



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:35 AM UTC

PDB ID : 6KW3 / pdb_00006kw3
EMDB ID : EMD-0777
Title : The ClassA RSC-Nucleosome Complex
Authors : Ye, Y.P.; Wu, H.; Chen, K.J.; Verma, N.; Cairns, B.; Gao, N.; Chen, Z.C.
Deposited on : 2019-09-05
Resolution : 7.13 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:

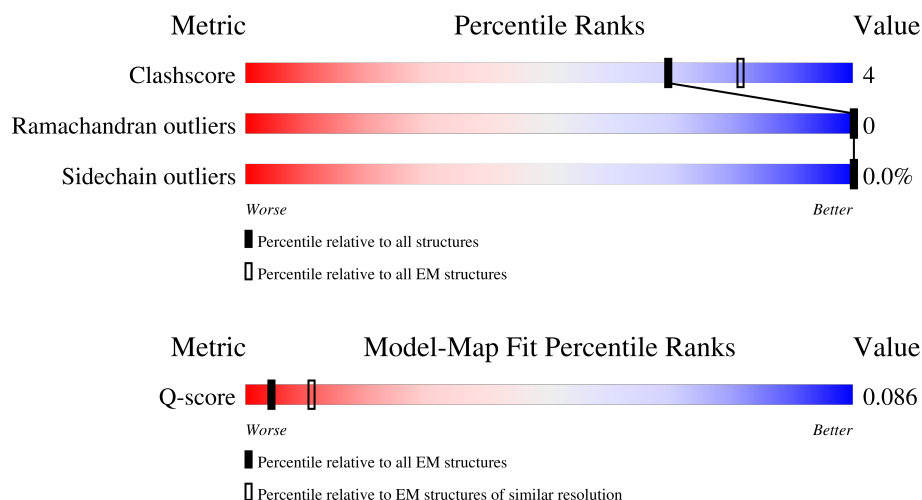
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 7.13 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	-
Q-score	-	25397	419 (6.63 - 7.61)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	103	
1	R	103	
2	N	136	
2	Q	136	

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Mol	Chain	Length	Quality of chain
3	O	130	
3	S	130	
4	U	167	
5	V	167	
6	J	1359	
6	W	1359	
6	Y	1359	
7	f	477	
8	h	157	
9	F	435	
10	D	557	
10	H	557	
11	M	581	
12	I	483	
13	G	426	
14	A	502	
15	E	78	
16	C	883	
17	K	885	
18	X	625	
19	L	889	
20	P	126	
20	T	126	
21	g	467	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 45514 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	82	Total	C	N	O	S	0	0
			657	416	128	112	1		
1	R	87	Total	C	N	O	S	0	0
			703	443	142	117	1		

- Molecule 2 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	98	Total	C	N	O	S	0	0
			810	511	157	139	3		
2	Q	95	Total	C	N	O	S	0	0
			784	494	151	136	3		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	O	107	Total	C	N	O	0	0
			823	519	161	143		
3	S	107	Total	C	N	O	0	0
			823	519	161	143		

- Molecule 4 is a DNA chain called DNA 167.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	146	Total	C	N	O	P	0	0
			2977	1414	542	875	146		

- Molecule 5 is a DNA chain called DNA 167.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V	146	Total	C	N	O	P	0	0
			3009	1425	561	877	146		

- Molecule 6 is a protein called Nuclear protein STH1/NPS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	W	69	Total	C	N	O	S	0	0
			592	364	121	105	2		
6	J	235	Total	C	N	O	S	0	0
			1814	1136	327	349	2		
6	Y	548	Total	C	N	O	S	0	0
			4503	2873	780	832	18		

- Molecule 7 is a protein called Actin-related protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	f	398	Total	C	N	O	S	3	0
			3219	2075	527	602	15		

- Molecule 8 is a protein called Regulator of Ty1 transposition protein 102.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	54	Total	C	N	O	S	0	0
			490	313	84	92	1		

- Molecule 9 is a protein called Chromatin structure-remodeling complex subunit RSC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	118	Total	C	N	O	S	0	0
			964	601	164	197	2		

- Molecule 10 is a protein called Chromatin structure-remodeling complex protein RSC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	393	Total	C	N	O	S	0	0
			3215	2036	552	613	14		
10	D	305	Total	C	N	O	S	0	0
			2510	1613	416	471	10		

- Molecule 11 is a protein called Chromatin structure-remodeling complex subunit RSC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	384	Total	C	N	O	S	0	0
			3058	1970	497	574	17		

- Molecule 12 is a protein called Chromatin structure-remodeling complex protein RSC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	244	Total	C	N	O	S	0	0
			1944	1234	328	377	5		

