



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:43 AM UTC

PDB ID : 5GAP / pdb_00005gap
EMDB ID : EMD-8014
Title : Body region of the U4/U6.U5 tri-snRNP
Authors : Nguyen, T.H.D.; Galej, W.P.; Oubridge, C.; Bai, X.C.; Newman, A.; Scheres, S.; Nagai, K.
Deposited on : 2015-12-15
Resolution : 3.60 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:

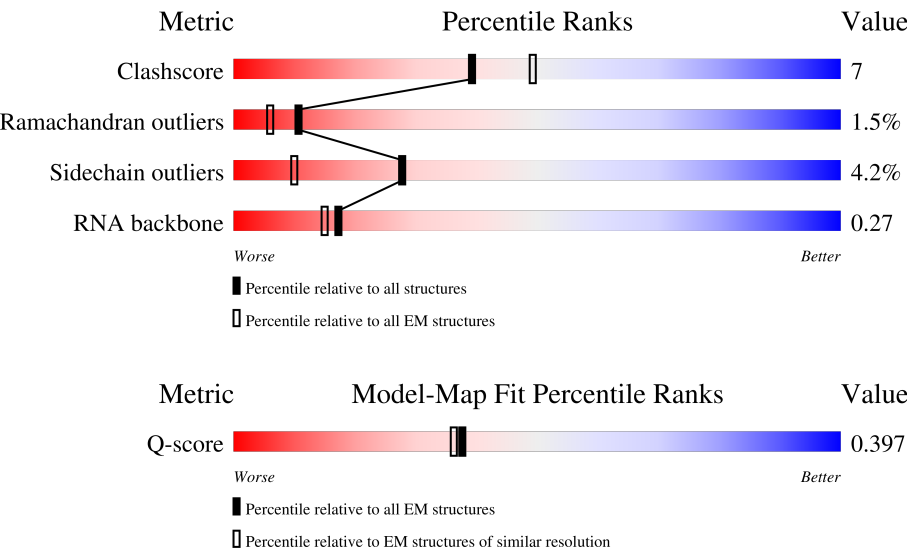
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.60 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.



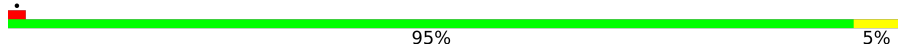
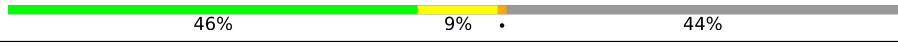
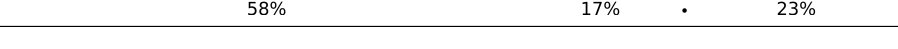
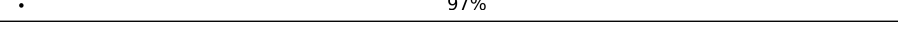
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	V	67	
2	W	112	
3	U	214	

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Mol	Chain	Length	Quality of chain
4	x	82	
5	A	2413	
6	H	465	
7	J	899	
8	D	143	
9	F	494	
10	G	469	
11	K	126	
12	B	2163	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 31576 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called U4 snRNA, 5' region, nucleotides 1-67.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	V	67	Total	C	N	O	P	0	0
			1426	637	247	475	67		

- Molecule 2 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	W	56	Total	C	N	O	P	0	0
			1190	533	210	391	56		

- Molecule 3 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	U	20	Total	C	N	O	P	0	0
			414	186	64	144	20		

- Molecule 4 is a protein called unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	x	82	Total	C	N	O	0	0
			410	246	82	82		

- Molecule 5 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	1349	Total	C	N	O	S	0	0
			11066	7094	1901	2031	40		

- Molecule 6 is a protein called U4/U6 small nuclear ribonucleoprotein PRP4.

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

- Molecule 7 is a protein called Pre-mRNA-splicing factor 6.

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

- Molecule 8 is a protein called Spliceosomal protein DIB1.

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

- Molecule 9 is a protein called Pre-mRNA-processing factor 31.

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

- Molecule 10 is a protein called U4/U6 small nuclear ribonucleoprotein PRP3.

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

- Molecule 11 is a protein called 13 kDa ribonucleoprotein-associated protein.

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

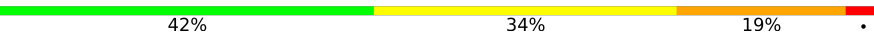
- Molecule 12 is a protein called Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	71	Total	C	N	O	S	0	0
			522	326	89	106	1		

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.

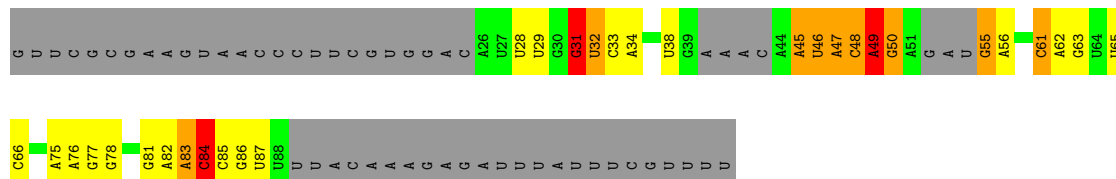
- Molecule 1: U4 snRNA, 5' region, nucleotides 1-67

Chain V: 



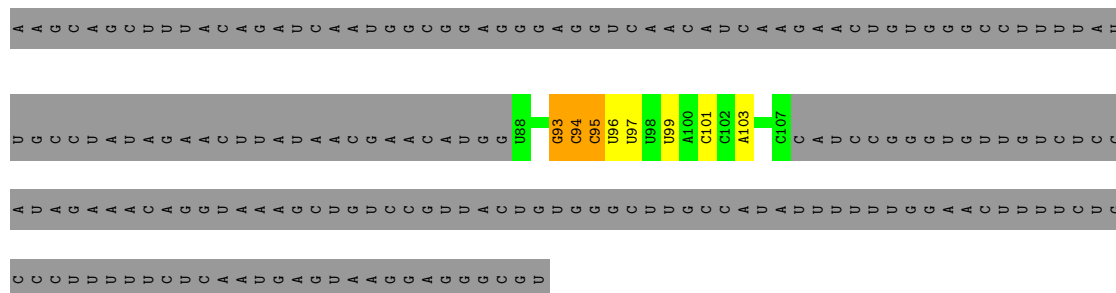
- Molecule 2: U6 snRNA

Chain W: 

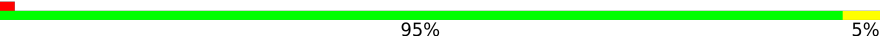


- Molecule 3: U5 snRNA

Chain U: 



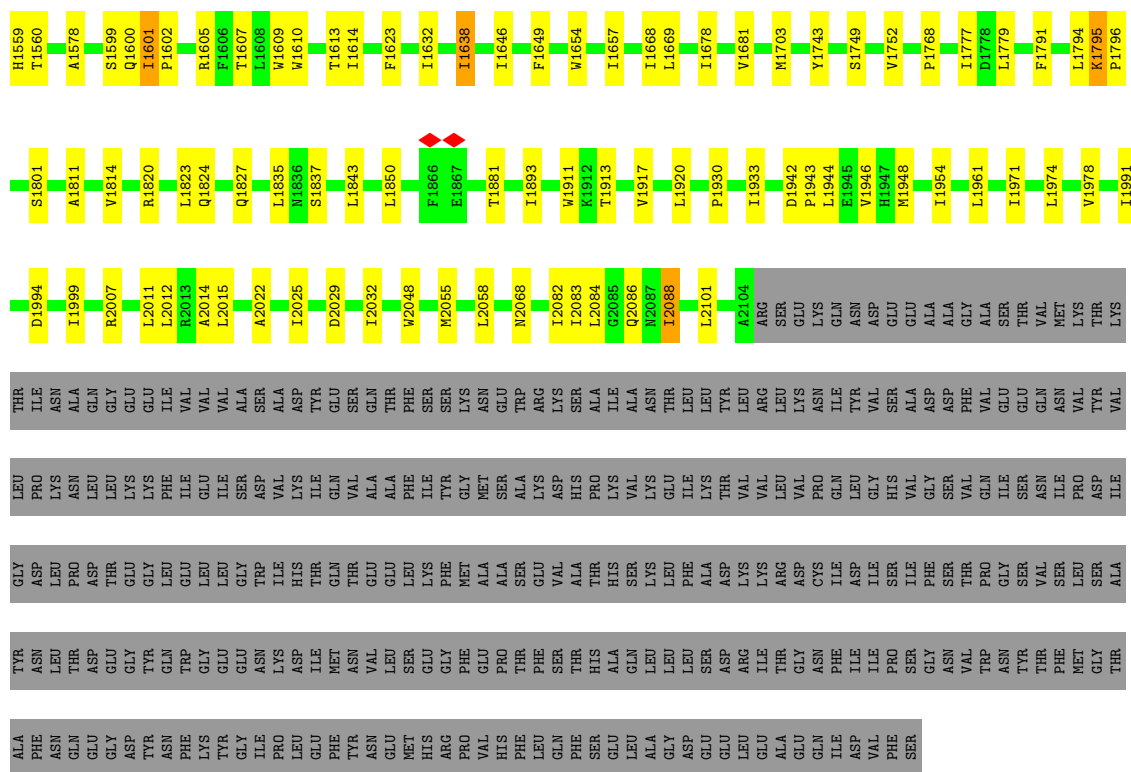
- Molecule 4: unknown protein

Chain x: 



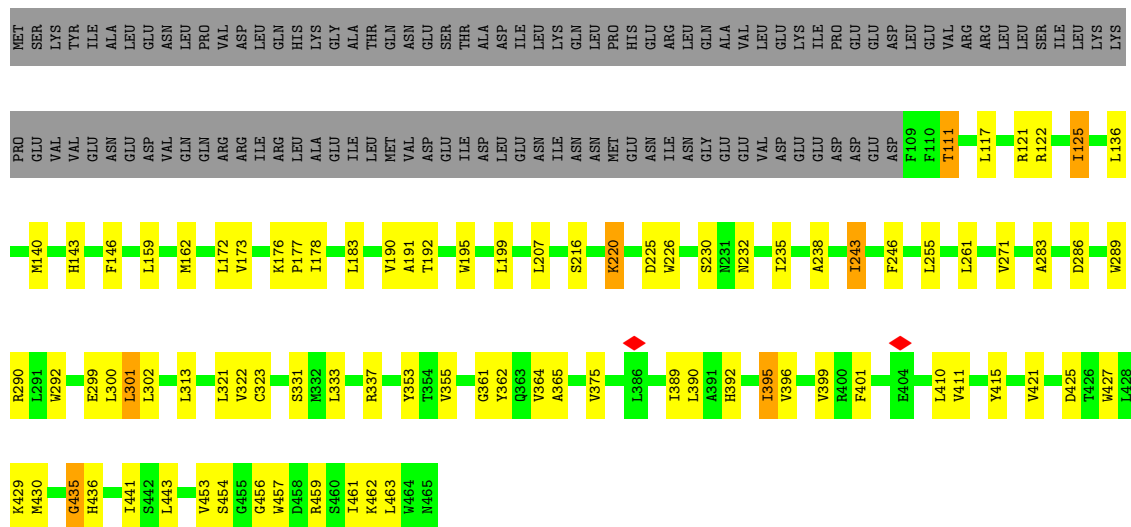
Chain A: 46% 9% . 44%





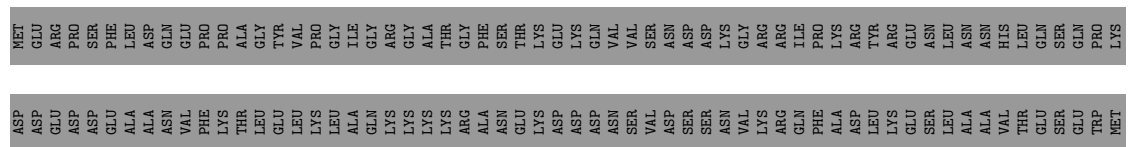
• Molecule 6: U4/U6 small nuclear ribonucleoprotein PRP4

