39	0.52
4:3:950:ALA:HB2	4:3:989:TYR:CZ	2.41	0.52
17:v:1:MET:HG2	17:v:6:GLU:H	1.75	0.52
4:3:209:THR:HA	4:3:224:TYR:O	2.10	0.52
7:6:22:LEU:HG	7:6:69:ALA:HB2	1.92	0.52
4:3:460:TRP:CZ3	4:3:505:THR:HG23	2.44	0.52
2:1:680:LEU:HB3	2:1:681:PRO:HD3	1.92	0.52
5:4:34:LEU:HA	5:4:37:GLY:O	2.10	0.52
4:3:464:ARG:NH2	4:3:473:TYR:OH	2.43	0.51
4:3:950:ALA:CB	4:3:989:TYR:OH	2.44	0.51
5:4:16:TYR:HA	5:4:57:GLY:O	2.10	0.51
4:3:69:ARG:NH2	4:3:74:THR:O	2.43	0.51
2:1:968:GLU:OE1	2:1:971:MET:SD	2.68	0.51
2:1:524:ARG:HH11	2:1:566:LEU:HD11	1.74	0.51
4:3:428:GLY:HA3	4:3:433:SER:HA	1.93	0.51
1:A:210:G:N3	1:A:210:G:C2'	2.73	0.51
4:3:138:GLN:HG3	4:3:161:HIS:HE1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:1032:TRP:O	4:3:1048:ASP:HA	2.10	0.51
4:3:875:ASN:OD1	4:3:875:ASN:N	2.33	0.51
6:5:27:PRO:CG	6:5:83:CYS:HB3	2.35	0.51
2:1:1256:HIS:ND1	2:1:1261:VAL:HG11	2.26	0.51
3:2:476:GLU:OE1	3:2:478:HIS:NE2	2.43	0.51
6:5:77:LEU:HG	6:5:89:VAL:HG11	1.92	0.51
4:3:703:ARG:HD3	4:3:710:GLU:OE2	2.11	0.51
4:3:980:LYS:HG3	17:v:215:VAL:HG13	1.92	0.51
4:3:1159:ASP:HB3	4:3:1162:SER:HB3	1.92	0.51
2:1:614:ARG:HB3	2:1:615:PRO:HD3	1.93	0.51
4:3:384:THR:OG1	4:3:385:PHE:N	2.44	0.51
2:1:933:CYS:SG	2:1:970:LEU:HD21	2.51	0.50
3:2:633:LEU:C	3:2:635:ALA:N	2.69	0.50
1:A:202:A:OP1	2:1:1149:LYS:HE3	2.11	0.50
1:A:206:C:H4'	1:A:207:A:O5'	2.11	0.50
2:1:1075:ARG:HA	2:1:1078:VAL:CG2	2.39	0.50
4:3:564:VAL:HG22	4:3:580:ARG:HG2	1.93	0.50
4:3:678:VAL:HG23	4:3:688:ASP:OD1	2.11	0.50
4:3:522:ASP:O	4:3:538:THR:HG23	2.11	0.50
4:3:589:CYS:SG	4:3:640:LEU:HD12	2.52	0.50
4:3:716:SER:OG	4:3:717:SER:N	2.45	0.50
4:3:757:ILE:HG13	4:3:757:ILE:O	2.12	0.50
4:3:318:ASP:HB2	4:3:323:THR:HG21	1.94	0.50
4:3:722:SER:HB3	4:3:731:LEU:HD13	1.92	0.50
2:1:823:MET:HG2	2:1:833:LEU:HD22	1.92	0.50
2:1:1124:SER:O	2:1:1127:THR:OG1	2.30	0.50
4:3:118:GLY:HA2	4:3:132:ILE:HD11	1.94	0.50
4:3:430:GLY:H	4:3:784:THR:HG22	1.77	0.49
3:2:644:SER:CA	5:4:65:GLU:CB	2.91	0.49
3:2:691:ALA:HB2	17:v:190:LEU:HG	1.94	0.49
4:3:1057:ARG:HH11	4:3:1057:ARG:CG	2.13	0.49
2:1:619:ASN:CG	2:1:624:VAL:HG21	2.37	0.49
4:3:552:ARG:HD3	4:3:600:GLN:O	2.12	0.49
4:3:623:ASP:HB2	4:3:626:GLN:HG3	1.93	0.49
3:2:694:PHE:CE1	17:v:187:ARG:NH1	2.75	0.49
2:1:1180:ARG:HH21	2:1:1180:ARG:CB	2.26	0.49
1:A:210:G:N3	1:A:210:G:C3'	2.75	0.48
4:3:546:LYS:HG3	4:3:588:VAL:O	2.13	0.48
14:l:15:VAL:O	16:n:33:GLY:HA3	2.12	0.48
3:2:700:GLU:HA	3:2:703:ILE:HD12	1.94	0.48
4:3:333:VAL:HG11	4:3:349:VAL:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:619:ASN:OD1	2:1:620:MET:N	2.45	0.48
4:3:429:ARG:HH21	4:3:429:ARG:CG	2.13	0.48
4:3:720:TRP:CE3	4:3:731:LEU:HG	2.49	0.48
2:1:614:ARG:N	2:1:615:PRO:CD	2.76	0.48
2:1:641:ILE:CD1	2:1:675:MET:HE2	2.24	0.48
2:1:1002:ASN:HD22	2:1:1002:ASN:HA	1.50	0.48
3:2:691:ALA:HA	17:v:190:LEU:HD11	1.96	0.48
1:A:211:U:H2'	1:A:213:C:OP2	2.14	0.48
2:1:129:SEP:O3P	2:1:150:ARG:NH2	2.30	0.48
3:2:553:MET:HE3	17:v:1:MET:HE1	1.94	0.48
7:6:22:LEU:CD2	7:6:60:ILE:HD12	2.44	0.48
2:1:936:VAL:CG2	2:1:954:LEU:HD23	2.44	0.48
4:3:123:VAL:HG12	4:3:130:VAL:HG23	1.96	0.48
4:3:530:ASP:OD1	4:3:532:ARG:HG2	2.13	0.48
2:1:130:PRO:HG2	2:1:150:ARG:HD2	1.95	0.47
2:1:1033:GLU:OE1	2:1:1070:LYS:HE2	2.15	0.47
4:3:987:ALA:HB3	4:3:1007:GLU:HG2	1.96	0.47
2:1:933:CYS:SG	2:1:970:LEU:HD11	2.54	0.47
6:5:80:PHE:CD2	6:5:82:VAL:HG23	2.50	0.47
2:1:540:MET:HE3	2:1:577:VAL:HG22	1.95	0.47
2:1:671:ILE:HG23	2:1:675:MET:HG3	1.95	0.47
2:1:758:ASP:OD1	2:1:758:ASP:N	2.48	0.47
4:3:49:LYS:CG	4:3:51:HIS:CE1	2.92	0.47
7:6:45:ILE:HD11	7:6:50:ASN:HB3	1.97	0.47
2:1:933:CYS:O	2:1:937:LEU:HB2	2.15	0.47
2:1:1109:ARG:O	2:1:1112:THR:CG2	2.63	0.47
4:3:629:SER:OG	4:3:686:LEU:HD12	2.15	0.47
4:3:1118:VAL:HG22	4:3:1128:ILE:HG22	1.96	0.47
5:4:67:ALA:O	5:4:70:ALA:HB3	2.15	0.47
9:H:39:G:H2'	9:H:40:G:O4'	2.15	0.47
17:v:201:TRP:CH2	17:v:224:PRO:HD3	2.49	0.47
4:3:399:ASP:OD1	4:3:400:GLU:N	2.48	0.47
2:1:128:ILE:HB	6:5:96:ARG:HB3	1.97	0.47
7:6:30:CYS:O	7:6:34:ASP:HA	2.15	0.47
5:4:12:ASP:O	5:4:67:ALA:HB2	2.10	0.46
4:3:54:LEU:CD2	4:3:99:PHE:CD2	2.96	0.46
9:H:14:A:C6	17:v:10:TRP:HB3	2.50	0.46
2:1:929:LEU:HD22	2:1:962:MET:HE2	1.96	0.46
2:1:971:MET:CE	2:1:1003:VAL:CG1	2.88	0.46
4:3:952:ILE:HG12	4:3:961:ILE:HG12	1.96	0.46
6:5:48:ILE:HG12	6:5:62:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:77:LEU:CG	6:5:89:VAL:HG11	2.45	0.46
2:1:1094:LEU:HD22	2:1:1128:VAL:HB	1.97	0.46
5:4:12:ASP:CB	5:4:67:ALA:HB3	2.43	0.46
4:3:136:GLU:HB3	4:3:166:LEU:HD23	1.98	0.46
4:3:515:ALA:HB1	4:3:526:HIS:NE2	2.31	0.46
2:1:641:ILE:HG12	2:1:675:MET:HE2	1.96	0.46
2:1:982:LEU:HD12	2:1:1019:ARG:HG2	1.97	0.46
2:1:1032:GLN:O	2:1:1036:ILE:HG22	2.15	0.46
4:3:643:VAL:O	4:3:663:LEU:HD12	2.16	0.46
3:2:691:ALA:CB	17:v:190:LEU:CG	2.94	0.46
4:3:137:LYS:O	4:3:137:LYS:HD3	2.15	0.46
4:3:353:PHE:HE2	4:3:429:ARG:NH1	2.13	0.46
4:3:173:VAL:HB	4:3:181:MET:HB2	1.98	0.46
4:3:1004:ASP:OD1	4:3:1005:VAL:N	2.49	0.46
4:3:1017:ASN:HB3	17:v:194:LEU:HD21	1.97	0.45
2:1:716:ALA:O	2:1:719:TYR:N	2.40	0.45
4:3:430:GLY:HA3	4:3:431:PRO:HD2	1.84	0.45
9:H:38:G:C2'	9:H:39:G:H5''	2.46	0.45
3:2:632:TRP:HB3	5:4:76:MET:CB	2.47	0.45
2:1:675:MET:HB2	2:1:679:ILE:HG23	1.97	0.45
3:2:648:LEU:HD12	3:2:649:LYS:H	1.81	0.45
4:3:702:PHE:HE2	4:3:715:MET:SD	2.40	0.45
4:3:1164:ARG:C	4:3:1170:VAL:HG22	2.41	0.45
1:A:210:G:N3	1:A:210:G:H2'	2.32	0.45
4:3:593:ALA:HB3	4:3:602:SER:OG	2.16	0.45
4:3:614:VAL:HG11	4:3:667:ILE:HD13	1.98	0.45
4:3:675:LEU:HD22	4:3:691:THR:HG22	1.99	0.45
2:1:1258:ALA:HB3	2:1:1261:VAL:HG12	1.98	0.45
3:2:565:ASP:OD1	3:2:565:ASP:N	2.47	0.45
4:3:519:VAL:HG23	4:3:524:ILE:HG12	1.98	0.45
2:1:770:MET:HE3	2:1:801:VAL:HG11	1.98	0.45
4:3:553:GLN:NE2	4:3:619:LEU:HD13	2.32	0.45
4:3:574:LEU:HD23	4:3:574:LEU:HA	1.78	0.45
4:3:675:LEU:HD23	4:3:691:THR:HA	1.99	0.45
2:1:1109:ARG:CA	2:1:1112:THR:HG22	2.47	0.44
4:3:444:VAL:HG22	4:3:767:LEU:HD22	1.98	0.44
4:3:563:LEU:HD12	4:3:581:LYS:HD3	1.99	0.44
2:1:1206:ASP:OD1	2:1:1206:ASP:N	2.50	0.44
4:3:485:LEU:HD23	4:3:491:VAL:CG1	2.47	0.44
2:1:524:ARG:HG2	8:7:1:MET:HE2	1.99	0.44
2:1:1136:TYR:HD1	2:1:1147:VAL:CG2	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:520:TYR:CD1	4:3:522:ASP:HB2	2.53	0.44
4:3:638:GLU:HA	4:3:638:GLU:OE1	2.16	0.44
5:4:12:ASP:CA	5:4:67:ALA:HB1	2.44	0.44
2:1:1044:ASP:HB3	2:1:1083:TYR:CD1	2.53	0.44
2:1:1250:CYS:HA	2:1:1265:TYR:CE2	2.51	0.44
2:1:1303:ILE:HD12	2:1:1303:ILE:HA	1.78	0.44
3:2:691:ALA:HB2	17:v:190:LEU:CG	2.48	0.44
4:3:12:THR:O	4:3:34:ARG:NH1	2.50	0.44
2:1:732:TRP:HA	2:1:732:TRP:CE3	2.53	0.44
3:2:573:ASP:OD1	3:2:577:LYS:HE3	2.18	0.44
4:3:42:ARG:HB2	4:3:53:LEU:HD11	1.99	0.44
4:3:720:TRP:HE3	4:3:731:LEU:HG	1.80	0.44
2:1:1262:ARG:NH1	8:7:24:ALA:O	2.47	0.44
4:3:485:LEU:HD23	4:3:491:VAL:HG12	2.00	0.44