- Molecule 13 is a protein called Chromatin structure-remodeling complex subunit SFH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	246	Total	C	N	O	S	0	0
			1996	1271	337	380	8		

- Molecule 14 is a protein called Chromatin structure-remodeling complex protein RSC58.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A	365	Total	C	N	O	S	0	0
			3007	1942	509	547	9		

- Molecule 15 is a protein called High temperature lethal protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	58	Total	C	N	O	S	0	0
			477	295	86	92	4		

- Molecule 16 is a protein called Chromatin structure-remodeling complex protein RSC30.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	C	33	Total	C	N	O	S	0	0
			269	177	39	52	1		

- Molecule 17 is a protein called Chromatin structure-remodeling complex protein RSC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	42	Total	C	N	O	S	0	0
			347	225	57	63	2		

- Molecule 18 is a protein called Chromatin structure-remodeling complex subunit RSC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	147	Total	C	N	O	S	0	0
			1220	776	202	234	8		

- Molecule 19 is a protein called Chromatin structure-remodeling complex subunit RSC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	85	Total	C	N	O	S	0	0
			669	428	120	119	2		

- Molecule 20 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	93	Total	C	N	O	S	0	0
			725	456	130	137	2		
20	P	93	Total	C	N	O	S	0	0
			717	450	128	137	2		

- Molecule 21 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	g	395	Total	C	N	O	S	1	0
			3191	2048	522	614	7		

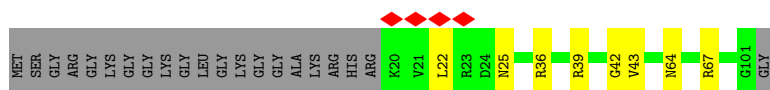
- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
22	H	1	Total	Zn	0
			1	1	

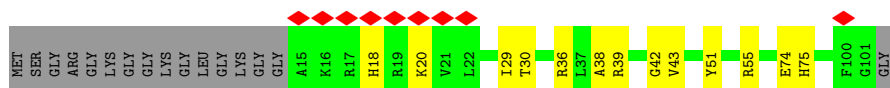
3 Residue-property plots [i](#)

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.