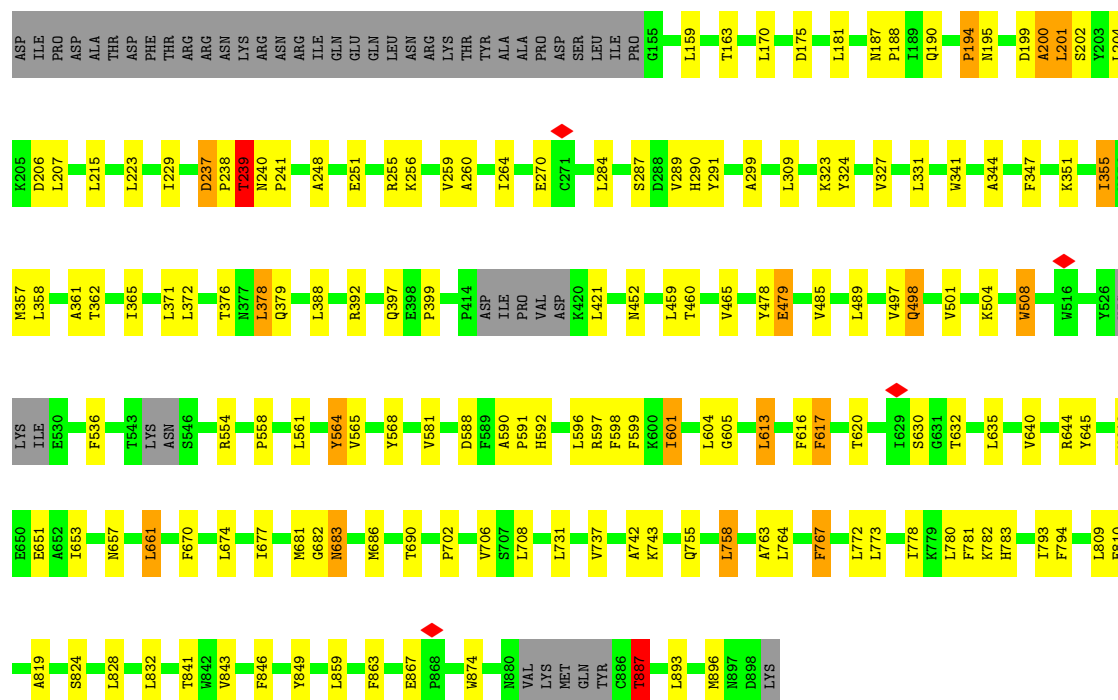
Chain H: 58% 17% 23%



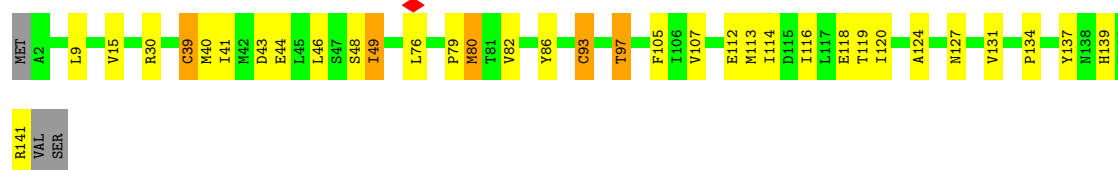
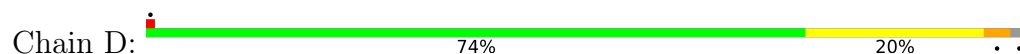
• Molecule 7: Pre-mRNA-splicing factor 6

Chain J: 64% 15% 19%





• Molecule 8: Spliceosomal protein DIB1



• Molecule 9: Pre-mRNA-processing factor 31





[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	140155	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.326	Depositor
Minimum map value	-0.232	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	543.39996, 543.39996, 543.39996	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.43, 1.43, 1.43	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	V	0.41	0/1593	0.88	5/2480 (0.2%)
2	W	0.41	0/1328	0.94	8/2061 (0.4%)
3	U	0.40	0/459	0.77	1/710 (0.1%)
5	A	0.54	1/11327 (0.0%)	1.04	14/15348 (0.1%)
6	H	0.51	0/2845	0.93	3/3843 (0.1%)
7	J	0.57	0/5934	1.21	8/8039 (0.1%)
8	D	0.56	0/1172	1.06	2/1578 (0.1%)
9	F	0.58	0/3273	1.19	9/4413 (0.2%)
10	G	0.54	0/2687	0.99	3/3611 (0.1%)
11	K	0.61	0/949	1.18	1/1292 (0.1%)
12	B	0.61	0/529	1.13	0/716
All	All	0.54	1/32096 (0.0%)	1.07	54/44091 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	A	0	3
9	F	0	1
12	B	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1369	ASN	CA-C	-5.24	1.46	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	95	C	C4'-C3'-O3'	8.08	121.52	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	49	A	C2'-C3'-O3'	7.76	121.14	109.50
7	J	239	THR	N-CA-C	7.75	120.62	111.71
5	A	1369	ASN	CA-C-O	-7.45	112.66	120.55
1	V	17	A	C2'-C3'-O3'	7.36	124.74	113.70
7	J	355	ILE	CB-CA-C	-7.09	102.89	111.97
1	V	39	C	C2'-C3'-O3'	6.95	119.93	109.50
5	A	979	SER	C-N-CD	-6.95	105.32	120.60
1	V	31	U	C4'-C3'-O3'	6.68	119.42	109.40
11	K	125	LEU	N-CA-C	6.45	118.00	110.97
1	V	19	U	C2'-C3'-O3'	6.35	119.02	109.50
9	F	197	ILE	N-CA-CB	6.32	119.14	110.54
9	F	74	LEU	CA-C-N	-6.26	113.69	119.82
9	F	74	LEU	C-N-CA	-6.26	113.69	119.82
10	G	349	ASN	CA-C-N	6.22	125.63	118.85
10	G	349	ASN	C-N-CA	6.22	125.63	118.85
9	F	379	PHE	N-CA-C	6.22	120.87	113.28
9	F	117	ILE	N-CA-CB	6.21	118.99	110.54
5	A	1361	VAL	N-CA-C	-6.14	103.85	110.23
2	W	55	G	C2'-C3'-O3'	6.11	122.87	113.70
5	A	811	ILE	N-CA-CB	6.08	117.67	110.55
5	A	1021	PRO	N-CA-C	5.97	117.98	110.70
9	F	222	ILE	N-CA-C	5.94	119.37	111.17
5	A	1752	VAL	N-CA-CB	5.90	118.56	110.54
9	F	46	ILE	N-CA-C	5.89	117.33	110.62
2	W	83	A	C2'-C3'-O3'	5.85	118.27	109.50
7	J	601	ILE	CB-CA-C	-5.84	104.50	111.97
2	W	31	G	O4'-C4'-C3'	-5.82	100.28	106.10
9	F	307	CYS	N-CA-C	-5.81	104.64	110.97
5	A	1942	ASP	O-C-N	5.77	124.94	120.38
7	J	564	TYR	CB-CA-C	-5.69	101.94	110.88
10	G	297	VAL	N-CA-CB	5.65	117.80	110.57
7	J	617	PHE	CB-CA-C	5.62	120.12	110.79
7	J	201	LEU	N-CA-C	-5.61	105.93	112.89
8	D	97	THR	N-CA-C	5.60	118.92	111.75
2	W	48	C	C3'-C2'-O2'	5.58	119.06	110.70
2	W	48	C	C2'-C3'-O3'	5.56	122.04	113.70
5	A	1601	ILE	CB-CA-C	-5.52	108.50	114.35
5	A	1795	LYS	O-C-N	5.51	125.38	120.48
8	D	116	ILE	N-CA-CB	5.51	118.03	110.54
2	W	84	C	C4'-C3'-O3'	5.46	117.60	109.40
5	A	816	ILE	N-CA-CB	5.39	117.88	110.54
6	H	125	ILE	N-CA-CB	5.37	117.85	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2082	ILE	N-CA-C	5.33	115.43	110.42
7	J	887	THR	N-CA-C	5.32	121.58	109.81
5	A	1814	VAL	CB-CA-C	-5.32	105.16	111.97
1	V	44	G	C2'-C3'-O3'	5.28	117.42	109.50
6	H	238	ALA	N-CA-C	5.19	115.39	108.38
7	J	378	LEU	N-CA-C	5.19	116.63	110.97
2	W	63	G	C3'-C2'-O2'	5.16	118.44	110.70
9	F	155	ASP	N-CA-C	5.15	125.42	111.00
5	A	990	ILE	CB-CA-C	-5.10	105.44	111.97
6	H	395	ILE	CB-CA-C	-5.08	105.76	111.45
5	A	1279	VAL	N-CA-C	5.06	115.86	108.53

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	1278	VAL	Peptide
5	A	1994	ASP	Peptide
5	A	979	SER	Peptide
12	B	423	ILE	Peptide
9	F	154	SER	Peptide

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	V	1426	0	716	22	0
2	W	1190	0	603	14	0
3	U	414	0	213	4	0
4	x	410	0	89	3	0
5	A	11066	0	11078	149	0
6	H	2789	0	2725	56	0
7	J	5822	0	5792	110	0
8	D	1151	0	1138	19	0
9	F	3218	0	3297	55	0
10	G	2632	0	2599	28	0
11	K	936	0	987	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	B	522	0	506	6	0
All	All	31576	0	29743	443	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 7.