4:3:566:PHE:HD1	4:3:576:GLU:HA	1.83	0.44
4:3:55:THR:O	4:3:55:THR:HG23	2.16	0.44
4:3:170:VAL:CG2	4:3:184:CYS:SG	2.97	0.44
4:3:640:LEU:HD23	4:3:665:LEU:HD11	1.99	0.44
2:1:936:VAL:HG11	2:1:955:ILE:HG13	2.00	0.44
4:3:185:LEU:HB3	4:3:206:GLN:NE2	2.32	0.44
4:3:475:ILE:HD13	4:3:484:VAL:HG23	2.00	0.44
4:3:965:LYS:HG3	4:3:966:LEU:HD12	2.00	0.44
3:2:691:ALA:CB	17:v:190:LEU:HD11	2.48	0.43
4:3:460:TRP:HZ3	4:3:505:THR:HG23	1.82	0.43
4:3:603:ARG:NH1	4:3:620:ASP:HB2	2.33	0.43
4:3:678:VAL:HB	4:3:687:SER:HB3	2.00	0.43
3:2:495:ARG:NH2	4:3:1026:ASP:OD2	2.52	0.43
4:3:274:ARG:HH21	4:3:274:ARG:HD3	1.67	0.43
6:5:87:LEU:HD12	6:5:87:LEU:HA	1.86	0.43
2:1:550:HIS:CG	7:6:100:TYR:CD2	3.06	0.43
2:1:563:LEU:HB3	2:1:566:LEU:HD12	2.00	0.43
2:1:1125:PRO:O	2:1:1129:LEU:HB2	2.19	0.43
4:3:318:ASP:HB2	4:3:323:THR:CG2	2.48	0.43
6:5:27:PRO:HG3	6:5:85:ARG:CD	2.44	0.43
9:H:83:G:H2'	9:H:84:C:C6	2.54	0.43
2:1:1050:VAL:HG21	2:1:1055:TRP:CZ2	2.52	0.43
4:3:537:LYS:HA	4:3:537:LYS:HD3	1.84	0.43
9:H:38:G:C2'	9:H:39:G:C5'	2.97	0.43
2:1:572:HIS:HB2	2:1:612:THR:HG23	2.01	0.43
2:1:577:VAL:HG12	2:1:577:VAL:O	2.17	0.43
2:1:884:ILE:HG23	2:1:888:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:v:201:TRP:CZ3	17:v:211:LYS:HG3	2.53	0.43
2:1:1023:ILE:O	2:1:1023:ILE:HG22	2.19	0.43
4:3:669:LEU:HD12	4:3:673:VAL:CG2	2.47	0.43
4:3:1001:ILE:HG13	4:3:1038:LEU:HD11	2.00	0.43
2:1:1183:VAL:HA	2:1:1186:GLN:HG2	2.00	0.43
4:3:47:THR:CG2	4:3:49:LYS:CG	2.84	0.43
6:5:35:MET:HE2	6:5:35:MET:HB2	1.90	0.43
2:1:937:LEU:HD23	2:1:937:LEU:HA	1.79	0.43
2:1:1287:ILE:HG13	8:7:32:LEU:HD21	2.00	0.43
2:1:1302:TYR:OH	8:7:57:GLU:OE2	2.37	0.43
13:k:68:GLU:HA	13:k:97:SER:O	2.19	0.43
17:v:212:ASP:OD1	17:v:213:GLU:N	2.52	0.43
4:3:675:LEU:CD2	4:3:691:THR:CG2	2.92	0.42
4:3:1099:GLU:HG3	4:3:1121:THR:HG21	2.01	0.42
1:A:209:U:H4'	1:A:210:G:C5	2.53	0.42
1:A:217:U:H6	1:A:217:U:C5'	2.29	0.42
2:1:1086:LYS:HA	2:1:1086:LYS:HD3	1.86	0.42
2:1:476:ASP:N	2:1:476:ASP:OD1	2.50	0.42
4:3:406:PRO:O	4:3:427:CYS:CB	2.67	0.42
2:1:1119:VAL:HA	2:1:1122:THR:HG22	2.01	0.42
3:2:691:ALA:CB	17:v:190:LEU:CD2	2.87	0.42
4:3:274:ARG:NH2	4:3:309:ASP:OD1	2.53	0.42
4:3:931:VAL:HG23	4:3:936:LYS:HB3	2.01	0.42
1:A:219:U:O2	1:A:219:U:O2'	2.31	0.42
2:1:123:ARG:HA	2:1:126:MET:HE2	2.01	0.42
4:3:532:ARG:HE	4:3:532:ARG:HB2	1.68	0.42
6:5:76:HIS:ND1	6:5:76:HIS:C	2.73	0.42
17:v:196:LEU:O	17:v:201:TRP:HB2	2.20	0.42
3:2:630:PRO:HA	3:2:631:PRO:HD3	1.78	0.42
4:3:956:GLN:HE22	4:3:998:HIS:CE1	2.37	0.42
4:3:1052:ASN:OD1	4:3:1052:ASN:N	2.50	0.42
9:H:74:A:H5'	9:H:80:U:OP2	2.18	0.42
17:v:194:LEU:HD23	17:v:194:LEU:HA	1.85	0.42
2:1:1114:VAL:O	2:1:1118:ILE:HG12	2.20	0.42
3:2:632:TRP:CB	5:4:76:MET:CB	2.97	0.42
4:3:1120:THR:HG22	4:3:1126:ILE:HG12	2.00	0.42
2:1:1133:MET:HG2	2:1:1172:LEU:HD22	2.01	0.42
4:3:133:SER:HB2	4:3:139:LYS:HG2	2.02	0.42
4:3:715:MET:HE2	4:3:715:MET:HB3	1.90	0.42
4:3:34:ARG:HE	4:3:39:GLU:CD	2.28	0.42
4:3:563:LEU:HD21	4:3:590:MET:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:1220:PHE:HE1	2:1:1261:VAL:HA	1.85	0.42
4:3:610:VAL:O	4:3:610:VAL:HG23	2.20	0.42
17:v:39:ASP:OD1	17:v:39:ASP:N	2.33	0.42
5:4:17:VAL:CA	5:4:85:ARG:O	2.45	0.41
2:1:403:GLU:O	2:1:406:ALA:HB3	2.20	0.41
2:1:619:ASN:ND2	2:1:624:VAL:HG21	2.35	0.41
2:1:885:ASP:N	2:1:885:ASP:OD1	2.50	0.41
4:3:246:SER:O	4:3:260:ASN:ND2	2.54	0.41
4:3:1130:VAL:CG1	4:3:1215:TYR:CE2	2.84	0.41
2:1:793:LYS:HG3	2:1:839:GLU:HG3	2.02	0.41
4:3:642:ILE:HG22	4:3:663:LEU:HD11	2.02	0.41
2:1:1120:ALA:HB2	2:1:1128:VAL:HG21	2.02	0.41
4:3:510:LEU:O	4:3:510:LEU:HG	2.20	0.41
4:3:601:ARG:NH2	4:3:621:PRO:HD3	2.35	0.41
4:3:1194:SER:HB2	4:3:1199:ARG:O	2.20	0.41
9:H:79:U:C3'	9:H:80:U:H5'	2.51	0.41
2:1:1129:LEU:HD23	2:1:1129:LEU:HA	1.75	0.41
4:3:520:TYR:CE1	4:3:522:ASP:HB2	2.55	0.41
7:6:7:ASP:OD1	7:6:7:ASP:N	2.52	0.41
2:1:675:MET:HB2	2:1:679:ILE:CG2	2.51	0.41
2:1:1304:LEU:HA	2:1:1304:LEU:HD23	1.82	0.41
4:3:694:LEU:HD12	4:3:694:LEU:O	2.20	0.41
1:A:207:A:O4'	7:6:102:ARG:HG3	2.21	0.41
4:3:668:GLY:HA3	4:3:699:VAL:HG23	2.03	0.41
4:3:761:THR:HG21	4:3:763:ARG:NH2	2.31	0.41
4:3:968:ARG:HB2	4:3:970:TYR:HE2	1.81	0.41
4:3:981:CYS:SG	4:3:981:CYS:O	2.78	0.41
4:3:1004:ASP:OD2	4:3:1007:GLU:CB	2.55	0.41
9:H:50:A:H2'	9:H:51:A:C8	2.55	0.41
2:1:721:ILE:HG12	2:1:757:MET:HA	2.02	0.41
3:2:710:GLU:OE2	4:3:1057:ARG:NH2	2.53	0.41
4:3:583:MET:HE1	4:3:607:VAL:HG21	2.02	0.41
7:6:29:LYS:HA	7:6:35:SER:O	2.21	0.41
8:7:44:MET:HE3	8:7:44:MET:HB3	1.94	0.41
1:A:211:U:C2'	1:A:213:C:OP2	2.69	0.41
2:1:1167:TYR:CZ	3:2:581:LYS:HE2	2.56	0.41
4:3:506:LEU:HA	4:3:506:LEU:HD23	1.90	0.41
4:3:834:LEU:O	4:3:837:GLU:HB3	2.21	0.41
17:v:1:MET:CG	17:v:6:GLU:HB3	2.51	0.41
2:1:1245:ARG:O	2:1:1249:TYR:HD1	2.04	0.41
4:3:1052:ASN:HB3	4:3:1096:HIS:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:1129:LEU:HD23	4:3:1129:LEU:HA	1.93	0.41
7:6:102:ARG:HH12	9:H:17:A:H1'	1.86	0.41
17:v:1:MET:HG2	17:v:6:GLU:HB3	2.02	0.41
2:1:157:ARG:NH1	6:5:103:THR:OG1	2.54	0.40
4:3:673:VAL:HG12	4:3:693:TYR:HA	2.03	0.40
17:v:33:GLU:HB3	17:v:63:ARG:HH22	1.85	0.40
2:1:1200:TYR:CD1	2:1:1239:VAL:O	2.74	0.40
2:1:1291:ASP:OD1	2:1:1291:ASP:N	2.51	0.40
4:3:138:GLN:HA	4:3:161:HIS:ND1	2.35	0.40
4:3:503:THR:OG1	4:3:504:PRO:HD2	2.21	0.40
4:3:988:ASN:HB2	4:3:1004:ASP:OD1	2.21	0.40
2:1:774:ILE:HD13	2:1:774:ILE:HA	1.83	0.40
7:6:42:LEU:HD11	7:6:68:ASP:HB3	2.03	0.40
17:v:33:GLU:N	17:v:33:GLU:OE1	2.55	0.40
2:1:479:LEU:HD13	2:1:479:LEU:HA	1.84	0.40
2:1:968:GLU:HA	2:1:971:MET:CG	2.48	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	
2	1	964/1304 (74%)	948 (98%)	16 (2%)	0	100	100
3	2	206/895 (23%)	197 (96%)	9 (4%)	0	100	100
4	3	1184/1217 (97%)	1137 (96%)	47 (4%)	0	100	100
5	4	76/424 (18%)	71 (93%)	5 (7%)	0	100	100
6	5	107/125 (86%)	104 (97%)	3 (3%)	0	100	100
7	6	103/110 (94%)	98 (95%)	5 (5%)	0	100	100
8	7	79/86 (92%)	78 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	h	76/126 (60%)	74 (97%)	2 (3%)	0	100	100
11	i	84/240 (35%)	82 (98%)	2 (2%)	0	100	100
12	j	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
13	k	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
14	l	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
15	m	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
16	n	64/76 (84%)	62 (97%)	2 (3%)	0	100	100
17	v	115/230 (50%)	113 (98%)	2 (2%)	0	100	100
All	All	3368/5248 (64%)	3263 (97%)	105 (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	
2	1	842/1103 (76%)	797 (95%)	45 (5%)	20	42
3	2	163/776 (21%)	157 (96%)	6 (4%)	30	51
4	3	1031/1050 (98%)	997 (97%)	34 (3%)	33	55
6	5	97/109 (89%)	96 (99%)	1 (1%)	68	76
7	6	90/95 (95%)	88 (98%)	2 (2%)	45	64
8	7	72/77 (94%)	72 (100%)	0	100	100
17	v	104/199 (52%)	100 (96%)	4 (4%)	29	51
All	All	2399/3409 (70%)	2307 (96%)	92 (4%)	30	51