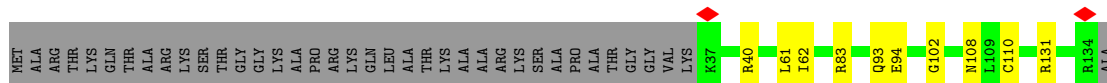
- Molecule 1: Histone H4



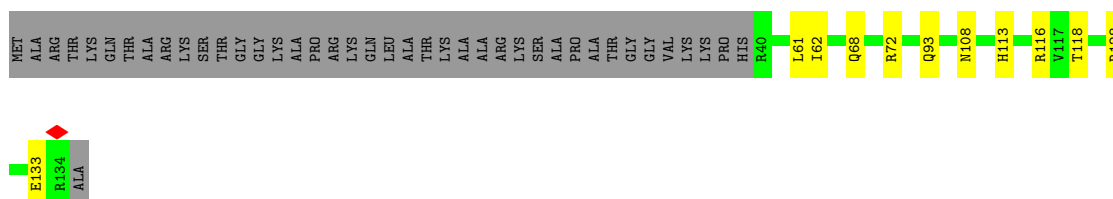
- Molecule 1: Histone H4



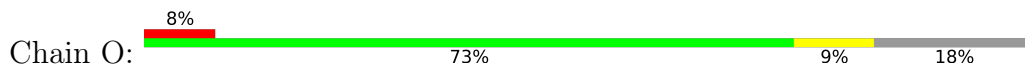
- Molecule 2: Histone H3.2



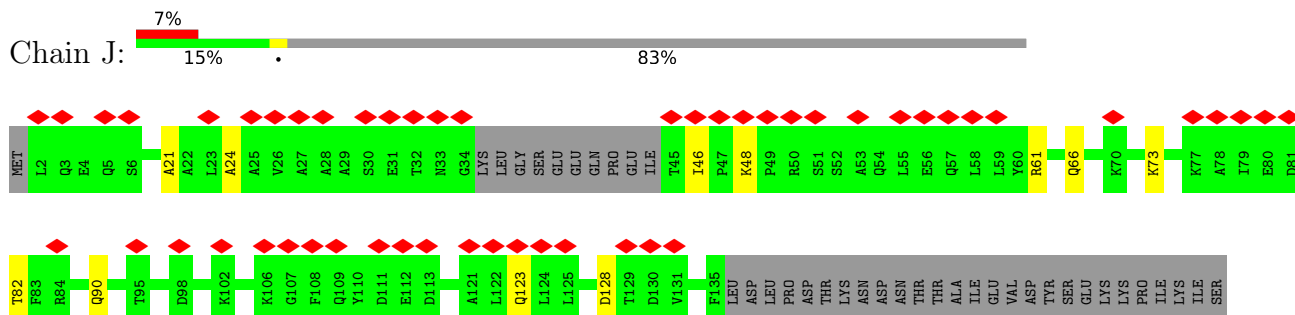
- Molecule 2: Histone H3.2



- Molecule 3: Histone H2A



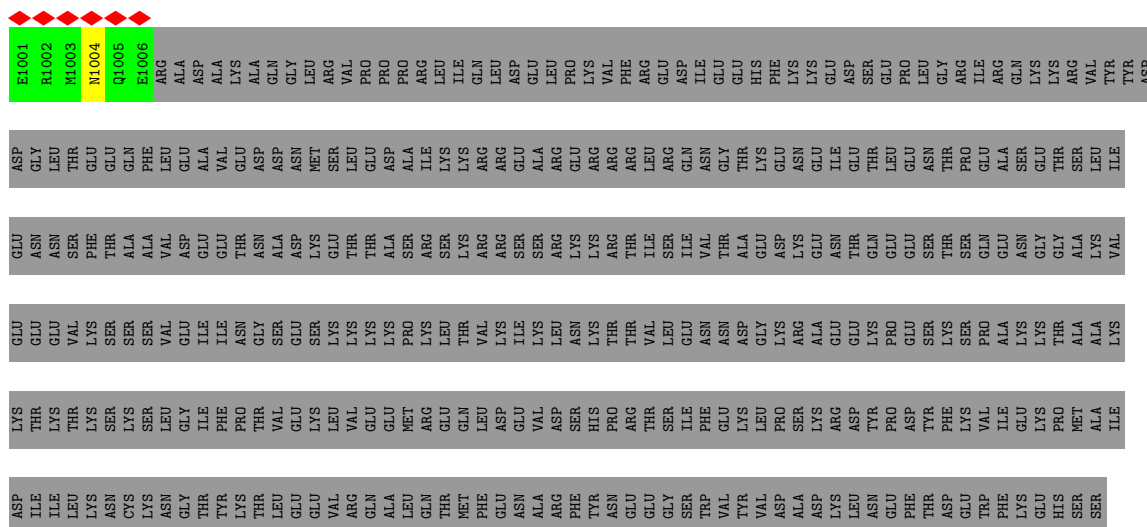
- Molecule 6: Nuclear protein STH1/NPS1



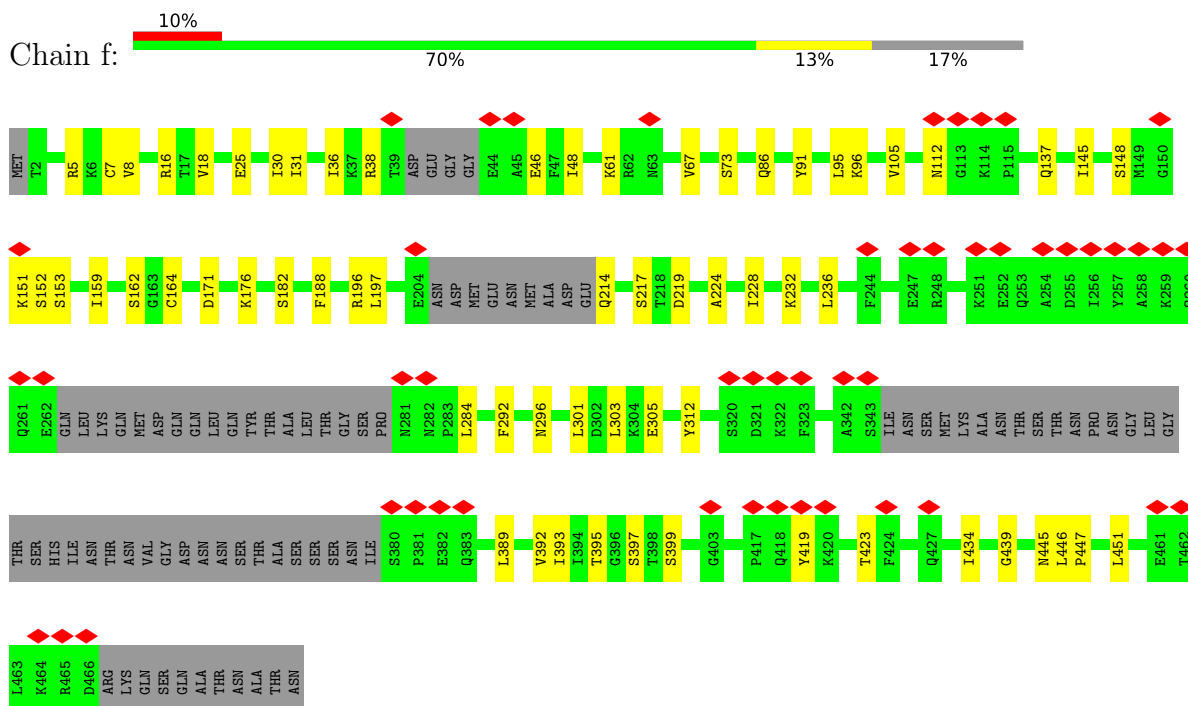


Chain Y:

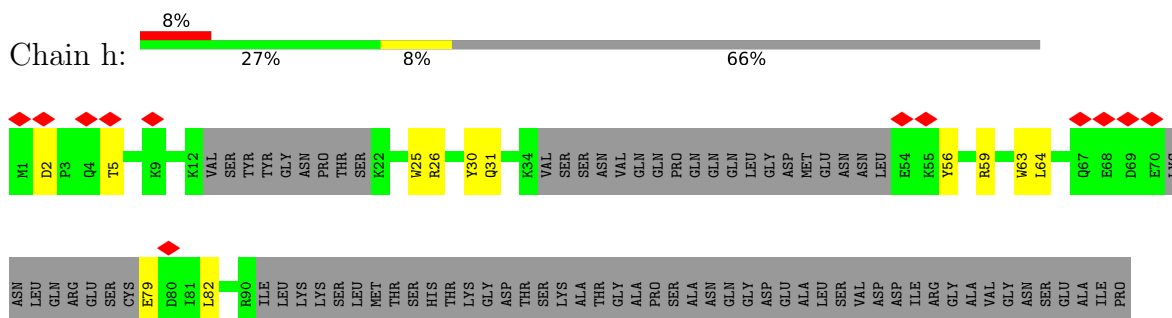


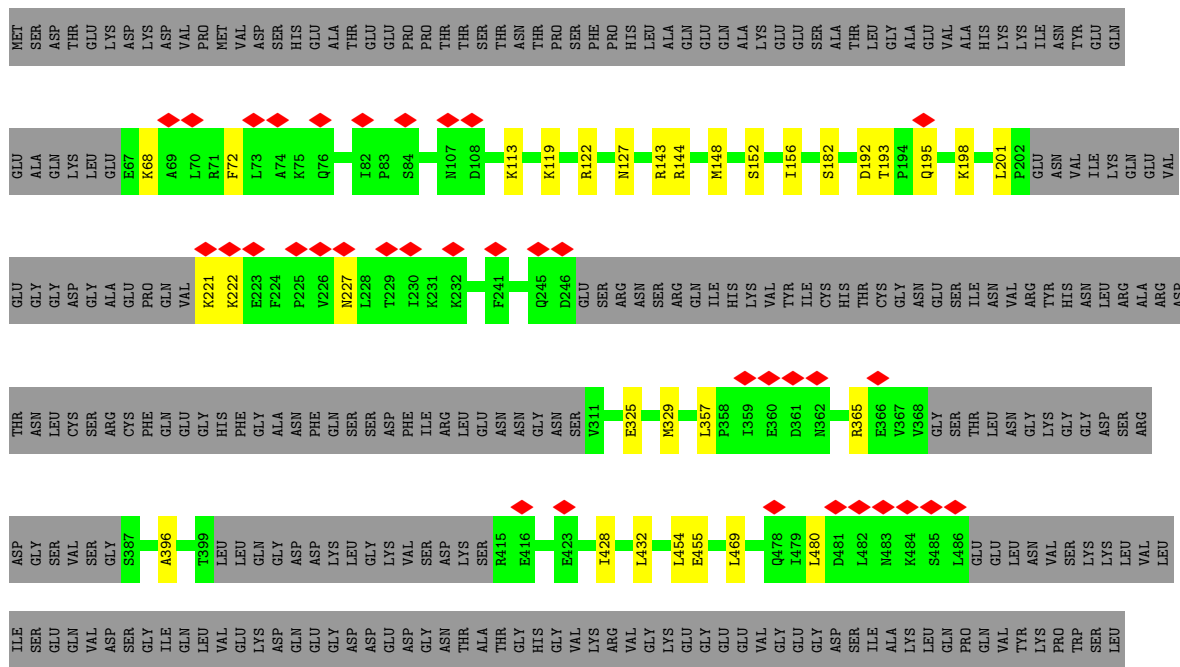


- Molecule 7: Actin-related protein 7

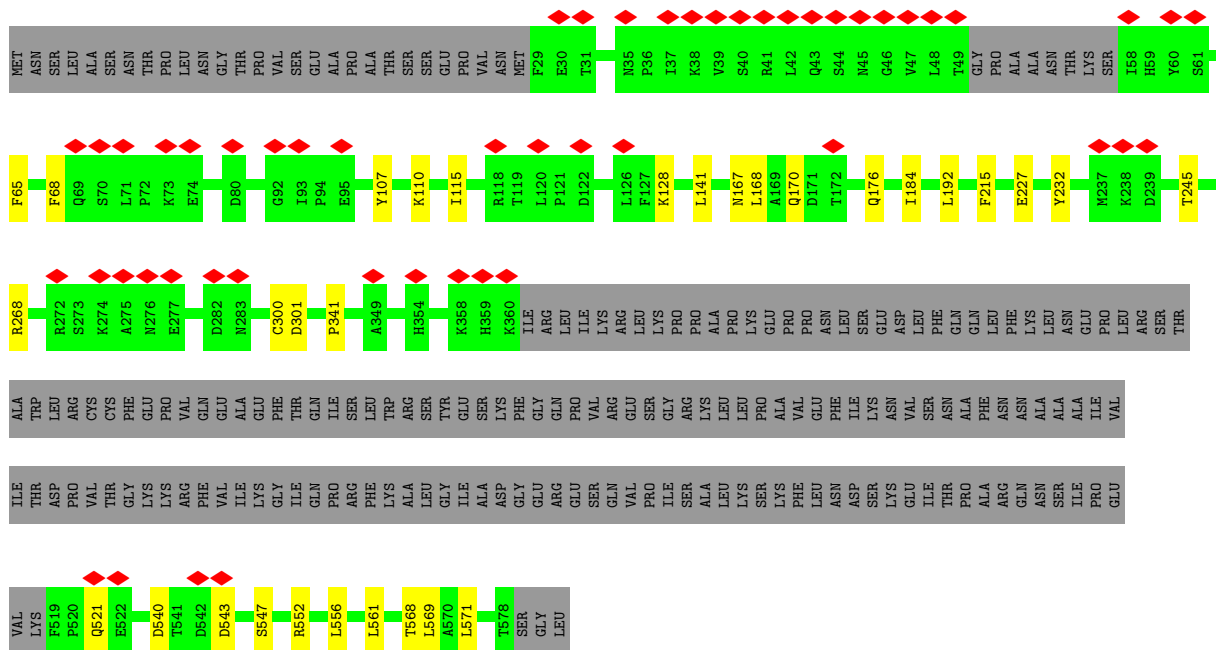


- Molecule 8: Regulator of Ty1 transposition protein 102