All (443) 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)
5:A:1275:MET:HE3	5:A:1281:ASN:CG	1.83	1.02
5:A:1578:ALA:HB1	5:A:1602:PRO:HB3	1.40	1.02
5:A:1275:MET:HE3	5:A:1281:ASN:ND2	1.86	0.91
9:F:112:MET:HE2	9:F:203:ILE:HD12	1.61	0.82
10:G:272:VAL:HG12	10:G:280:VAL:HG21	1.59	0.81
5:A:1067:ASN:HB2	5:A:1083:THR:HG21	1.64	0.80
7:J:199:ASP:O	7:J:201:LEU:N	2.14	0.79
9:F:347:ALA:HB1	9:F:348:PRO:HD2	1.69	0.74
7:J:598:PHE:HA	7:J:601:ILE:HD12	1.68	0.74
11:K:16:LEU:HD21	11:K:124:LEU:HD11	1.69	0.74
11:K:24:VAL:HG13	11:K:33:LEU:CD1	2.19	0.72
6:H:441:ILE:HG22	6:H:456:GLY:HA2	1.69	0.72
7:J:361:ALA:HB1	7:J:371:LEU:HD13	1.72	0.72
1:V:18:A:OP2	9:F:378:LYS:NZ	2.24	0.70
7:J:849:TYR:CD2	7:J:859:LEU:HD11	2.27	0.70
8:D:86:TYR:CD2	8:D:124:ALA:HB1	2.27	0.69
5:A:960:THR:HG21	9:F:455:PHE:CZ	2.29	0.68
5:A:1668:ILE:HD13	5:A:1801:SER:HB3	1.76	0.68
5:A:1050:LEU:HD22	5:A:1170:MET:HE3	1.76	0.67
5:A:1946:VAL:HG21	7:J:229:ILE:HG21	1.77	0.66
11:K:16:LEU:CD2	11:K:124:LEU:HD11	2.25	0.66
7:J:264:ILE:HD13	7:J:284:LEU:HD11	1.78	0.66
5:A:1948:MET:HE1	5:A:1954:ILE:HD12	1.77	0.66
10:G:346:ASN:HD22	10:G:419:MET:HE2	1.60	0.65
7:J:863:PHE:CE1	7:J:893:LEU:HD11	2.32	0.65
5:A:1835:LEU:HD21	5:A:1843:LEU:HD11	1.79	0.64
9:F:135:LEU:HD22	9:F:208:TRP:CD1	2.33	0.64
7:J:351:LYS:O	7:J:355:ILE:HG13	1.98	0.64
7:J:251:GLU:OE2	7:J:259:VAL:HG23	1.99	0.62
7:J:597:ARG:HE	7:J:620:THR:HG22	1.64	0.62
7:J:601:ILE:HD13	7:J:640:VAL:HG11	1.80	0.62
5:A:1092:PHE:O	5:A:1093:LYS:C	2.42	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:74:LEU:HB3	9:F:75:PRO:HD3	1.80	0.62
3:U:93:G:N1	3:U:94:C:C4	2.68	0.62
9:F:53:LEU:HD22	9:F:73:ILE:HG12	1.81	0.62
11:K:24:VAL:HG22	11:K:102:ILE:HD11	1.82	0.61
5:A:1342:LEU:CD2	5:A:1360:LEU:HD21	2.30	0.61
6:H:411:VAL:HG12	6:H:443:LEU:HD21	1.81	0.61
5:A:1063:PHE:CE1	5:A:1086:ASN:HB3	2.35	0.61
5:A:1089:VAL:HG22	5:A:1098:VAL:HG22	1.82	0.61
7:J:452:ASN:CB	7:J:497:VAL:HG21	2.30	0.61
9:F:127:LEU:HD11	9:F:140:VAL:HG11	1.82	0.61
6:H:283:ALA:HB2	6:H:313:LEU:HG	1.83	0.61
5:A:1559:HIS:HB3	5:A:1613:THR:HG21	1.82	0.60
5:A:2025:ILE:HD12	5:A:2058:LEU:HD22	1.83	0.60
4:x:30:UNK:O	4:x:34:UNK:N	2.33	0.60
11:K:64:LEU:CD2	11:K:98:ILE:HD13	2.31	0.60
5:A:1578:ALA:CB	5:A:1602:PRO:HB3	2.25	0.60
6:H:192:THR:HG21	6:H:461:ILE:CD1	2.32	0.60
2:W:31:G:H4'	2:W:32:U:OP1	2.01	0.60
1:V:58:G:H2'	1:V:59:C:O4'	2.02	0.60
7:J:204:LEU:HD23	9:F:433:ASN:HD22	1.66	0.60
9:F:233:VAL:HG11	9:F:237:ILE:HG21	1.84	0.59
5:A:1669:LEU:HD13	5:A:1703:MET:HE3	1.85	0.59
5:A:1971:ILE:HD11	5:A:2012:LEU:HD21	1.83	0.59
5:A:1082:ILE:HD13	5:A:1113:ILE:HD11	1.84	0.59
3:U:93:G:N2	3:U:94:C:C2	2.70	0.59
7:J:465:VAL:HG11	7:J:501:VAL:HG22	1.84	0.59
7:J:702:PRO:O	7:J:706:VAL:HG23	2.02	0.59
6:H:395:ILE:HD11	6:H:415:TYR:CD1	2.38	0.59
7:J:613:LEU:O	7:J:617:PHE:CD2	2.56	0.59
10:G:342:PHE:HB3	10:G:424:ILE:HD11	1.85	0.59
7:J:590:ALA:HB3	7:J:591:PRO:HD3	1.85	0.58
9:F:218:ILE:O	9:F:222:ILE:HG23	2.04	0.58
10:G:341:VAL:HG11	10:G:463:PHE:CD1	2.39	0.58
7:J:341:TRP:CD1	7:J:365:ILE:HD11	2.39	0.58
8:D:86:TYR:CG	8:D:124:ALA:HB1	2.38	0.58
5:A:1023:LEU:HD13	5:A:1451:PHE:CD1	2.39	0.58
6:H:375:VAL:HG11	6:H:427:TRP:CH2	2.39	0.58
7:J:204:LEU:HD22	9:F:380:ARG:O	2.04	0.57
7:J:758:LEU:HD21	11:K:75:ASN:HB2	1.86	0.57
7:J:536:PHE:HB3	7:J:564:TYR:CZ	2.40	0.57
6:H:162:MET:HB3	6:H:421:VAL:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1312:PHE:CE2	5:A:1360:LEU:HD23	2.40	0.56
10:G:368:LEU:HD13	10:G:370:LEU:HD13	1.87	0.56
5:A:808:ILE:O	5:A:811:ILE:HG22	2.05	0.56
5:A:1599:SER:O	5:A:1602:PRO:HD2	2.05	0.56
6:H:159:LEU:HD13	6:H:430:MET:HE2	1.87	0.56
2:W:84:C:H3'	10:G:350:PRO:HB3	1.88	0.56
7:J:201:LEU:O	7:J:202:SER:C	2.49	0.56
10:G:365:LEU:HD22	10:G:382:VAL:HG12	1.88	0.56
5:A:1394:LEU:HD11	5:A:1553:ILE:HD13	1.88	0.55
11:K:64:LEU:HD22	11:K:98:ILE:HD13	1.88	0.55
12:B:387:GLU:O	12:B:388:GLN:CB	2.54	0.55
5:A:1339:LEU:HD21	5:A:1402:ALA:HB2	1.88	0.55
7:J:327:VAL:HG11	7:J:344:ALA:HB2	1.89	0.55
5:A:1275:MET:HE3	5:A:1281:ASN:OD1	2.07	0.55
7:J:846:PHE:CD1	7:J:859:LEU:HD13	2.42	0.55
8:D:46:LEU:HD21	8:D:113:MET:HE2	1.88	0.55
5:A:1961:LEU:HG	5:A:2084:LEU:HG	1.88	0.55
7:J:215:LEU:HD13	9:F:398:GLN:NE2	2.22	0.55
9:F:98:PHE:HA	9:F:101:ILE:HG22	1.88	0.55
1:V:10:C:H2'	1:V:11:A:O4'	2.06	0.54
5:A:882:ILE:CD1	5:A:1238:LEU:HD21	2.37	0.54
10:G:352:ILE:HD12	10:G:400:ILE:HG23	1.89	0.54
11:K:54:MET:HB3	11:K:64:LEU:HD11	1.89	0.54
1:V:58:G:C6	1:V:59:C:C4	2.96	0.54
2:W:49:A:O2'	2:W:50:G:OP2	2.22	0.54
5:A:831:ARG:NH2	5:A:978:ILE:HG23	2.22	0.54
9:F:194:ARG:O	9:F:197:ILE:HG13	2.08	0.54
7:J:616:PHE:O	7:J:620:THR:HG23	2.06	0.54
5:A:874:ILE:HD13	5:A:1065:LEU:HD22	1.90	0.53
9:F:329:LEU:HD22	11:K:60:PRO:HG3	1.90	0.53
7:J:204:LEU:CD1	9:F:381:LEU:HD23	2.38	0.53
11:K:39:GLU:O	11:K:43:THR:HG23	2.08	0.53
6:H:390:LEU:HB3	10:G:428:TRP:CE3	2.43	0.53
7:J:299:ALA:HB1	7:J:309:LEU:HD13	1.90	0.53
12:B:423:ILE:HG23	12:B:424:PRO:HD3	1.91	0.53
7:J:617:PHE:CD2	7:J:644:ARG:CZ	2.91	0.53
5:A:1354:GLU:N	5:A:1355:PRO:CD	2.72	0.53
7:J:204:LEU:HD23	9:F:433:ASN:ND2	2.23	0.53
2:W:77:G:H2'	2:W:78:G:O4'	2.09	0.53
5:A:1946:VAL:HG21	7:J:229:ILE:CG2	2.39	0.52
6:H:436:HIS:HA	6:H:462:LYS:HE3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:40:ALA:O	11:K:43:THR:OG1	2.21	0.52
5:A:1933:ILE:HD12	5:A:1948:MET:HE2	1.91	0.52
5:A:1168:ILE:HD12	5:A:1170:MET:HE2	1.91	0.52
7:J:215:LEU:HD13	9:F:398:GLN:HE22	1.74	0.52
5:A:765:ASP:CG	7:J:163:THR:HG21	2.35	0.52
5:A:1791:PHE:CE2	5:A:1794:LEU:HD22	2.44	0.52
7:J:781:PHE:CZ	7:J:793:ILE:HG13	2.45	0.52
9:F:106:LYS:O	9:F:109:ILE:HG22	2.09	0.52
5:A:939:LEU:HD21	9:F:445:ILE:HD11	1.92	0.52
5:A:1393:GLU:HG3	9:F:391:MET:HE2	1.92	0.52
7:J:376:THR:HG22	7:J:388:LEU:HD13	1.91	0.51
7:J:737:VAL:HG22	7:J:767:PHE:CD1	2.44	0.51
5:A:753:TYR:HB2	8:D:41:ILE:HD11	1.92	0.51
5:A:1063:PHE:CZ	5:A:1086:ASN:HB3	2.46	0.51
7:J:561:LEU:HB3	7:J:596:LEU:HD21	1.92	0.51
9:F:268:LEU:HD13	9:F:270:HIS:CE1	2.45	0.51
5:A:1600:GLN:NE2	8:D:134:PRO:O	2.43	0.51
6:H:192:THR:HG21	6:H:461:ILE:HD13	1.92	0.51
7:J:204:LEU:HD11	9:F:381:LEU:HD23	1.92	0.51
7:J:601:ILE:HG12	7:J:617:PHE:CZ	2.46	0.51
7:J:605:GLY:HA3	7:J:887:THR:HG21	1.92	0.51
9:F:145:GLU:HG3	9:F:197:ILE:HD11	1.91	0.51
11:K:24:VAL:HG13	11:K:33:LEU:HD11	1.93	0.51
1:V:35:G:N2	1:V:43:C:C2	2.79	0.51
5:A:1669:LEU:HB3	5:A:1681:VAL:HG21	1.93	0.51
7:J:843:VAL:HG21	7:J:896:MET:HE3	1.93	0.51
5:A:2015:LEU:HD23	5:A:2022:ALA:HB3	1.93	0.51
6:H:207:LEU:HD22	6:H:463:LEU:HG	1.91	0.51
10:G:382:VAL:HG21	10:G:392:TYR:CD2	2.45	0.51
9:F:57:LEU:HD21	9:F:108:ASN:HA	1.92	0.51
3:U:93:G:C2	3:U:94:C:C4	2.99	0.51
5:A:982:TYR:CD2	5:A:1104:ILE:HG23	2.46	0.51
5:A:1066:LEU:HD11	5:A:1113:ILE:HG23	1.93	0.51
5:A:1387:VAL:HG12	5:A:1610:TRP:CE3	2.46	0.51
9:F:74:LEU:HD13	9:F:78:VAL:HB	1.93	0.51
6:H:246:PHE:HB3	6:H:255:LEU:HD22	1.93	0.50
7:J:238:PRO:C	7:J:240:ASN:HA	2.35	0.50
7:J:661:LEU:HD22	7:J:670:PHE:HB3	1.92	0.50
11:K:53:ILE:HD11	11:K:102:ILE:HG12	1.92	0.50
5:A:788:GLU:HB2	7:J:181:LEU:HD23	1.93	0.50
5:A:1318:GLY:O	5:A:1321:MET:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:778:ILE:HG23	7:J:794:PHE:CE1	2.47	0.50
5:A:1578:ALA:HB1	5:A:1602:PRO:CB	2.28	0.50
5:A:1387:VAL:HG12	5:A:1610:TRP:CD2	2.47	0.50
9:F:298:VAL:HG12	9:F:302:MET:HB2	1.92	0.50
5:A:1275:MET:CE	5:A:1281:ASN:ND2	2.70	0.50
9:F:102:ILE:N	9:F:103:PRO:CD	2.75	0.50
6:H:111:THR:HG22	10:G:216:TYR:HB3	1.94	0.49
11:K:26:GLN:HB3	11:K:110:ILE:HG21	1.94	0.49
7:J:372:LEU:O	7:J:376:THR:HG23	2.12	0.49
1:V:21:C:H2'	1:V:22:G:O4'	2.12	0.49
5:A:1560:THR:HG21	5:A:1609:TRP:NE1	2.27	0.49
5:A:1893:ILE:HD12	5:A:1978:VAL:HG22	1.95	0.49
6:H:425:ASP:HB2	10:G:174:LEU:HD23	1.93	0.49
9:F:320:GLN:HE22	9:F:326:ASN:HB3	1.78	0.49
6:H:122:ARG:O	6:H:125:ILE:HG12	2.13	0.49
7:J:601:ILE:HG12	7:J:617:PHE:CE1	2.47	0.49
10:G:368:LEU:HD11	10:G:381:ILE:HD12	1.94	0.49
6:H:390:LEU:HD13	10:G:428:TRP:HB2	1.95	0.49
7:J:465:VAL:CG1	7:J:501:VAL:HG22	2.43	0.49
5:A:1183:THR:HG23	5:A:1221:ASN:HB3	1.94	0.49
5:A:1933:ILE:HG21	5:A:1944:LEU:HD21	1.94	0.49
1:V:34:G:H2'	1:V:35:G:O4'	2.12	0.49
5:A:1791:PHE:CZ	5:A:1794:LEU:HD22	2.47	0.49
7:J:195:ASN:O	7:J:199:ASP:N	2.46	0.49
7:J:207:LEU:HD12	9:F:382:SER:CB	2.43	0.49
1:V:22:G:C2	1:V:23:C:C2	3.00	0.48
7:J:248:ALA:HA	7:J:264:ILE:HD11	1.94	0.48
7:J:251:GLU:HB3	7:J:260:ALA:HB2	1.96	0.48
7:J:341:TRP:CE3	7:J:361:ALA:HB2	2.48	0.48
10:G:347:LEU:HD11	10:G:371:ARG:HD3	1.93	0.48
6:H:121:ARG:O	6:H:125:ILE:HG23	2.14	0.48
6:H:243:ILE:HG13	6:H:261:LEU:HD13	1.94	0.48
7:J:239:THR:N	7:J:240:ASN:HA	2.28	0.48
7:J:674:LEU:CD2	7:J:690:THR:HG21	2.43	0.48
5:A:1010:PRO:HG2	5:A:1012:TRP:CZ2	2.49	0.48
6:H:459:ARG:NH2	11:K:72:GLU:O	2.46	0.48
11:K:54:MET:HE2	11:K:78:TYR:HB2	1.95	0.48
1:V:22:G:C6	1:V:23:C:C4	3.02	0.48
7:J:190:GLN:O	7:J:194:PRO:HD2	2.13	0.48
5:A:1657:ILE:HA	5:A:1811:ALA:CB	2.44	0.48
7:J:170:LEU:HD13	7:J:175:ASP:OD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:404:GLY:O	12:B:407:GLN:HB2	2.13	0.48
5:A:1050:LEU:HD22	5:A:1170:MET:CE	2.42	0.48
6:H:176:LYS:HB3	6:H:177:PRO:HD2	1.95	0.48
7:J:256:LYS:HD2	7:J:259:VAL:HG22	1.96	0.48
7:J:674:LEU:HD22	7:J:690:THR:HG21	1.96	0.48
8:D:93:CYS:SG	8:D:120:ILE:HG21	2.54	0.48
11:K:54:MET:SD	11:K:64:LEU:CD1	3.02	0.48
5:A:1286:TRP:CZ2	5:A:1302:LEU:HD11	2.49	0.47
7:J:187:ASN:N	7:J:188:PRO:HD2	2.28	0.47
9:F:225:ILE:HG22	9:F:248:VAL:HG21	1.96	0.47
5:A:1407:ILE:HG21	5:A:1412:LEU:HD21	1.94	0.47
7:J:378:LEU:HD13	7:J:379:GLN:HA	1.96	0.47
5:A:1126:LEU:HD21	5:A:1161:TYR:CG	2.50	0.47
5:A:1820:ARG:O	5:A:1824:GLN:N	2.44	0.47
1:V:58:G:C5	1:V:59:C:C5	3.03	0.47
5:A:1974:LEU:O	5:A:1978:VAL:HG23	2.14	0.47
1:V:35:G:C2	1:V:43:C:C2	3.03	0.47
1:V:58:G:C2	1:V:59:C:C2	3.03	0.47
4:x:46:UNK:O	4:x:48:UNK:N	2.48	0.47
5:A:853:THR:O	5:A:857:ILE:HG12	2.14	0.47
7:J:645:TYR:O	7:J:649:ASN:N	2.46	0.47
9:F:130:LEU:HD11	9:F:178:SER:HB3	1.97	0.47
9:F:320:GLN:HE22	9:F:326:ASN:CB	2.28	0.47
5:A:770:MET:HE2	7:J:170:LEU:HD22	1.97	0.47
5:A:1414:TRP:HA	5:A:1558:GLU:HG2	1.95	0.47
5:A:2084:LEU:HD22	5:A:2086:GLN:CD	2.40	0.47
8:D:30:ARG:HA	8:D:82:VAL:HG12	1.95	0.47
5:A:1632:ILE:HD11	5:A:1649:PHE:CE1	2.49	0.47
5:A:1777:ILE:N	5:A:1777:ILE:HD12	2.30	0.47
6:H:125:ILE:HG22	6:H:337:ARG:HB3	1.95	0.47