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	120	LYS
2	1	412	TYR

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Mol	Chain	Res	Type
2	1	479	LEU
2	1	487	LEU
2	1	531	LEU
2	1	562	LYS
2	1	563	LEU
2	1	564	ASP
2	1	614	ARG
2	1	624	VAL
2	1	635	VAL
2	1	651	VAL
2	1	674	LEU
2	1	675	MET
2	1	677	CYS
2	1	680	LEU
2	1	721	ILE
2	1	872	ILE
2	1	909	VAL
2	1	936	VAL
2	1	976	VAL
2	1	997	LEU
2	1	1002	ASN
2	1	1003	VAL
2	1	1024	LEU
2	1	1038	LEU
2	1	1050	VAL
2	1	1058	ILE
2	1	1061	GLU
2	1	1112	THR
2	1	1113	THR
2	1	1119	VAL
2	1	1127	THR
2	1	1128	VAL
2	1	1180	ARG
2	1	1182	LEU
2	1	1184	HIS
2	1	1226	VAL
2	1	1227	ILE
2	1	1239	VAL
2	1	1260	LYS
2	1	1261	VAL
2	1	1264	VAL
2	1	1277	GLN

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Mol	Chain	Res	Type
2	1	1303	ILE
3	2	498	VAL
3	2	577	LYS
3	2	579	GLN
3	2	587	HIS
3	2	590	LEU
3	2	599	THR
4	3	47	THR
4	3	86	ARG
4	3	135	ILE
4	3	136	GLU
4	3	137	LYS
4	3	138	GLN
4	3	171	VAL
4	3	184	CYS
4	3	187	MET
4	3	295	THR
4	3	319	GLU
4	3	321	MET
4	3	322	VAL
4	3	425	VAL
4	3	429	ARG
4	3	607	VAL
4	3	609	LEU
4	3	610	VAL
4	3	612	ASN
4	3	614	VAL
4	3	615	ARG
4	3	686	LEU
4	3	689	THR
4	3	690	ARG
4	3	691	THR
4	3	773	VAL
4	3	943	THR
4	3	948	VAL
4	3	982	GLU
4	3	1007	GLU
4	3	1057	ARG
4	3	1064	ASP
4	3	1165	SER
4	3	1214	ARG
6	5	85	ARG