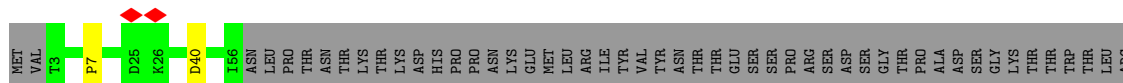


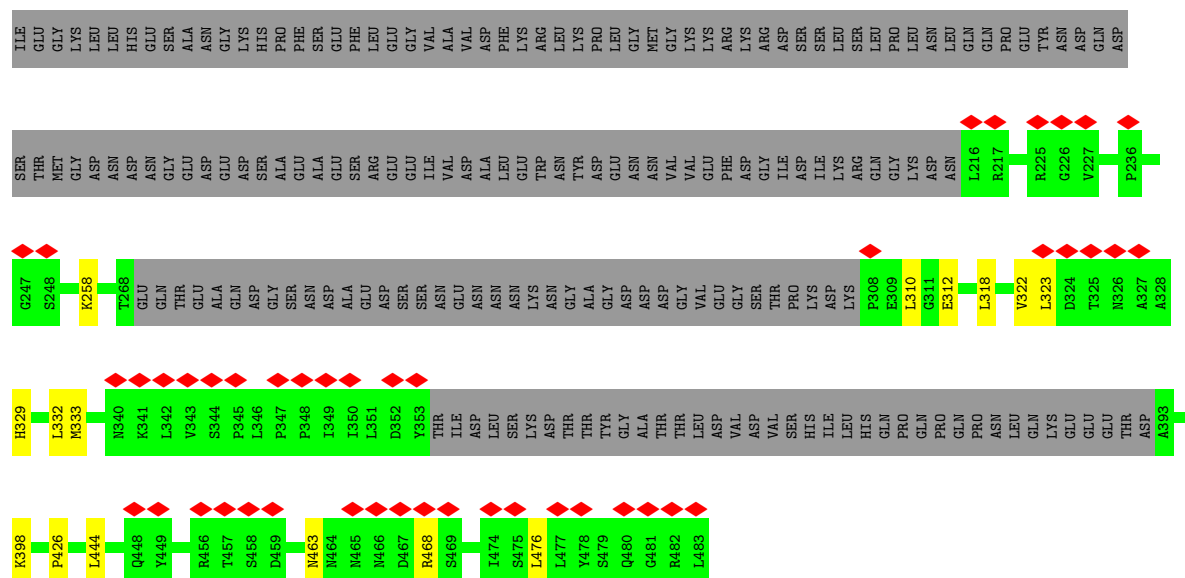


- Molecule 11: Chromatin structure-remodeling complex subunit RSC9

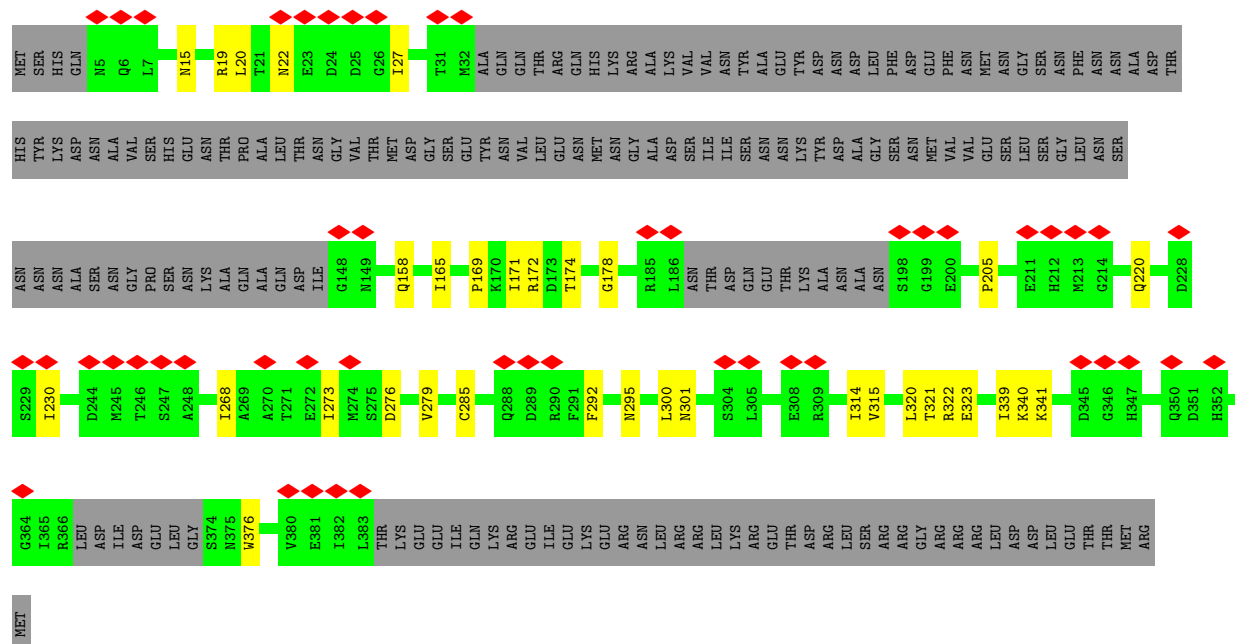


- Molecule 12: Chromatin structure-remodeling complex protein RSC6

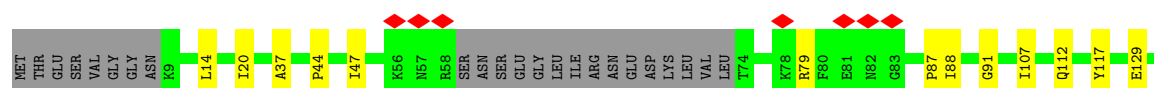




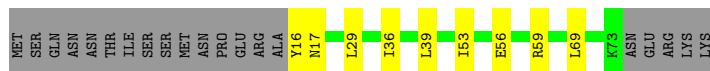
- Molecule 13: Chromatin structure-remodeling complex subunit SFH1