6:H:435:GLY:N	7:J:731:LEU:HD13	2.30	0.47
11:K:67:LEU:N	11:K:68:PRO:CD	2.76	0.47
9:F:277:SER:HB2	9:F:279:VAL:HG12	1.95	0.47
10:G:293:TRP:O	10:G:297:VAL:HG13	2.15	0.47
1:V:50:G:C6	1:V:51:U:N3	2.83	0.47
7:J:324:TYR:CD1	7:J:347:PHE:CE2	3.03	0.47
5:A:756:LEU:HD13	8:D:44:GLU:HG3	1.97	0.46
5:A:1632:ILE:HD11	5:A:1649:PHE:CD1	2.49	0.46
6:H:289:TRP:CD2	6:H:313:LEU:HD21	2.50	0.46
6:H:321:LEU:HD11	6:H:333:LEU:HB3	1.97	0.46
5:A:1144:PHE:CD2	5:A:1145:MET:HE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:498:GLN:HE21	7:J:498:GLN:N	2.13	0.46
5:A:1601:ILE:N	5:A:1602:PRO:CD	2.79	0.46
7:J:344:ALA:HB3	7:J:357:MET:HE2	1.98	0.46
5:A:1542:TYR:O	5:A:1546:VAL:HG23	2.16	0.46
7:J:323:LYS:O	7:J:327:VAL:HG23	2.16	0.46
11:K:79:VAL:HG13	11:K:121:ILE:HG12	1.98	0.46
5:A:1372:LYS:HG2	5:A:1383:PHE:CE2	2.51	0.46
5:A:1605:ARG:HG2	5:A:1823:LEU:HA	1.98	0.46
9:F:369:GLY:O	9:F:370:ARG:C	2.58	0.46
5:A:886:MET:HE2	5:A:1120:VAL:HG22	1.98	0.46
5:A:819:LYS:O	5:A:823:TRP:N	2.48	0.46
6:H:176:LYS:HB3	6:H:177:PRO:CD	2.46	0.46
7:J:289:VAL:HG23	7:J:290:HIS:N	2.31	0.46
1:V:37:U:H2'	1:V:39:C:C5	2.51	0.45
9:F:219:ALA:HA	9:F:239:ALA:HB2	1.97	0.45
5:A:1368:GLN:O	5:A:1372:LYS:HG3	2.16	0.45
6:H:235:ILE:HD11	6:H:243:ILE:HG13	1.98	0.45
6:H:365:ALA:HB2	6:H:375:VAL:HG13	1.98	0.45
7:J:706:VAL:HG22	7:J:742:ALA:CB	2.46	0.45
12:B:391:PHE:O	12:B:392:ARG:C	2.60	0.45
5:A:1115:GLN:HA	5:A:1115:GLN:OE1	2.17	0.45
7:J:568:TYR:CZ	7:J:581:VAL:HG21	2.52	0.45
11:K:54:MET:CG	11:K:64:LEU:HD11	2.46	0.45
5:A:914:LEU:HD22	5:A:1505:ASP:HB2	1.97	0.45
5:A:971:MET:HG3	5:A:979:SER:HA	1.99	0.45
7:J:159:LEU:O	7:J:163:THR:HG23	2.17	0.45
7:J:504:LYS:HG3	7:J:508:TRP:CZ3	2.51	0.45
2:W:49:A:C5	5:A:1646:ILE:HD13	2.51	0.45
5:A:1413:SER:N	5:A:1743:TYR:OH	2.50	0.45
6:H:173:VAL:HB	6:H:178:ILE:HD11	1.98	0.45
5:A:1335:TRP:CD1	5:A:1367:ILE:HG13	2.50	0.45
5:A:1911:TRP:CH2	5:A:1943:PRO:HA	2.52	0.45
6:H:323:CYS:SG	6:H:355:VAL:HG21	2.57	0.45
8:D:79:PRO:HA	8:D:80:MET:HE2	1.99	0.45
5:A:1092:PHE:O	5:A:1095:MET:N	2.50	0.45
5:A:1795:LYS:N	5:A:1796:PRO:CD	2.79	0.45
11:K:20:ILE:HD13	11:K:79:VAL:HG21	1.99	0.45
5:A:1614:ILE:HG22	5:A:1638:ILE:HD13	1.99	0.45
6:H:177:PRO:HB3	6:H:457:TRP:HA	1.99	0.45
6:H:243:ILE:HG12	6:H:261:LEU:HB2	1.99	0.45
8:D:9:LEU:HD13	8:D:15:VAL:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1850:LEU:HD12	5:A:1930:PRO:HG3	1.98	0.45
6:H:395:ILE:HD11	6:H:415:TYR:CE1	2.52	0.45
2:W:50:G:N3	2:W:50:G:C2'	2.80	0.44
5:A:1375:LEU:HD22	5:A:1607:THR:HG23	1.98	0.44
7:J:763:ALA:HB1	7:J:773:LEU:CD1	2.47	0.44
1:V:8:U:O2'	12:B:390:LYS:NZ	2.46	0.44
5:A:755:ASP:OD1	5:A:756:LEU:N	2.50	0.44
5:A:919:LEU:HD13	5:A:990:ILE:HD13	1.99	0.44
5:A:1021:PRO:O	5:A:1025:VAL:HG23	2.17	0.44
5:A:1946:VAL:CG2	7:J:229:ILE:HG21	2.47	0.44
6:H:117:LEU:HD13	6:H:301:LEU:HD12	1.98	0.44
7:J:478:TYR:O	7:J:479:GLU:CB	2.66	0.44
2:W:61:C:H2'	2:W:62:A:H8	1.82	0.44
5:A:1025:VAL:HG22	5:A:1262:MET:HG2	2.00	0.44
6:H:195:TRP:CG	6:H:220:LYS:HG3	2.52	0.44
6:H:390:LEU:HD13	10:G:428:TRP:CG	2.53	0.44
6:H:392:HIS:HD2	6:H:396:VAL:HG22	1.82	0.44
5:A:857:ILE:CG2	5:A:1095:MET:HE2	2.48	0.44
5:A:1085:LYS:O	5:A:1088:VAL:HG13	2.17	0.44
9:F:47:LEU:HD13	9:F:97:PHE:HB3	1.99	0.44
7:J:780:LEU:O	7:J:783:HIS:HB2	2.18	0.44
9:F:59:LEU:HD21	9:F:66:SER:HB3	1.99	0.44
8:D:97:THR:HG21	8:D:105:PHE:CE1	2.53	0.44
8:D:97:THR:O	8:D:141:ARG:NH2	2.51	0.44
10:G:250:LYS:HG2	10:G:251:MET:HE2	2.00	0.44
6:H:183:LEU:HD23	6:H:190:VAL:HB	1.99	0.44
7:J:201:LEU:HD23	9:F:379:PHE:CZ	2.52	0.44
5:A:1125:LEU:CD2	5:A:1230:ILE:HG23	2.47	0.44
5:A:1458:TRP:CH2	5:A:1494:LEU:HD11	2.53	0.44
7:J:604:LEU:HB3	7:J:613:LEU:CD2	2.48	0.44
5:A:1461:TYR:CE1	5:A:1494:LEU:HD13	2.52	0.43
1:V:58:G:C4	1:V:59:C:C6	3.06	0.43
5:A:1385:PRO:HB2	5:A:1437:ILE:HD11	1.99	0.43
5:A:1601:ILE:N	5:A:1602:PRO:HD2	2.33	0.43
5:A:1961:LEU:HD12	5:A:2084:LEU:HD23	2.00	0.43
9:F:434:GLN:O	9:F:435:ALA:C	2.62	0.43
5:A:1678:ILE:CD1	5:A:1703:MET:HE2	2.48	0.43
5:A:1320:LEU:HD23	5:A:1367:ILE:HD13	2.01	0.43
7:J:378:LEU:HD13	7:J:378:LEU:C	2.44	0.43
5:A:1837:SER:N	5:A:2084:LEU:HD21	2.34	0.43
8:D:39:CYS:SG	8:D:40:MET:N	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1657:ILE:HA	5:A:1811:ALA:HB1	2.01	0.43
7:J:686:MET:O	7:J:690:THR:HG23	2.19	0.43
2:W:34:A:N6	2:W:47:A:C8	2.87	0.43
5:A:1028:TRP:NE1	5:A:1032:ILE:HD11	2.34	0.43
6:H:159:LEU:CD1	6:H:430:MET:HE2	2.48	0.43
6:H:172:LEU:HD13	7:J:755:GLN:HG3	2.00	0.43
6:H:261:LEU:HB3	6:H:292:TRP:CZ3	2.53	0.43
7:J:737:VAL:HG22	7:J:767:PHE:CG	2.54	0.43
5:A:1047:ALA:HB3	5:A:1251:TYR:HB3	2.01	0.42
5:A:2011:LEU:HD23	5:A:2055:MET:HG3	2.01	0.42
6:H:125:ILE:HG22	6:H:337:ARG:CB	2.49	0.42
7:J:651:GLU:HG2	7:J:681:MET:HE1	2.00	0.42
4:x:30:UNK:O	4:x:34:UNK:CB	2.67	0.42
5:A:1070:LEU:HD21	5:A:1113:ILE:CD1	2.50	0.42
6:H:191:ALA:HB2	6:H:226:TRP:CZ2	2.54	0.42
7:J:207:LEU:HD12	9:F:382:SER:OG	2.19	0.42
7:J:846:PHE:CE1	7:J:859:LEU:HD13	2.55	0.42
8:D:120:ILE:HG22	8:D:131:VAL:CG1	2.50	0.42
2:W:34:A:C6	2:W:50:G:C6	3.07	0.42
7:J:565:VAL:HG11	7:J:599:PHE:CB	2.48	0.42
8:D:97:THR:HG22	8:D:141:ARG:HA	2.00	0.42
8:D:112:GLU:CD	8:D:137:TYR:OH	2.62	0.42
1:V:33:A:H2'	1:V:34:G:O4'	2.18	0.42
5:A:943:ALA:O	5:A:947:PRO:HA	2.20	0.42
6:H:401:PHE:CE1	6:H:410:LEU:HG	2.55	0.42
7:J:207:LEU:HD13	9:F:430:SER:CB	2.50	0.42
7:J:485:VAL:O	7:J:489:LEU:HG	2.19	0.42
2:W:81:G:H2'	2:W:82:A:C8	2.54	0.42
6:H:390:LEU:HD11	10:G:463:PHE:CD1	2.54	0.42
9:F:117:ILE:HD12	9:F:128:SER:CB	2.50	0.42
5:A:1601:ILE:HB	5:A:1602:PRO:HD3	2.01	0.42
9:F:114:ASN:HA	9:F:117:ILE:HG22	2.01	0.42
9:F:381:LEU:HD22	9:F:385:ARG:HB3	2.01	0.42
1:V:22:G:C4	1:V:23:C:C5	3.08	0.42
5:A:1933:ILE:CD1	5:A:1948:MET:HE2	2.50	0.42
6:H:207:LEU:HD13	6:H:463:LEU:HD21	2.01	0.42
7:J:358:LEU:O	7:J:362:THR:HG23	2.19	0.42
7:J:653:ILE:HG21	7:J:677:ILE:HD13	2.02	0.42
8:D:49:ILE:HD12	8:D:114:ILE:HG13	2.02	0.42
10:G:272:VAL:HG22	10:G:300:GLN:NE2	2.35	0.42
5:A:1837:SER:HB3	5:A:2084:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:77:G:H4'	11:K:113:GLN:HG3	2.01	0.42
5:A:1085:LYS:HG3	5:A:1107:LEU:HD13	2.02	0.42
5:A:1811:ALA:HA	5:A:2101:LEU:HD13	2.02	0.42
5:A:1881:THR:HG21	5:A:1920:LEU:HD23	2.02	0.42
6:H:140:MET:HA	6:H:143:HIS:CD2	2.55	0.42
7:J:341:TRP:HE3	7:J:357:MET:HE1	1.84	0.42
1:V:55:U:N3	7:J:200:ALA:O	2.53	0.42
2:W:65:U:H2'	2:W:66:C:C6	2.55	0.42
5:A:762:VAL:HG22	7:J:159:LEU:HD22	2.02	0.42
6:H:172:LEU:C	6:H:172:LEU:HD12	2.45	0.41
9:F:124:PHE:CE2	9:F:127:LEU:HD13	2.55	0.41
1:V:17:A:C2	1:V:18:A:C4	3.08	0.41
5:A:922:VAL:HG13	5:A:923:TYR:CD1	2.55	0.41
5:A:2083:ILE:HD11	10:G:287:ILE:HG12	2.02	0.41
6:H:290:ARG:NE	6:H:299:GLU:OE2	2.53	0.41
1:V:35:G:C2	1:V:36:A:C8	3.08	0.41
11:K:33:LEU:HD21	11:K:35:LYS:HG3	2.02	0.41
12:B:392:ARG:O	12:B:393:GLU:C	2.63	0.41
5:A:831:ARG:HH21	5:A:978:ILE:HG23	1.85	0.41
7:J:207:LEU:HD12	9:F:382:SER:HB2	2.03	0.41
7:J:392:ARG:HB3	7:J:397:GLN:HE22	1.84	0.41
2:W:45:A:C2'	2:W:46:U:OP1	2.69	0.41
2:W:45:A:C6	2:W:46:U:C4	3.08	0.41
3:U:93:G:C2	3:U:94:C:N3	2.89	0.41
5:A:804:MET:HE1	5:A:808:ILE:HG22	2.02	0.41
5:A:2012:LEU:HA	5:A:2015:LEU:HD12	2.03	0.41
7:J:824:SER:O	7:J:828:LEU:HG	2.20	0.41
5:A:1048:VAL:HG22	5:A:1250:VAL:HG22	2.02	0.41
5:A:2014:ALA:HB1	5:A:2058:LEU:HD23	2.03	0.41
5:A:2029:ASP:HB3	5:A:2032:ILE:HD12	2.03	0.41
6:H:390:LEU:HD11	10:G:463:PHE:HD1	1.85	0.41
7:J:682:GLY:O	7:J:683:ASN:C	2.63	0.41
7:J:706:VAL:HG22	7:J:742:ALA:HB1	2.03	0.41
8:D:119:THR:HG22	8:D:131:VAL:HG21	2.01	0.41
10:G:341:VAL:HG22	10:G:428:TRP:CB	2.50	0.41
5:A:788:GLU:CB	7:J:181:LEU:HD23	2.51	0.41
5:A:1073:ILE:HD13	5:A:1116:TYR:CD1	2.55	0.41
5:A:1654:TRP:CZ3	5:A:1779:LEU:HD12	2.56	0.41
5:A:1678:ILE:HD13	5:A:1703:MET:HE2	2.02	0.41
8:D:49:ILE:HG23	8:D:114:ILE:HG12	2.02	0.41
9:F:74:LEU:HD23	9:F:203:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:257:GLU:HA	10:G:260:ILE:HG22	2.02	0.41
5:A:1026:TYR:O	5:A:1029:THR:OG1	2.33	0.41
5:A:1038:ILE:HG23	5:A:1039:TRP:CD2	2.55	0.41
5:A:1320:LEU:HD11	5:A:1366:ARG:HB3	2.02	0.41
5:A:1346:PHE:O	5:A:1347:ARG:C	2.63	0.41
5:A:1375:LEU:HD23	5:A:1375:LEU:HA	1.97	0.41
5:A:1999:ILE:HD13	5:A:2007:ARG:NH2	2.36	0.41
7:J:215:LEU:CD2	9:F:400:VAL:HG22	2.51	0.41
7:J:632:THR:HA	7:J:635:LEU:HD21	2.02	0.41
7:J:778:ILE:CG2	7:J:810:GLU:HG3	2.51	0.41
10:G:363:LEU:HD11	10:G:391:PHE:CD2	2.56	0.41
1:V:19:U:H4'	1:V:20:A:C8	2.56	0.41
5:A:1321:MET:O	5:A:1322:ALA:CB	2.69	0.41
6:H:353:TYR:CZ	11:K:126:ILE:HD11	2.56	0.41
6:H:364:VAL:HG12	6:H:365:ALA:N	2.36	0.41
10:G:341:VAL:HG12	10:G:381:ILE:HG23	2.02	0.41
11:K:12:ALA:HB1	11:K:16:LEU:HD23	2.03	0.41
5:A:769:MET:HE2	5:A:769:MET:N	2.37	0.40
5:A:1039:TRP:CD2	5:A:1271:PRO:HG3	2.55	0.40
7:J:764:LEU:HD23	7:J:764:LEU:HA	1.96	0.40
9:F:108:ASN:OD1	9:F:112:MET:HE3	2.21	0.40
10:G:355:LYS:O	10:G:359:ASN:ND2	2.53	0.40
5:A:1913:THR:O	5:A:1917:VAL:HG23	2.21	0.40
5:A:2084:LEU:HB3	5:A:2086:GLN:HB3	2.02	0.40
5:A:1344:THR:HG21	5:A:1537:TRP:CD2	2.57	0.40
7:J:327:VAL:O	7:J:331:LEU:HG	2.21	0.40
9:F:119:LEU:CD1	9:F:197:ILE:HG22	2.50	0.40
10:G:339:CYS:SG	10:G:340:LYS:N	2.94	0.40
5:A:1216:ILE:HG13	5:A:1254:ASN:HB3	2.03	0.40
5:A:1458:TRP:CZ3	5:A:1494:LEU:HD11	2.56	0.40
6:H:183:LEU:HD21	6:H:453:VAL:HG21	2.03	0.40
6:H:410:LEU:HD23	6:H:410:LEU:HA	1.95	0.40
7:J:223:LEU:HD23	9:F:420:ALA:HB1	2.03	0.40
7:J:565:VAL:HG11	7:J:599:PHE:CG	2.56	0.40
7:J:617:PHE:CE2	7:J:644:ARG:HD3	2.56	0.40
5:A:816:ILE:HD12	5:A:817:LYS:N	2.36	0.40
6:H:399:VAL:CG1	6:H:410:LEU:HD22	2.51	0.40
6:H:453:VAL:HG22	6:H:463:LEU:HD22	2.04	0.40
7:J:207:LEU:C	7:J:207:LEU:HD23	2.46	0.40
7:J:344:ALA:HB3	7:J:357:MET:CE	2.52	0.40
9:F:200:ALA:HA	9:F:203:ILE:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:233:VAL:HG11	9:F:237:ILE:CG2	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	
5	A	1343/2413 (56%)	1226 (91%)	104 (8%)	13 (1%)	12	45
6	H	355/465 (76%)	301 (85%)	48 (14%)	6 (2%)	7	35
7	J	719/899 (80%)	650 (90%)	56 (8%)	13 (2%)	6	34
8	D	138/143 (96%)	126 (91%)	11 (8%)	1 (1%)	18	51
9	F	413/494 (84%)	364 (88%)	38 (9%)	11 (3%)	4	27
10	G	316/469 (67%)	283 (90%)	32 (10%)	1 (0%)	36	65
11	K	122/126 (97%)	111 (91%)	9 (7%)	2 (2%)	7	36
12	B	69/2163 (3%)	57 (83%)	8 (12%)	4 (6%)	1	13
All	All	3475/7172 (48%)	3118 (90%)	306 (9%)	51 (2%)	11	37