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Mol	Chain	Res	Type
7	6	25	LYS
7	6	95	LYS
17	v	1	MET
17	v	5	ARG
17	v	46	ILE
17	v	219	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	473	GLN
2	1	698	GLN
2	1	817	HIS
2	1	973	HIS
2	1	1002	ASN
2	1	1026	ASN
2	1	1225	HIS
2	1	1252	GLN
2	1	1283	HIS
2	1	1293	ASN
3	2	490	HIS
4	3	21	ASN
4	3	51	HIS
4	3	206	GLN
4	3	304	GLN
4	3	394	ASN
4	3	730	HIS
4	3	861	GLN
17	v	214	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	29/280 (10%)	13 (44%)	4 (13%)
9	H	48/150 (32%)	8 (16%)	0
All	All	77/430 (17%)	21 (27%)	4 (5%)

All (21) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	196	A
1	A	203	A
1	A	207	A
1	A	208	U
1	A	210	G
1	A	211	U
1	A	214	C
1	A	216	U
1	A	217	U
1	A	218	U
1	A	219	U
1	A	220	U
1	A	222	U
9	H	18	G
9	H	29	A
9	H	31	C
9	H	32	G
9	H	39	G
9	H	44	C
9	H	45	G
9	H	83	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	206	C
1	A	213	C
1	A	217	U
1	A	219	U

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	TPO	3	613	4	8,10,11	0.92	0	10,14,16	1.79	2 (20%)
2	SEP	1	129	2	8,9,10	1.13	1 (12%)	7,12,14	1.54	2 (28%)

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
4	TPO	3	613	4	-	1/9/11/13	-
2	SEP	1	129	2	-	5/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	129	SEP	P-O1P	2.26	1.57	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	613	TPO	P-OG1-CB	-4.97	109.81	123.33
4	3	613	TPO	O-C-CA	-2.31	118.83	124.77
2	1	129	SEP	O3P-P-OG	2.25	112.54	106.67
2	1	129	SEP	OG-CB-CA	2.19	110.28	108.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1	129	SEP	N-CA-CB-OG
2	1	129	SEP	C-CA-CB-OG
2	1	129	SEP	CB-OG-P-O1P
2	1	129	SEP	CB-OG-P-O2P
2	1	129	SEP	CB-OG-P-O3P
4	3	613	TPO	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	3	613	TPO	1	0
2	1	129	SEP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

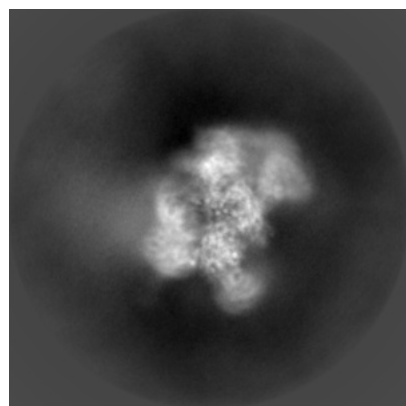
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39013. These allow visual inspection of the internal detail of the map and identification of artifacts.

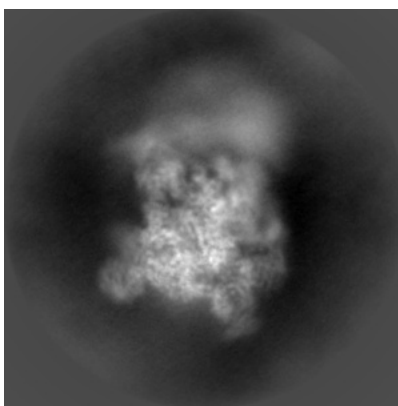
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

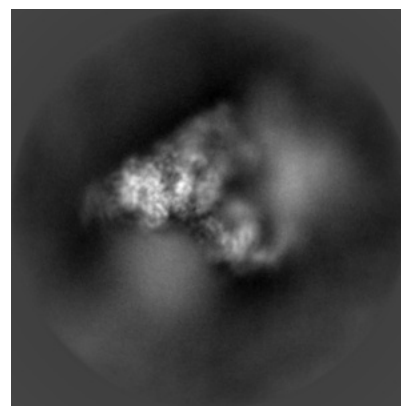
6.1.1 Primary map



X

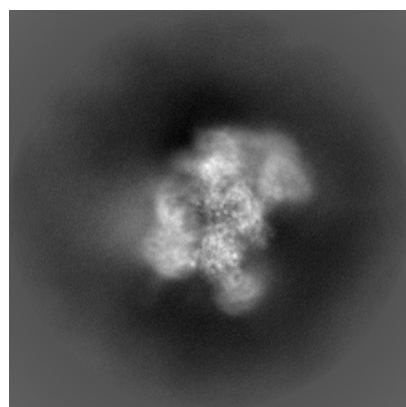


Y

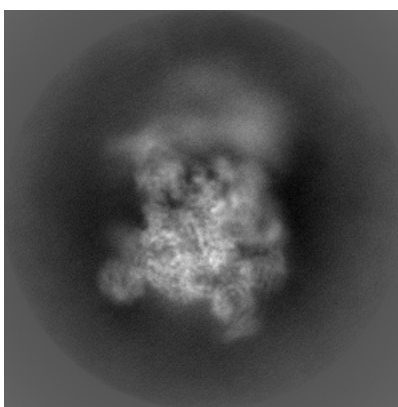


Z

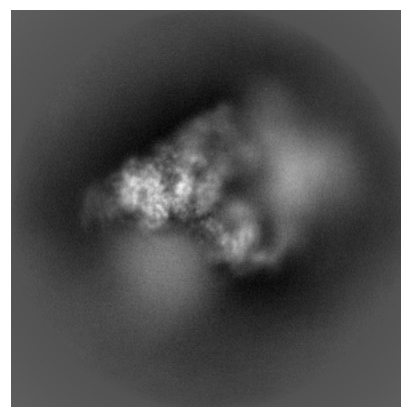
6.1.2 Raw map



X



Y

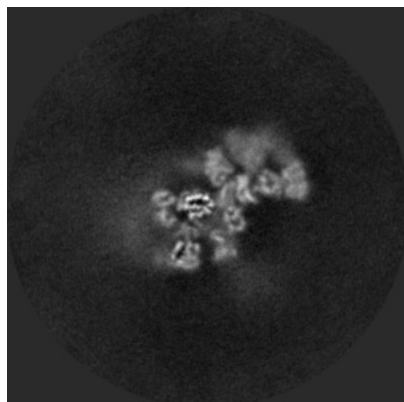


Z

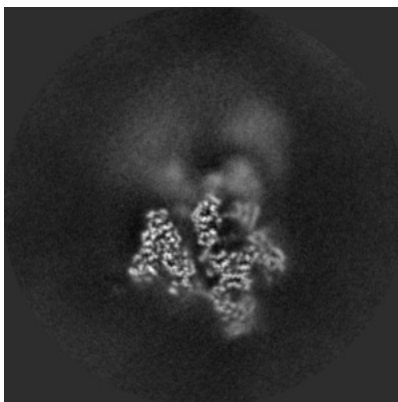
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