- Molecule 14: Chromatin structure-remodeling complex protein RSC58



- Molecule 15: High temperature lethal protein 1

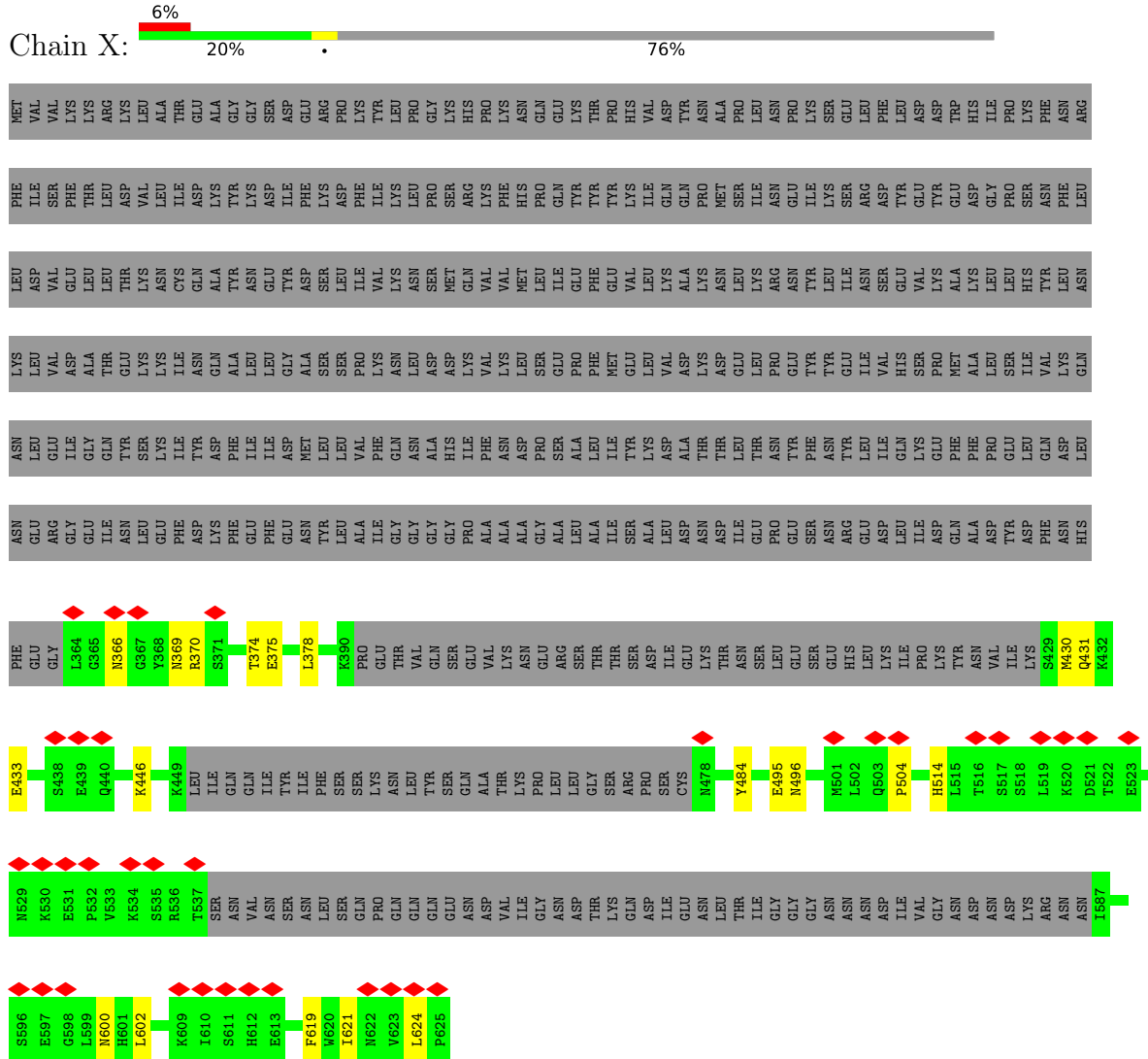


- Molecule 16: Chromatin structure-remodeling complex protein RSC30

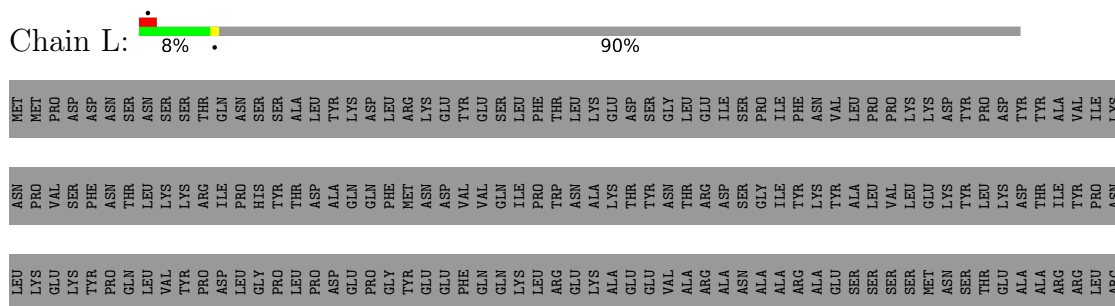