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	1093	LYS
5	A	1278	VAL
5	A	2088	ILE
6	H	362	TYR
7	J	479	GLU
7	J	592	HIS
7	J	683	ASN
9	F	74	LEU
9	F	363	PRO

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Mol	Chain	Res	Type
9	F	407	GLU
11	K	106	ASP
12	B	388	GLN
12	B	393	GLU
5	A	979	SER
6	H	361	GLY
7	J	200	ALA
8	D	127	ASN
9	F	59	LEU
9	F	79	ASP
9	F	148	ASN
9	F	165	ALA
9	F	435	ALA
12	B	424	PRO
5	A	980	PRO
5	A	1322	ALA
5	A	1623	PHE
5	A	1768	PRO
6	H	216	SER
6	H	435	GLY
7	J	867	GLU
9	F	58	ALA
9	F	146	ASN
9	F	365	LYS
5	A	1324	GLY
5	A	1535	LYS
5	A	2068	ASN
6	H	429	LYS
7	J	237	ASP
7	J	819	ALA
10	G	266	PRO
12	B	392	ARG
5	A	1386	ALA
6	H	230	SER
7	J	206	ASP
7	J	287	SER
7	J	399	PRO
5	A	1638	ILE
7	J	558	PRO
11	K	82	PRO
7	J	241	PRO
7	J	887	THR

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	
5	A	1216/2182 (56%)	1194 (98%)	22 (2%)	51	68
6	H	305/410 (74%)	288 (94%)	17 (6%)	19	47
7	J	627/813 (77%)	600 (96%)	27 (4%)	26	52
8	D	129/132 (98%)	119 (92%)	10 (8%)	11	38
9	F	346/445 (78%)	316 (91%)	30 (9%)	9	34
10	G	289/436 (66%)	281 (97%)	8 (3%)	38	60
11	K	102/104 (98%)	89 (87%)	13 (13%)	4	22
12	B	56/1955 (3%)	53 (95%)	3 (5%)	20	47
All	All	3070/6477 (47%)	2940 (96%)	130 (4%)	28	53

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	753	TYR
5	A	755	ASP
5	A	757	GLU
5	A	758	LEU
5	A	824	VAL
5	A	831	ARG
5	A	852	LEU
5	A	950	THR
5	A	965	LYS
5	A	971	MET
5	A	972	MET
5	A	1004	ASP
5	A	1103	LEU
5	A	1268	ARG
5	A	1276	GLU
5	A	1277	GLU
5	A	1512	ARG
5	A	1749	SER
5	A	1827	GLN

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Mol	Chain	Res	Type
5	A	1991	ILE
5	A	2048	TRP
5	A	2088	ILE
6	H	111	THR
6	H	136	LEU
6	H	146	PHE
6	H	199	LEU
6	H	220	LYS
6	H	225	ASP
6	H	232	ASN
6	H	243	ILE
6	H	271	VAL
6	H	286	ASP
6	H	300	LEU
6	H	301	LEU
6	H	302	LEU
6	H	322	VAL
6	H	331	SER
6	H	389	ILE
6	H	454	SER
7	J	194	PRO
7	J	237	ASP
7	J	239	THR
7	J	255	ARG
7	J	270	GLU
7	J	291	TYR
7	J	421	LEU
7	J	459	LEU
7	J	460	THR
7	J	498	GLN
7	J	508	TRP
7	J	554	ARG
7	J	588	ASP
7	J	613	LEU
7	J	630	SER
7	J	657	ASN
7	J	661	LEU
7	J	708	LEU
7	J	743	LYS
7	J	758	LEU
7	J	767	PHE
7	J	772	LEU