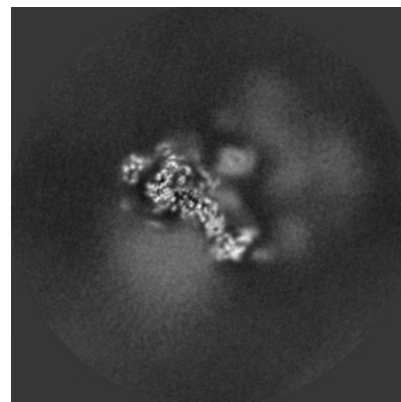
6.2.1 Primary map



X Index: 256

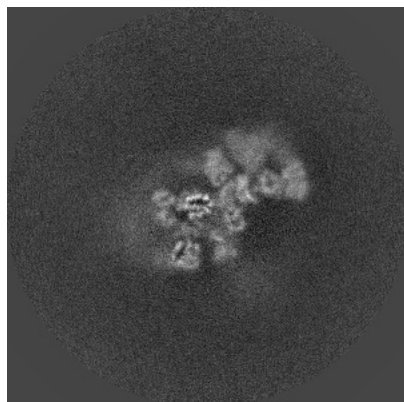


Y Index: 256

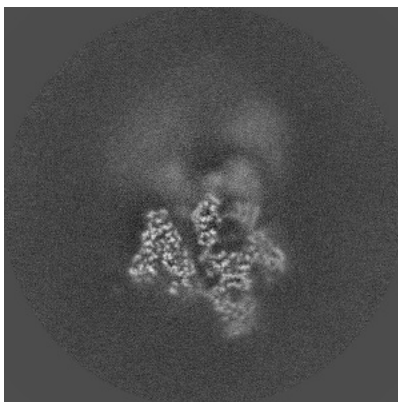


Z Index: 256

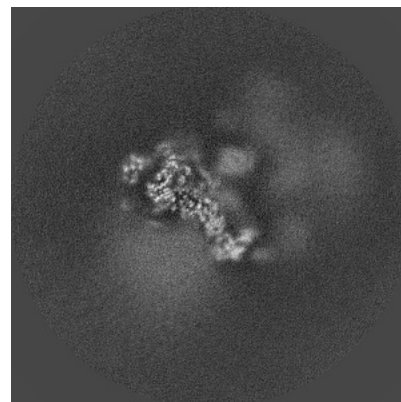
6.2.2 Raw map



X Index: 256



Y Index: 256

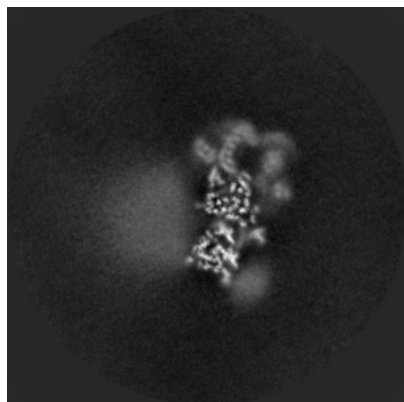


Z Index: 256

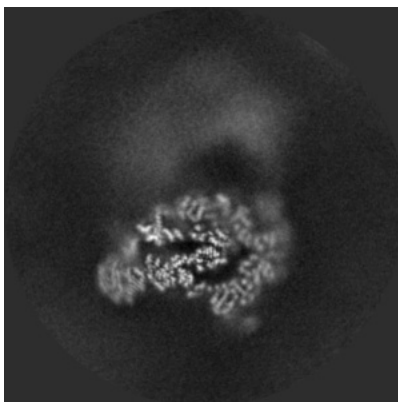
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

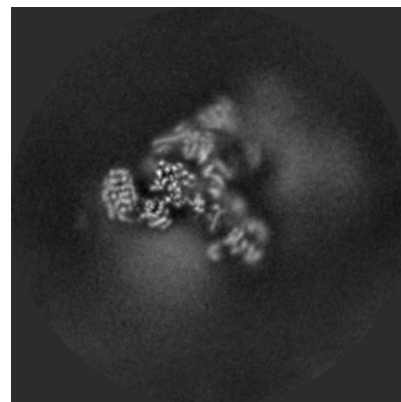
6.3.1 Primary map



X Index: 218

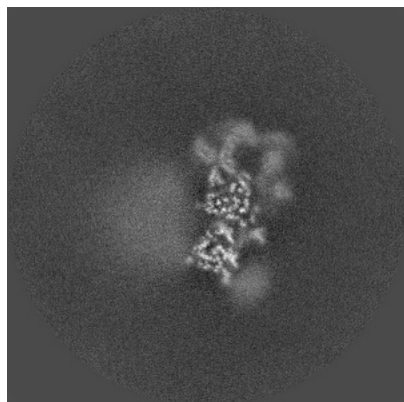


Y Index: 287

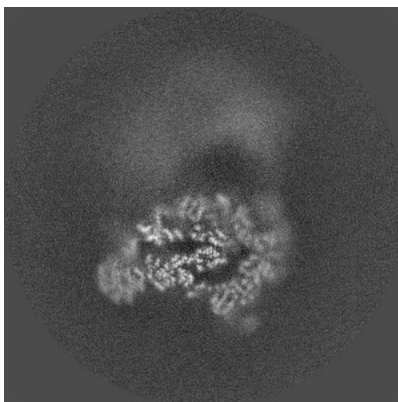


Z Index: 274

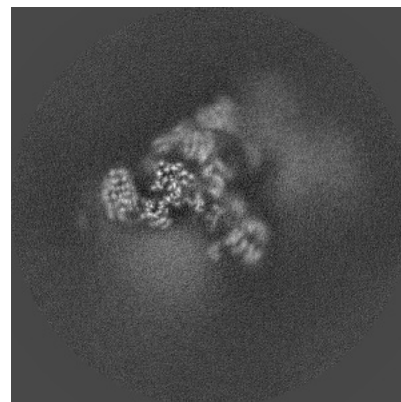
6.3.2 Raw map



X Index: 218



Y Index: 287

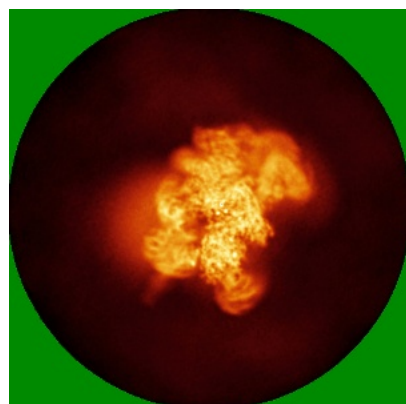


Z Index: 275

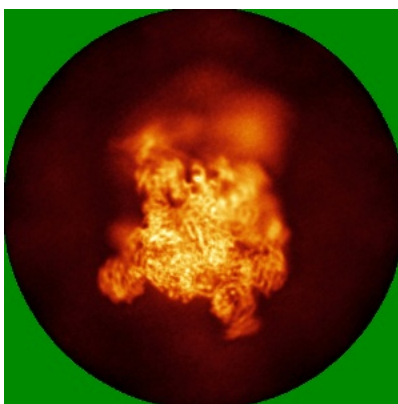
The images above show the largest variance slices of the map in three orthogonal directions.

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

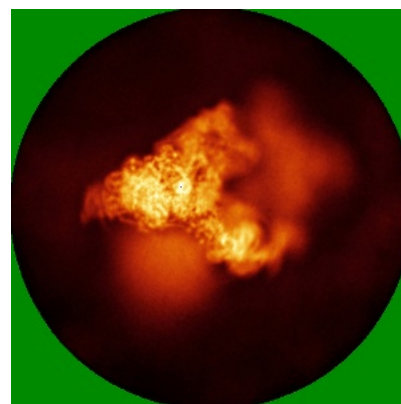
6.4.1 Primary map



X

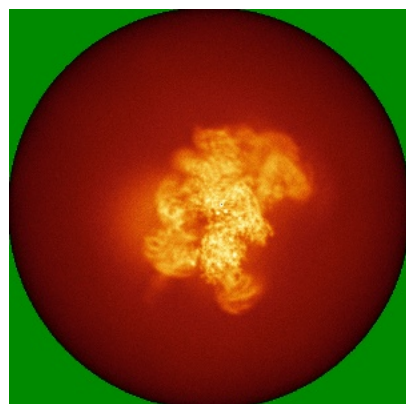


Y

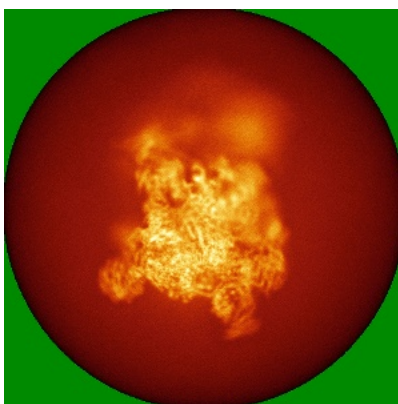


Z

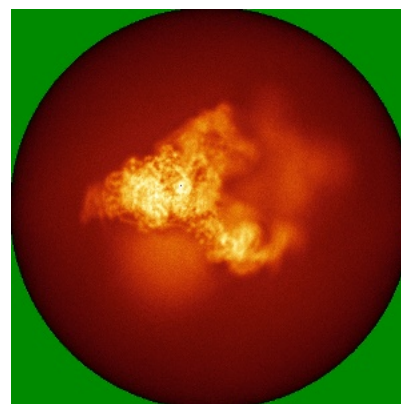
6.4.2 Raw map



X



Y

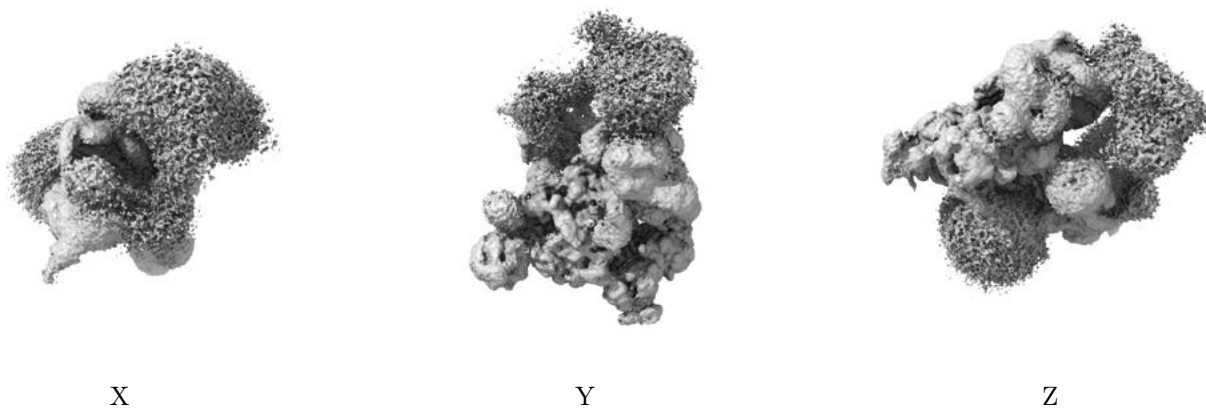


Z

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.