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Mol	Chain	Res	Type
7	J	782	LYS
7	J	809	LEU
7	J	832	LEU
7	J	841	THR
7	J	874	TRP
8	D	39	CYS
8	D	43	ASP
8	D	48	SER
8	D	49	ILE
8	D	76	LEU
8	D	80	MET
8	D	93	CYS
8	D	107	VAL
8	D	118	GLU
8	D	139	HIS
9	F	57	LEU
9	F	59	LEU
9	F	63	ASP
9	F	66	SER
9	F	67	LEU
9	F	74	LEU
9	F	77	ILE
9	F	81	LYS
9	F	82	ARG
9	F	84	LEU
9	F	85	GLN
9	F	117	ILE
9	F	120	TYR
9	F	153	GLU
9	F	154	SER
9	F	156	GLU
9	F	221	LYS
9	F	232	LEU
9	F	304	ARG
9	F	327	THR
9	F	364	LYS
9	F	376	LYS
9	F	378	LYS
9	F	384	VAL
9	F	391	MET
9	F	395	LYS
9	F	398	GLN

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Mol	Chain	Res	Type
9	F	401	LEU
9	F	410	LEU
9	F	419	GLN
10	G	189	THR
10	G	278	MET
10	G	285	GLN
10	G	329	MET
10	G	341	VAL
10	G	393	GLU
10	G	395	LEU
10	G	443	LYS
11	K	11	LEU
11	K	17	THR
11	K	21	LEU
11	K	33	LEU
11	K	34	LYS
11	K	53	ILE
11	K	64	LEU
11	K	69	LEU
11	K	79	VAL
11	K	93	VAL
11	K	113	GLN
11	K	119	ASP
11	K	120	LYS
12	B	387	GLU
12	B	390	LYS
12	B	396	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	760	ASN
5	A	907	ASN
5	A	1005	GLN
5	A	1030	GLN
5	A	1087	ASN
5	A	1190	ASN
5	A	1273	GLN
5	A	1281	ASN
5	A	1368	GLN
5	A	1516	GLN
5	A	1667	GLN

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Mol	Chain	Res	Type
5	A	1695	ASN
5	A	1737	GLN
5	A	1824	GLN
5	A	1831	GLN
5	A	1869	ASN
5	A	1907	GLN
5	A	2018	ASN
5	A	2047	GLN
6	H	200	GLN
6	H	385	GLN
6	H	388	GLN
6	H	465	ASN
7	J	281	ASN
7	J	397	GLN
7	J	498	GLN
7	J	537	GLN
7	J	578	GLN
7	J	673	GLN
7	J	733	ASN
7	J	755	GLN
7	J	762	GLN
7	J	795	GLN
7	J	802	GLN
8	D	87	HIS
9	F	171	GLN
9	F	196	GLN
9	F	240	GLN
9	F	292	GLN
9	F	299	HIS
9	F	320	GLN
9	F	322	ASN
9	F	331	HIS
9	F	434	GLN
10	G	276	ASN
11	K	38	ASN
11	K	45	ASN
11	K	113	GLN
12	B	420	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	V	66/67 (98%)	30 (45%)	6 (9%)
2	W	54/112 (48%)	20 (37%)	9 (16%)
3	U	19/214 (8%)	8 (42%)	1 (5%)
All	All	139/393 (35%)	58 (41%)	16 (11%)

All (58) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	V	2	U
1	V	11	A
1	V	18	A
1	V	19	U
1	V	20	A
1	V	22	G
1	V	25	U
1	V	26	A
1	V	29	A
1	V	31	U
1	V	32	G
1	V	33	A
1	V	34	G
1	V	35	G
1	V	36	A
1	V	37	U
1	V	39	C
1	V	40	G
1	V	41	U
1	V	44	G
1	V	45	A
1	V	46	G
1	V	55	U
1	V	56	U
1	V	57	U
1	V	59	C
1	V	64	U
1	V	65	G
1	V	66	A
1	V	67	A
2	W	28	U
2	W	29	U
2	W	31	G
2	W	32	U
2	W	33	C

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Mol	Chain	Res	Type
2	W	38	U
2	W	45	A
2	W	46	U
2	W	47	A
2	W	49	A
2	W	50	G
2	W	56	A
2	W	61	C
2	W	75	A
2	W	76	A
2	W	83	A
2	W	84	C
2	W	85	C
2	W	86	G
2	W	87	U
3	U	93	G
3	U	94	C
3	U	95	C
3	U	96	U
3	U	97	U
3	U	99	U
3	U	101	C
3	U	103	A

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	V	17	A
1	V	19	U
1	V	31	U
1	V	39	C
1	V	44	G
1	V	45	A
2	W	31	G
2	W	32	U
2	W	45	A
2	W	48	C
2	W	49	A
2	W	55	G
2	W	75	A
2	W	83	A
2	W	84	C

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Mol	Chain	Res	Type
3	U	95	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	x	1
5	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x	62:UNK	C	101:UNK	N	54.04
1	A	1860:VAL	C	1861:THR	N	4.50

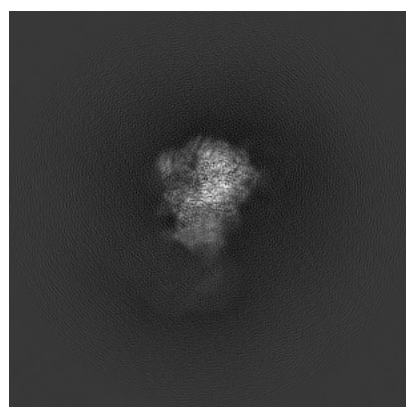
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8014. These allow visual inspection of the internal detail of the map and identification of artifacts.

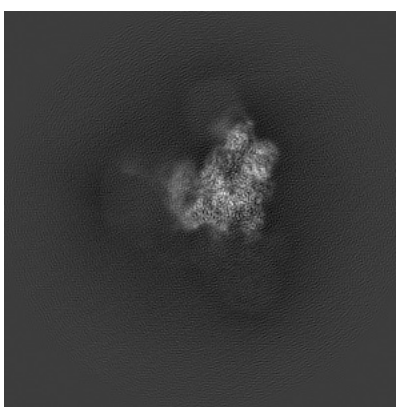
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

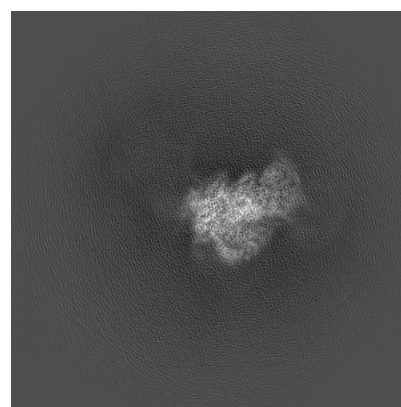
6.1.1 Primary map



X



Y

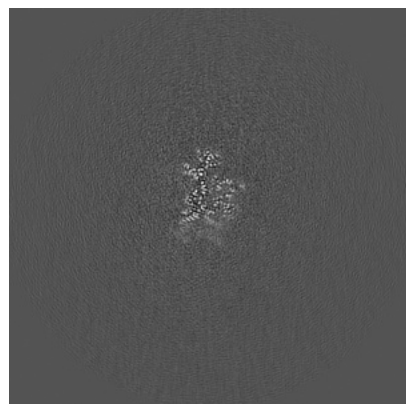


Z

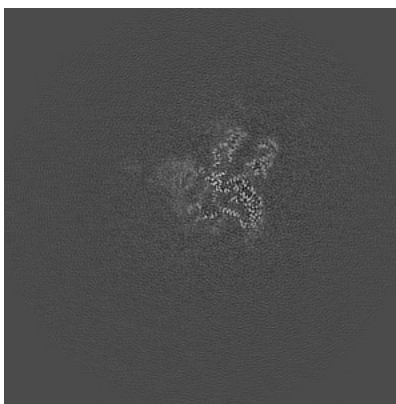
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

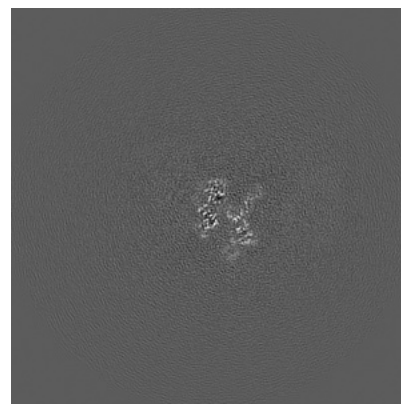
6.2.1 Primary map



X Index: 190



Y Index: 190

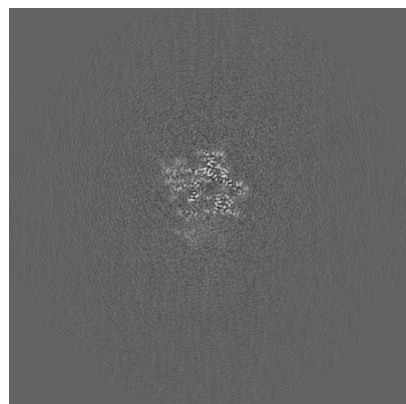


Z Index: 190

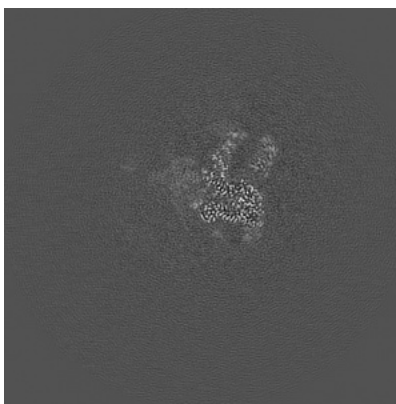
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

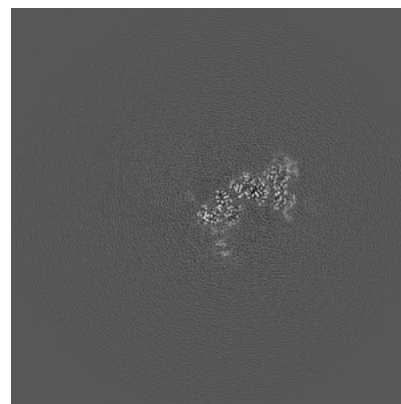
6.3.1 Primary map



X Index: 197



Y Index: 186

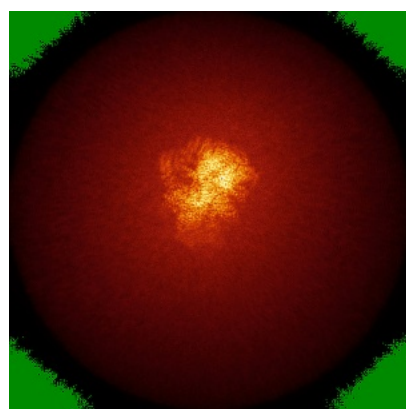


Z Index: 221

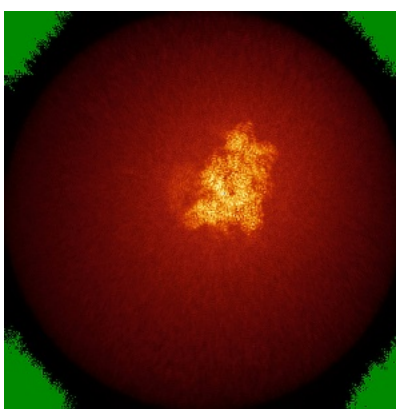
The images above show the largest variance slices of the map in three orthogonal directions.

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

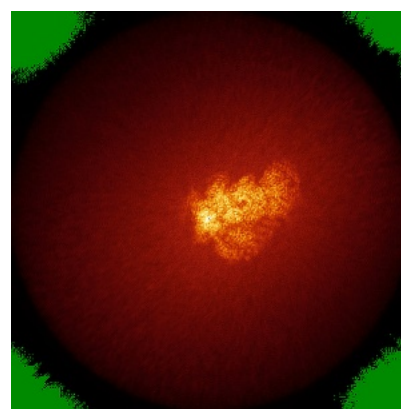
6.4.1 Primary map



X



Y

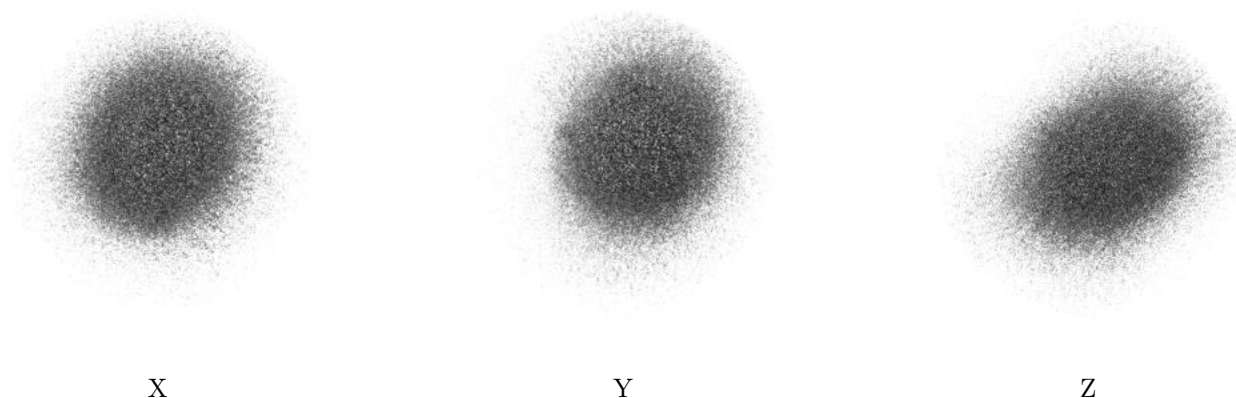


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

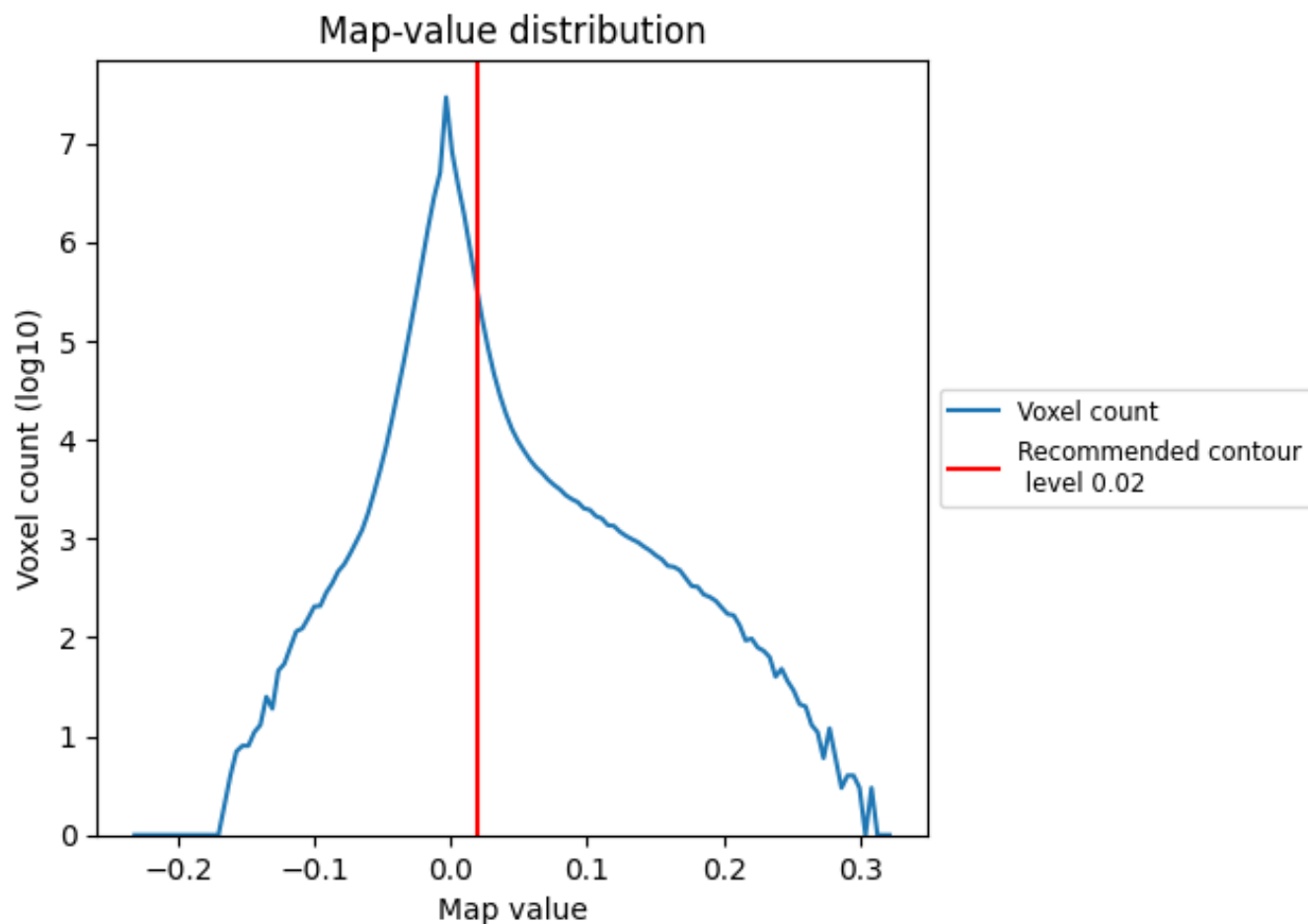
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

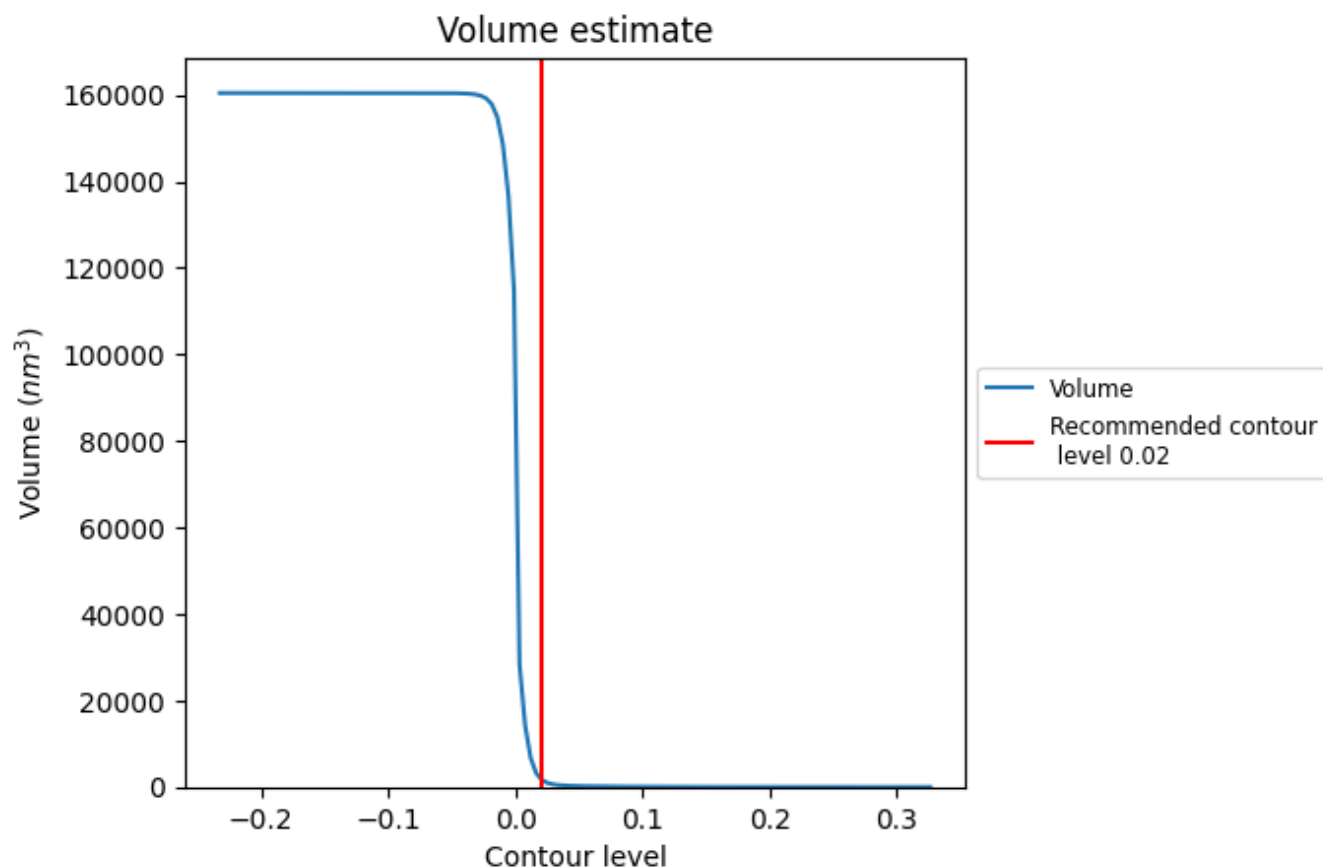
This section contains the results of statistical analysis of the map.

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.

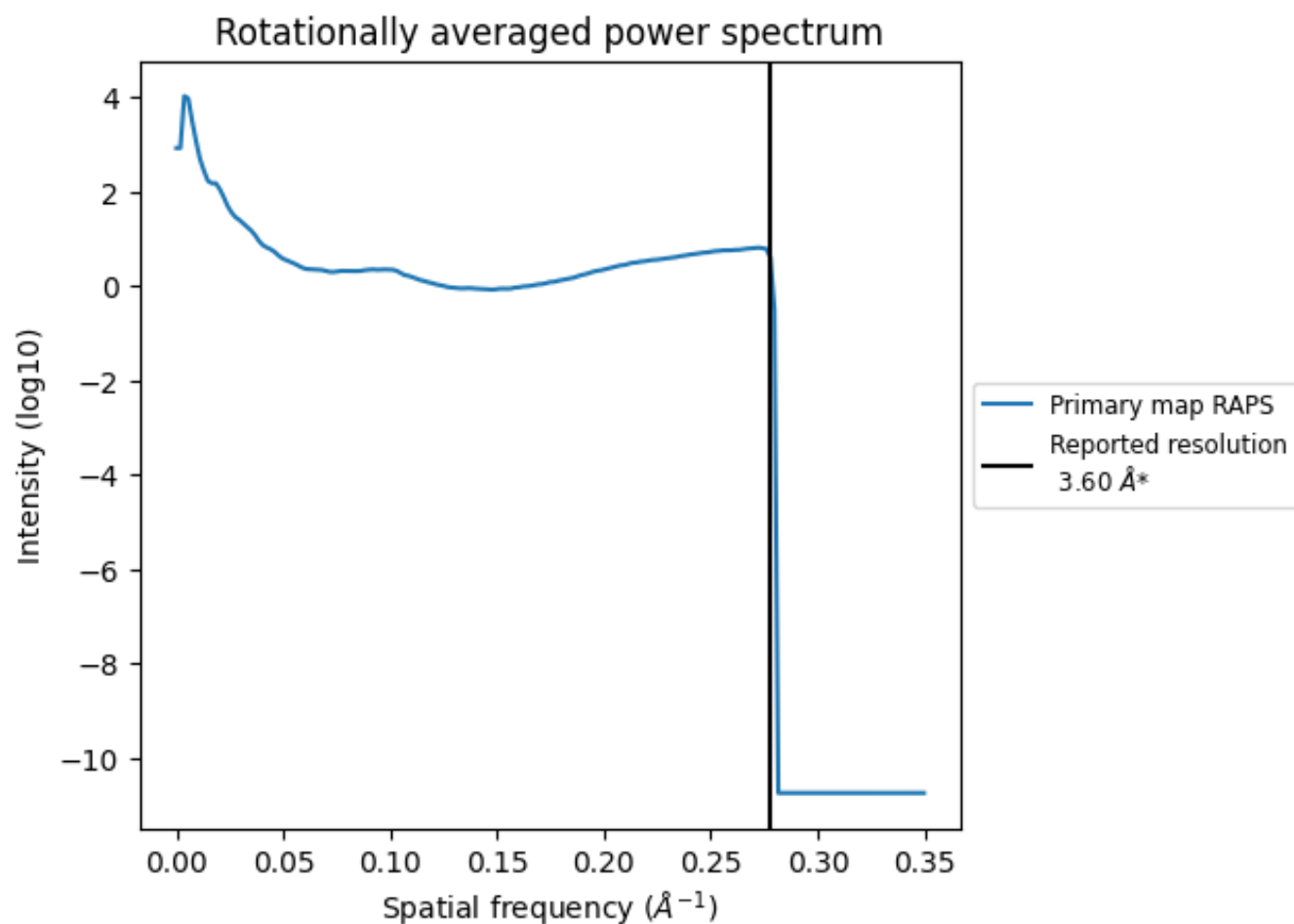
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1921 nm³; this corresponds to an approximate mass of 1735 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 ⓘ