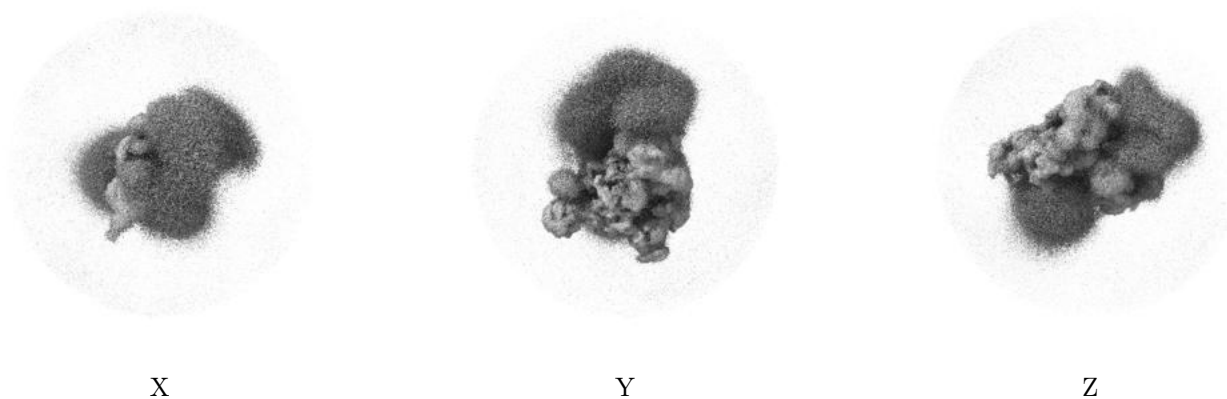
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. 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.

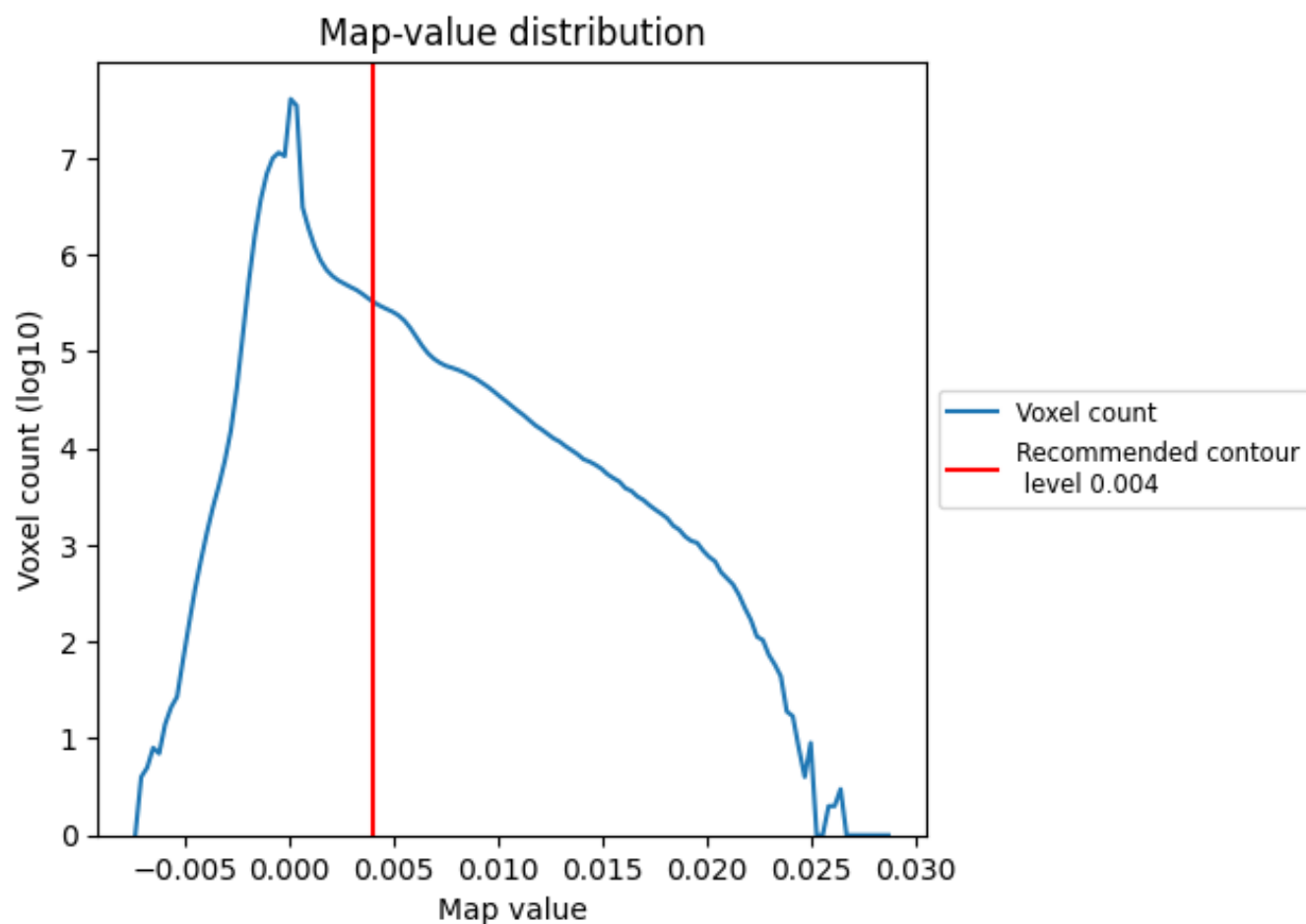
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

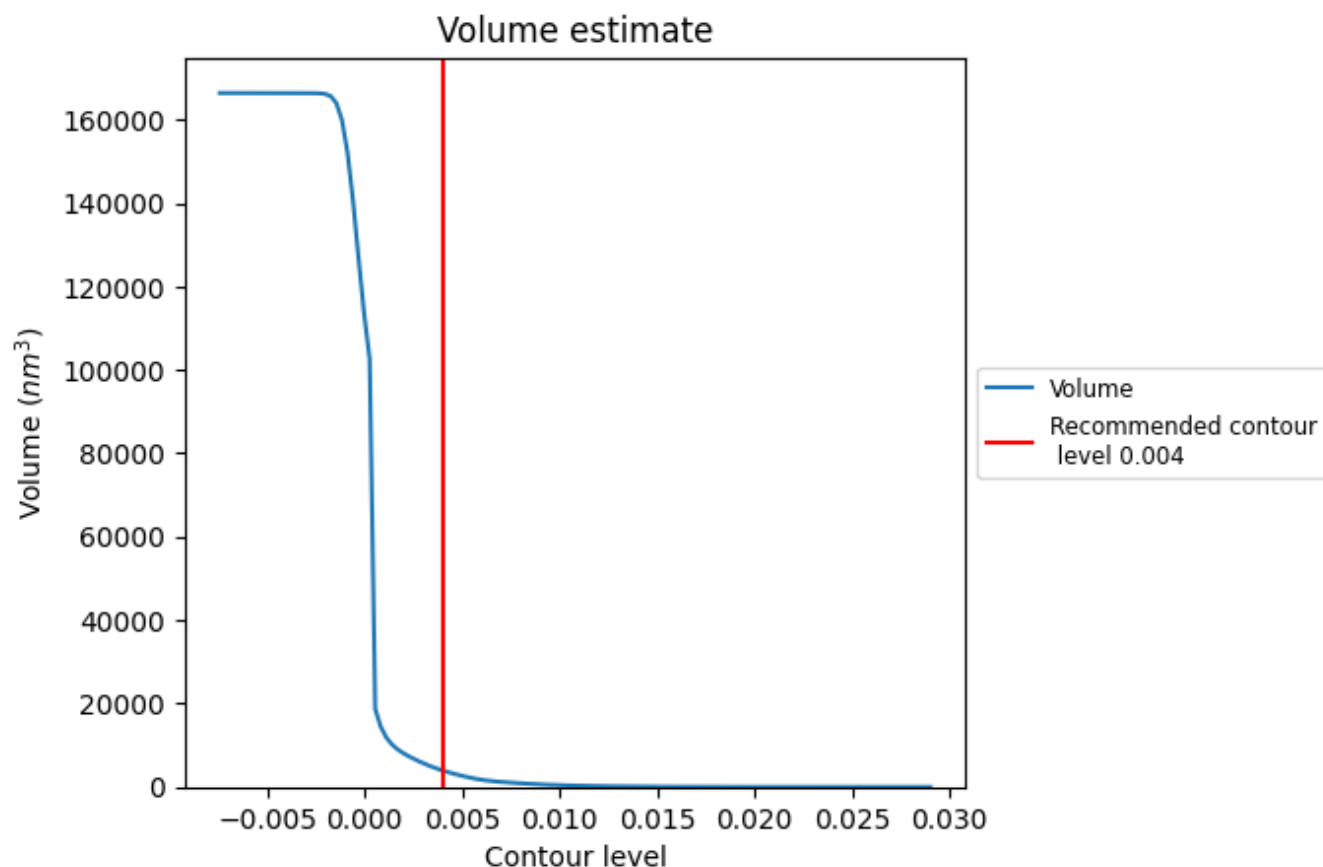
This section contains the results of statistical analysis of the map.