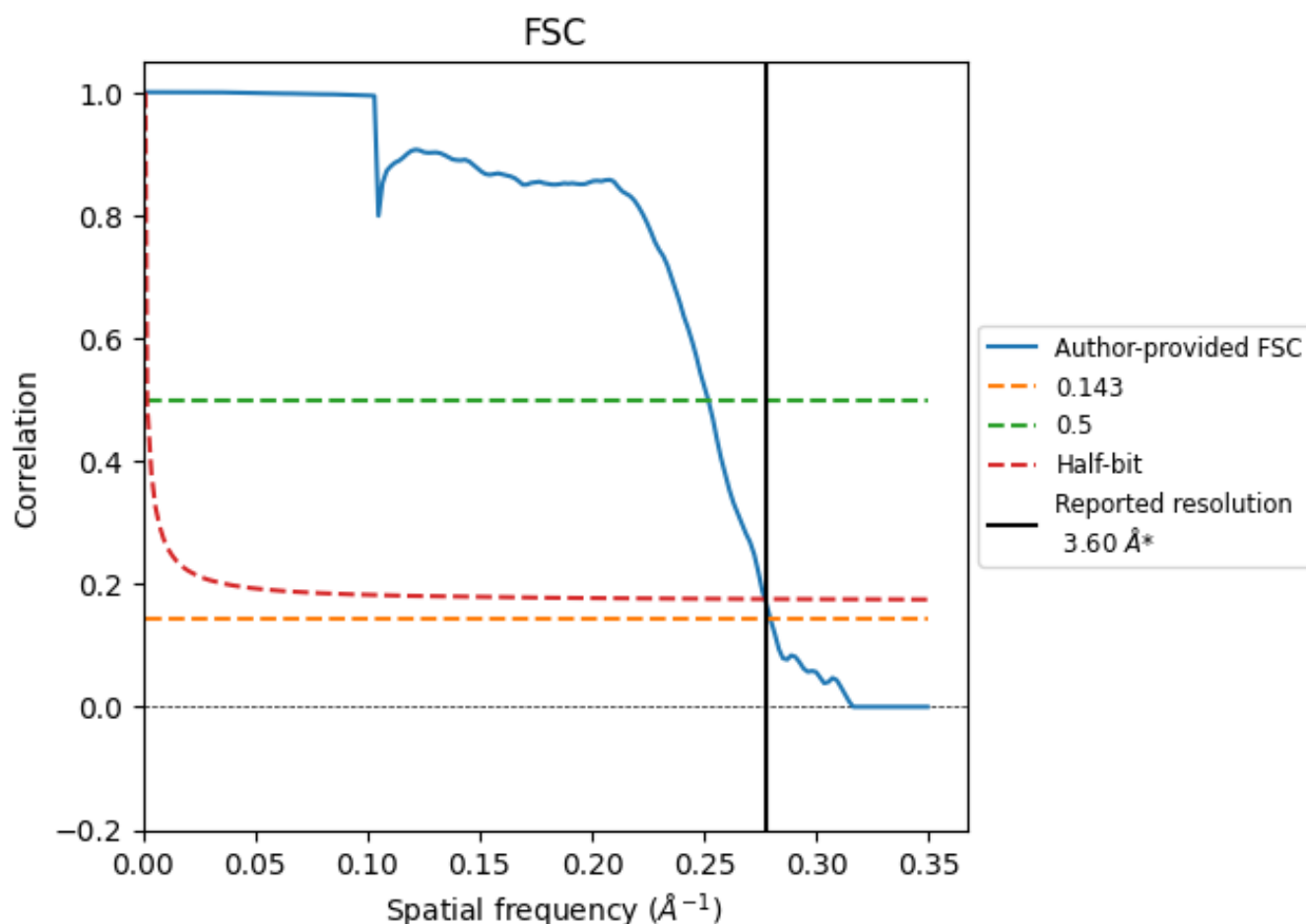


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

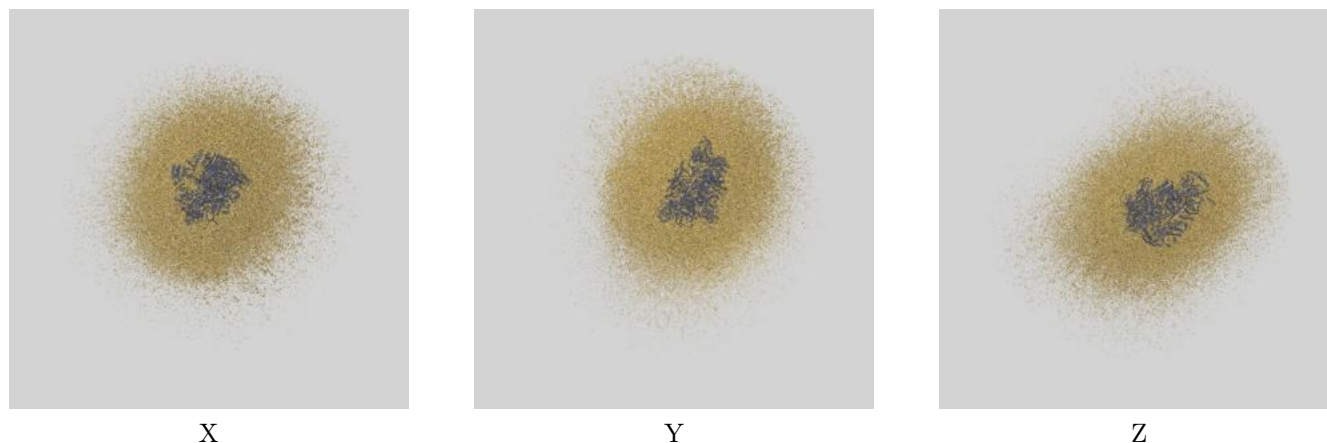
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	3.97	3.61
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

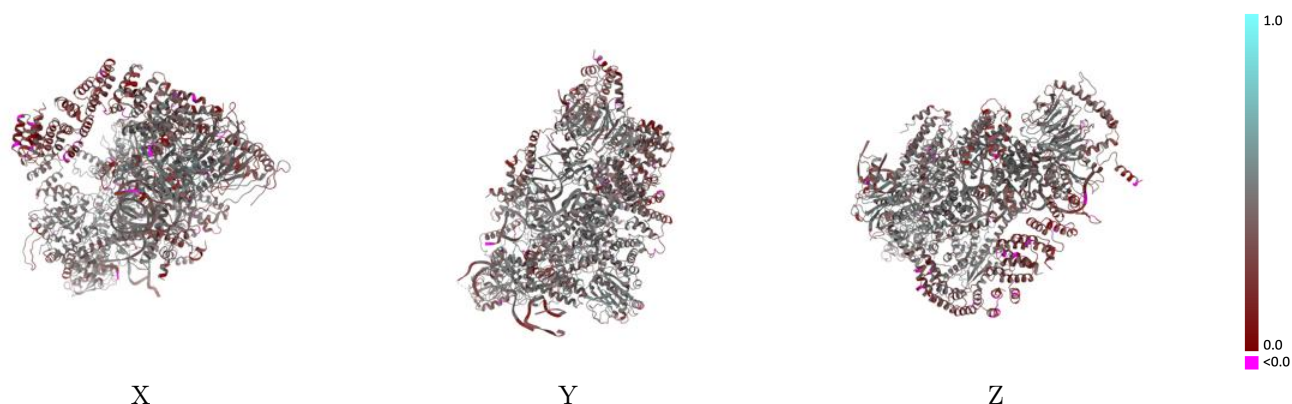
This section contains information regarding the fit between EMDB map EMD-8014 and PDB model 5GAP. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



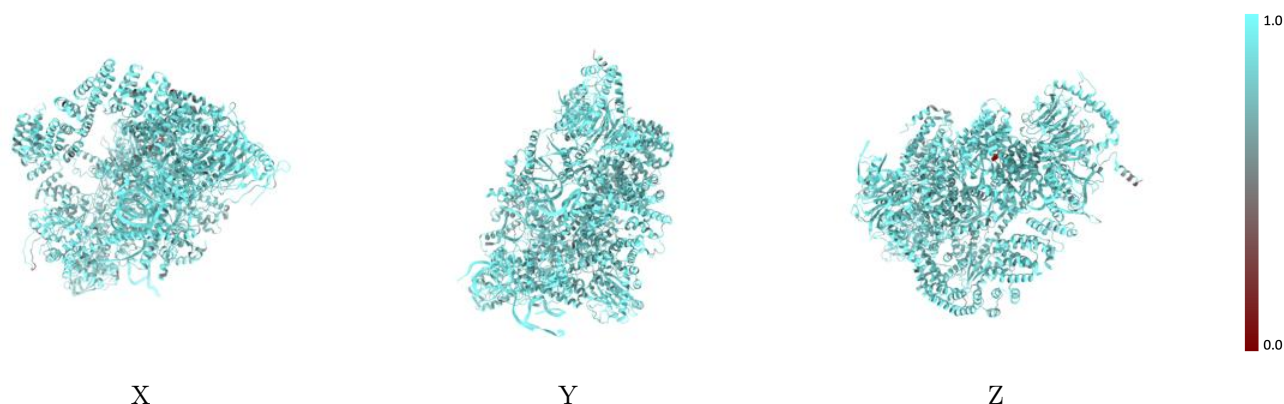
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



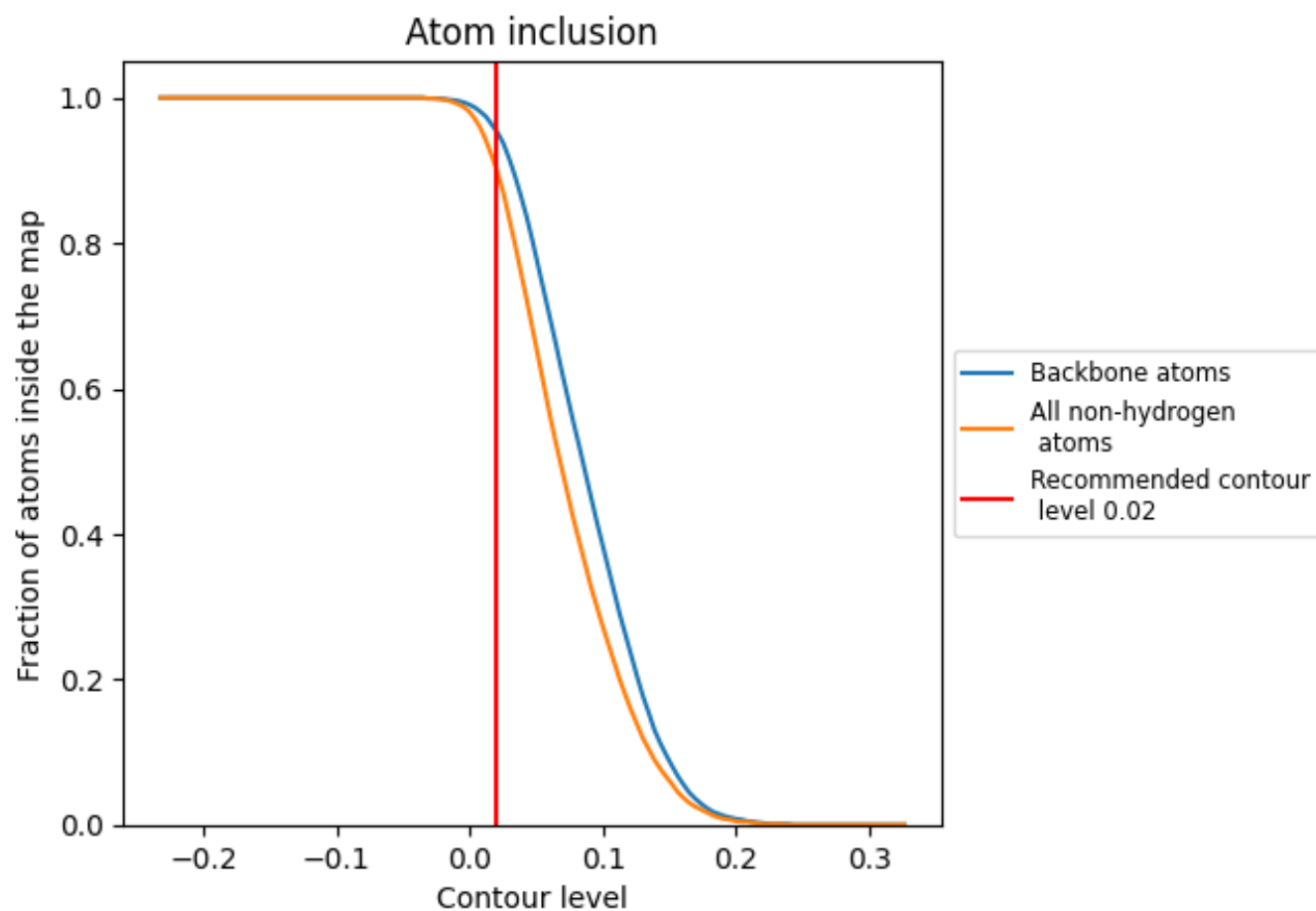
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 90% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9020	0.3970
A	0.9040	0.4340
B	0.8190	0.3180
D	0.8950	0.4260
F	0.8990	0.4110
G	0.8870	0.3770
H	0.8950	0.4080
J	0.8810	0.3130
K	0.9130	0.4670
U	0.9250	0.2810
V	0.9670	0.4390
W	0.9640	0.3760
x	0.9390	0.4020

1.0

0.0

<0.0