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.

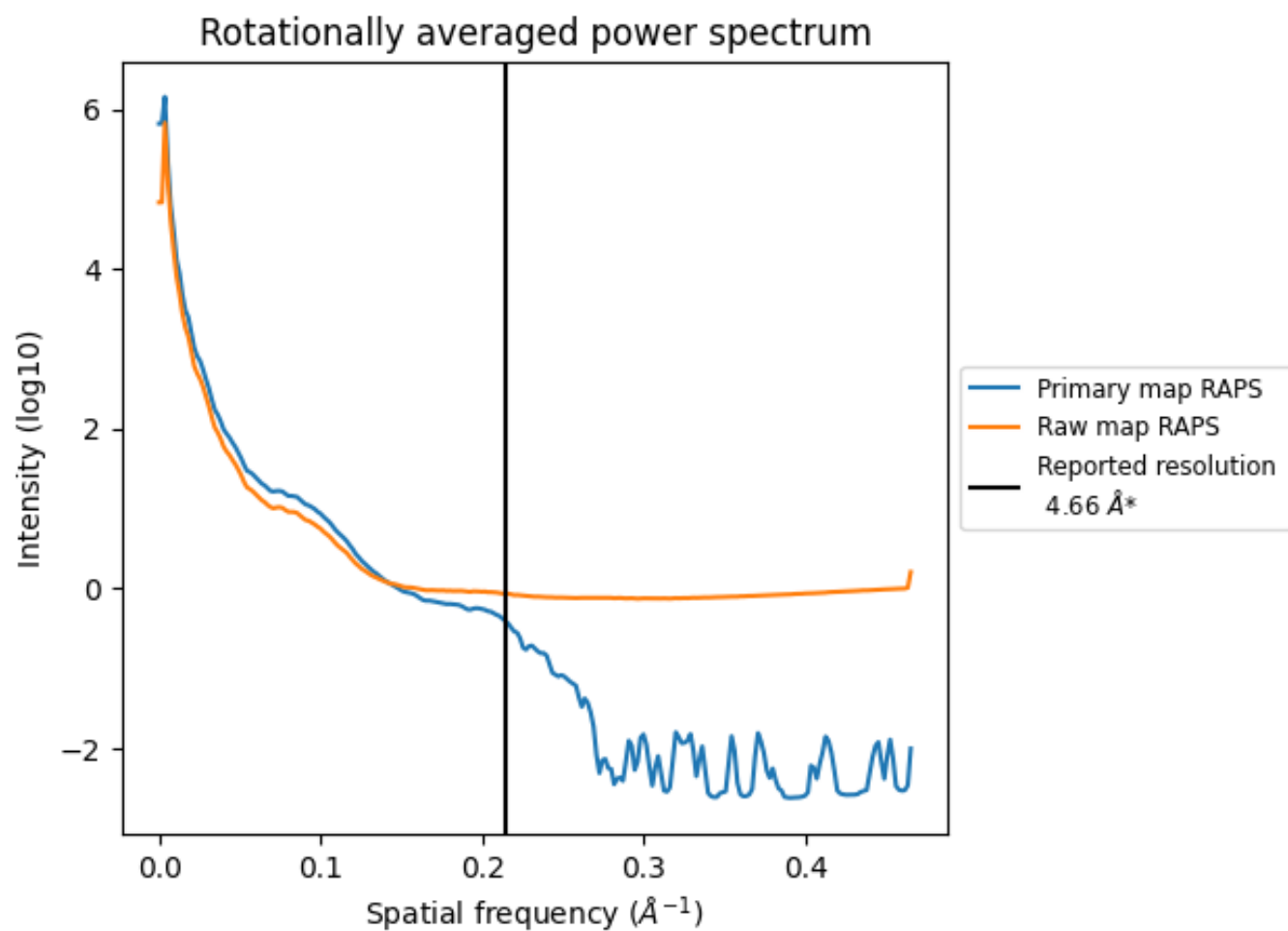
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3947 nm^3 ; this corresponds to an approximate mass of 3565 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 ⓘ

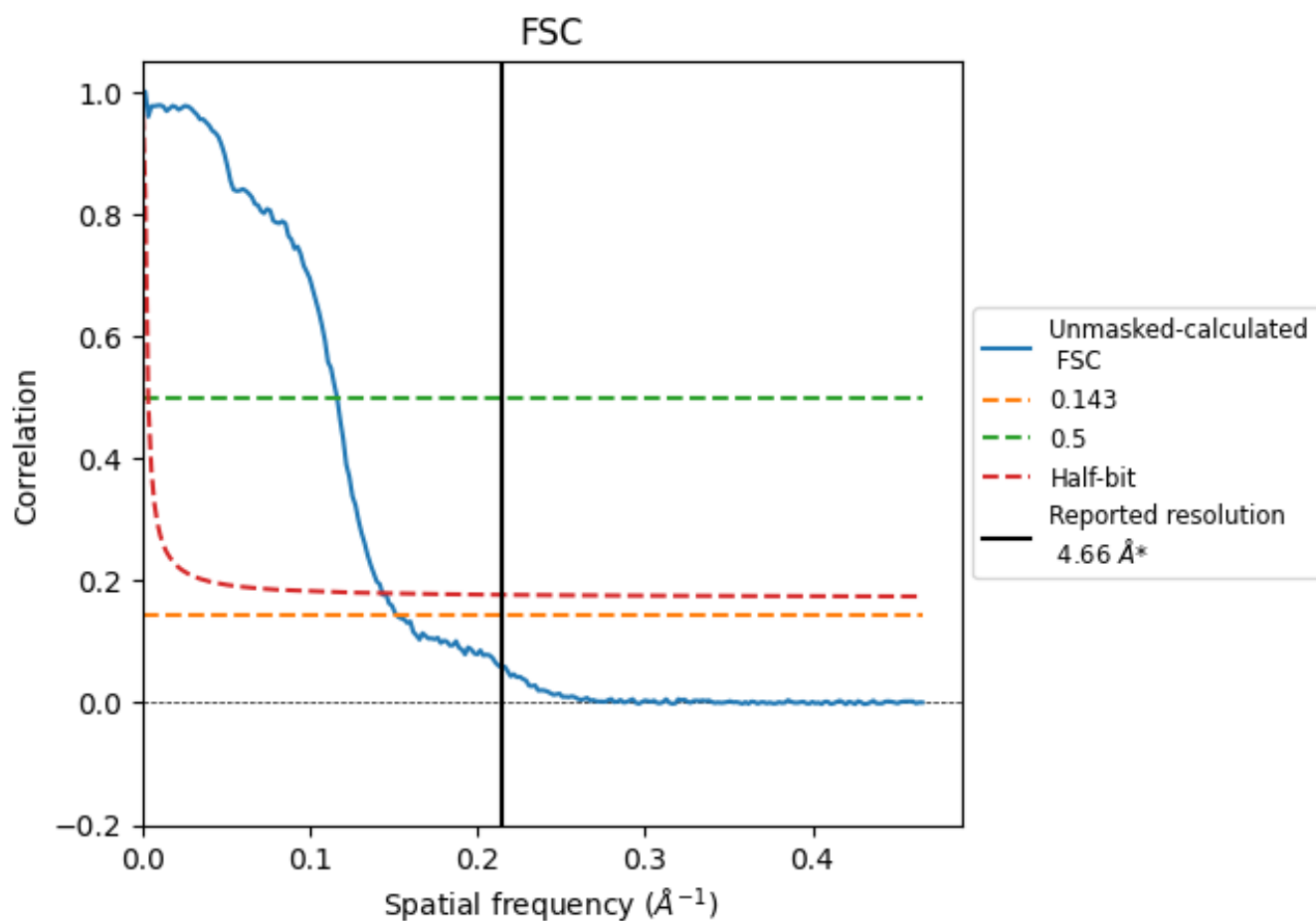


*Reported resolution corresponds to spatial frequency of 0.215 Å⁻¹

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 0.215 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

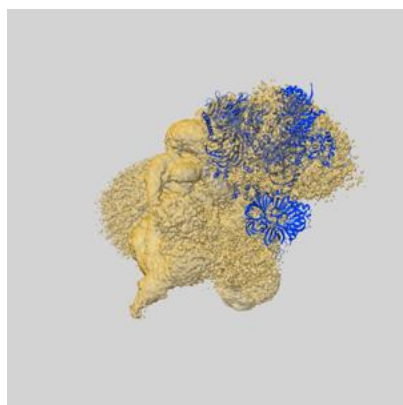
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.66	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.58	8.61	6.98

*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 6.58 differs from the reported value 4.66 by more than 10 %

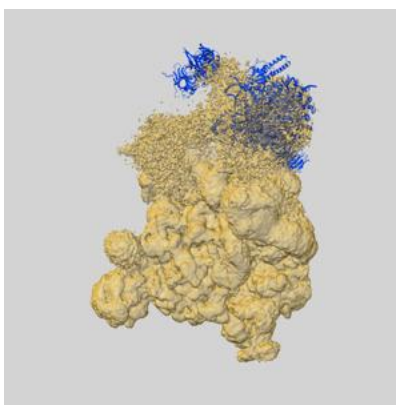
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39013 and PDB model 8Y7E. Per-residue inclusion information can be found in section [3](#) on page [7](#).

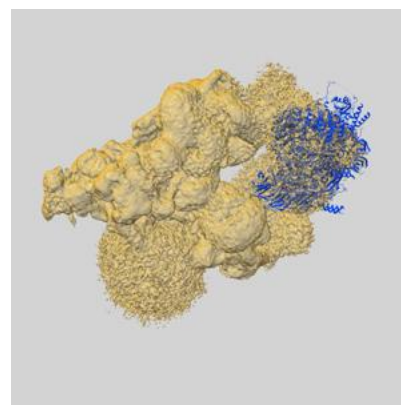
9.1 Map-model overlay [i](#)



X



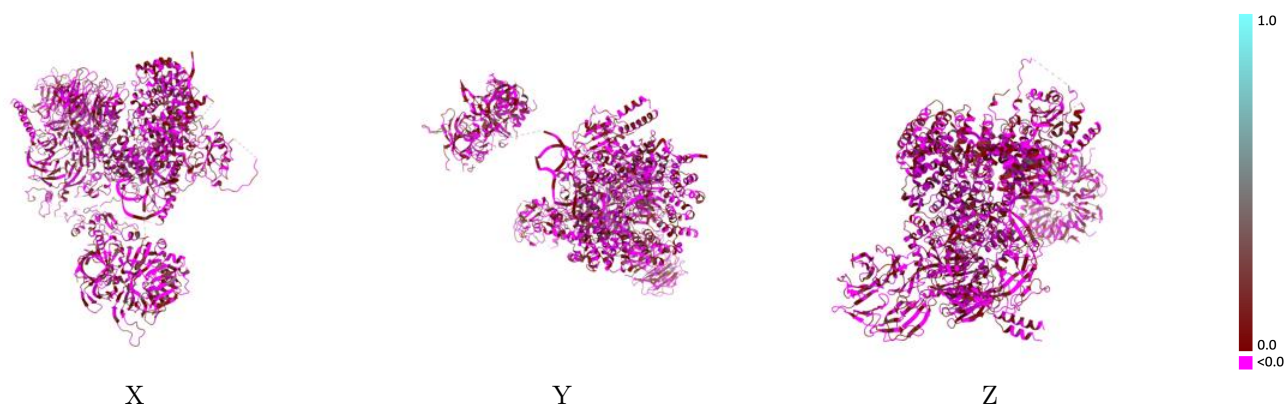
Y



Z

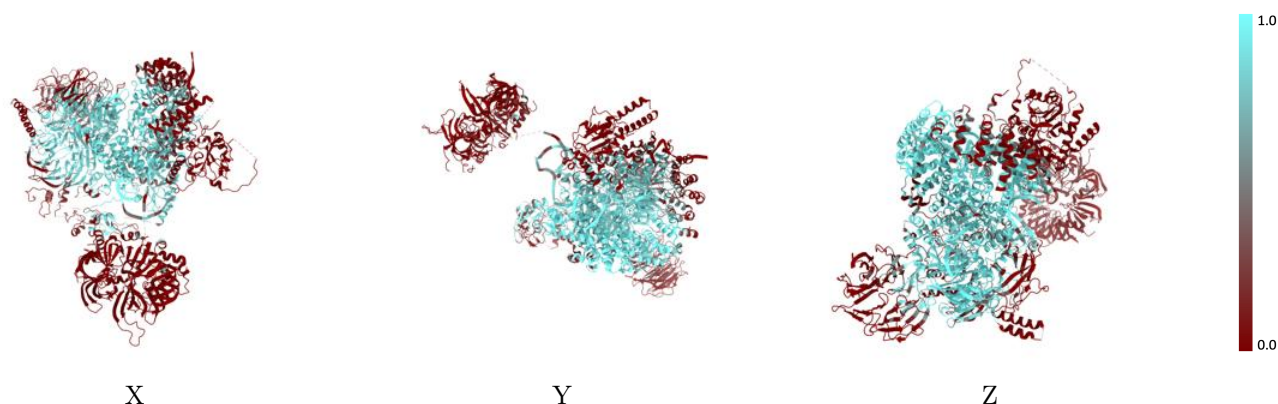
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



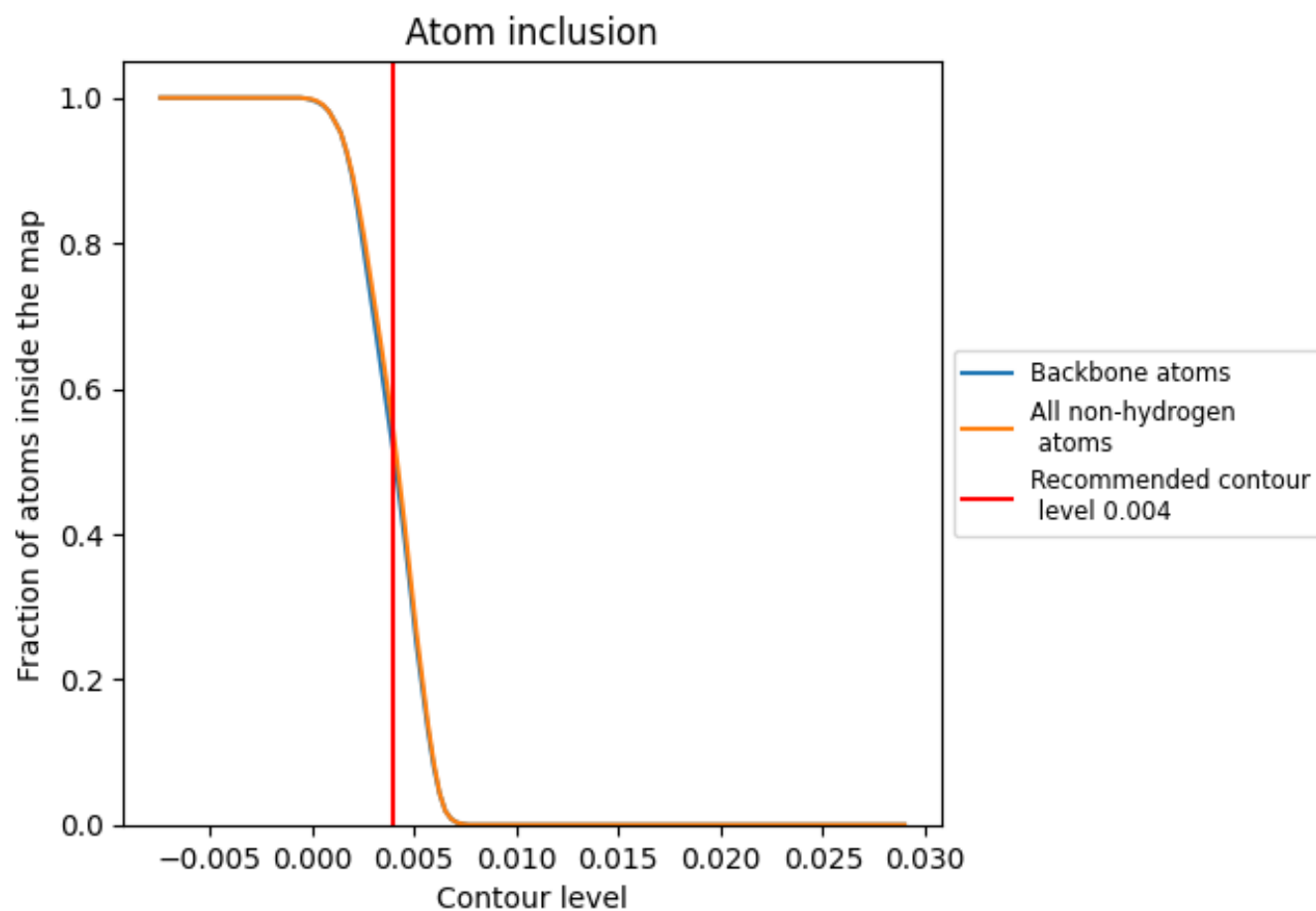
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).

9.4 Atom inclusion ⓘ



At the recommended contour level, 51% of all backbone atoms, 54% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5360	 0.0040
1	 0.6200	 0.0090
2	 0.5260	 -0.0010
3	 0.5810	 0.0000
4	 0.5640	 0.0030
5	 0.0000	 0.0060
6	 0.9870	 0.0010
7	 0.9910	 0.0150
A	 0.6460	 -0.0180
H	 0.6210	 -0.0230
h	 0.0000	 0.0170
i	 0.0000	 0.0100
j	 0.0150	 0.0490
k	 0.0310	 0.0100
l	 0.0080	 0.0150
m	 0.0440	 0.0150
n	 0.0000	 -0.0200
v	 0.5860	 0.0190