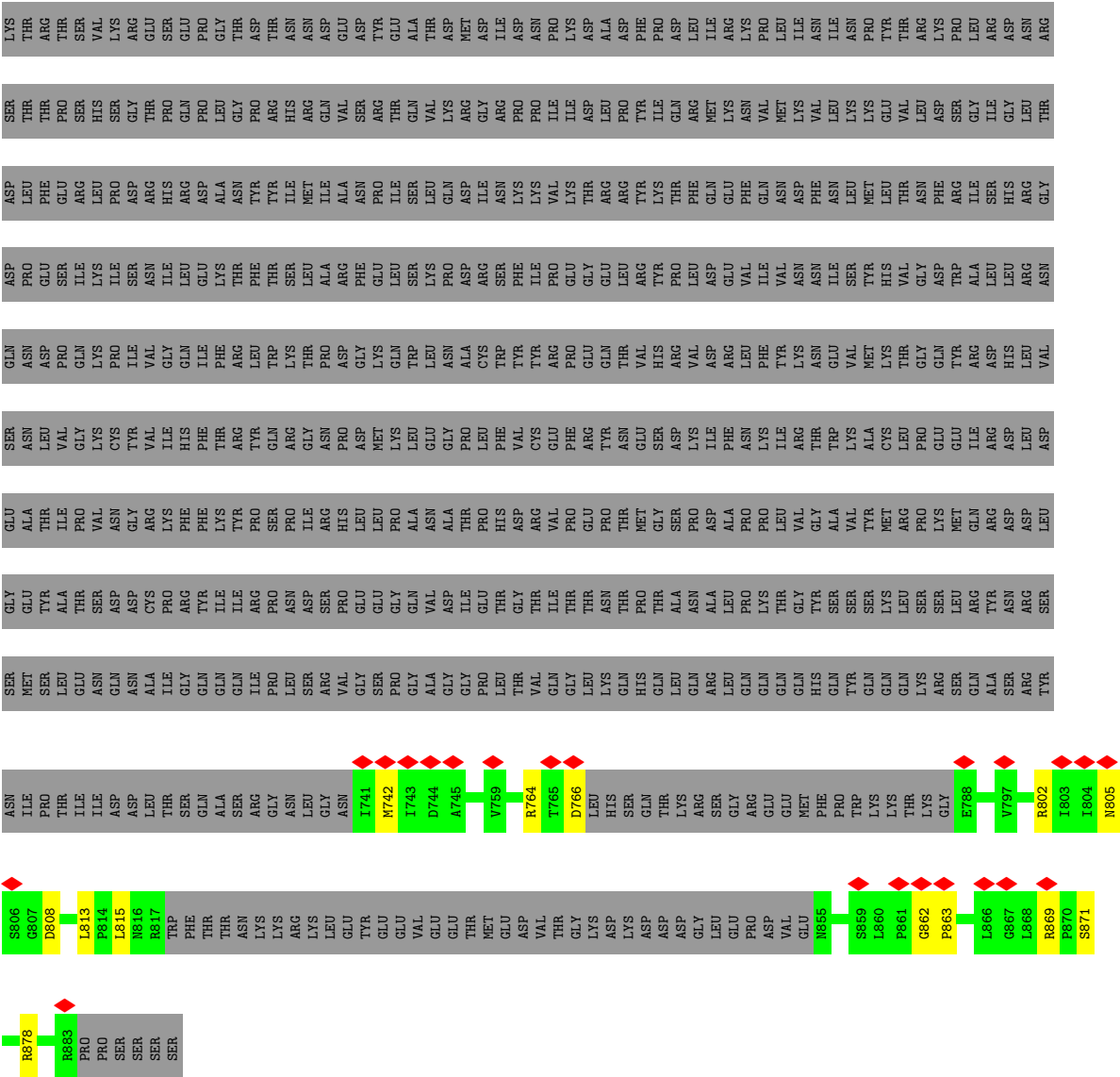


● Molecule 18: Chromatin structure-remodeling complex subunit RSC4

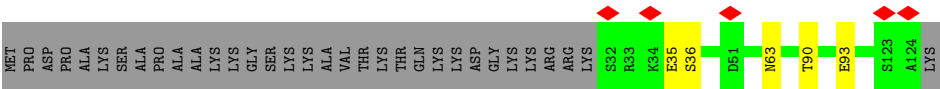


- Molecule 19: Chromatin structure-remodeling complex subunit RSC2





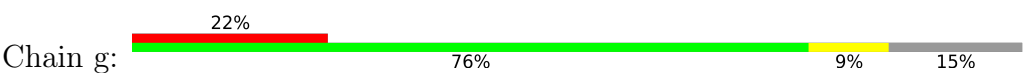
• Molecule 20: Histone H4

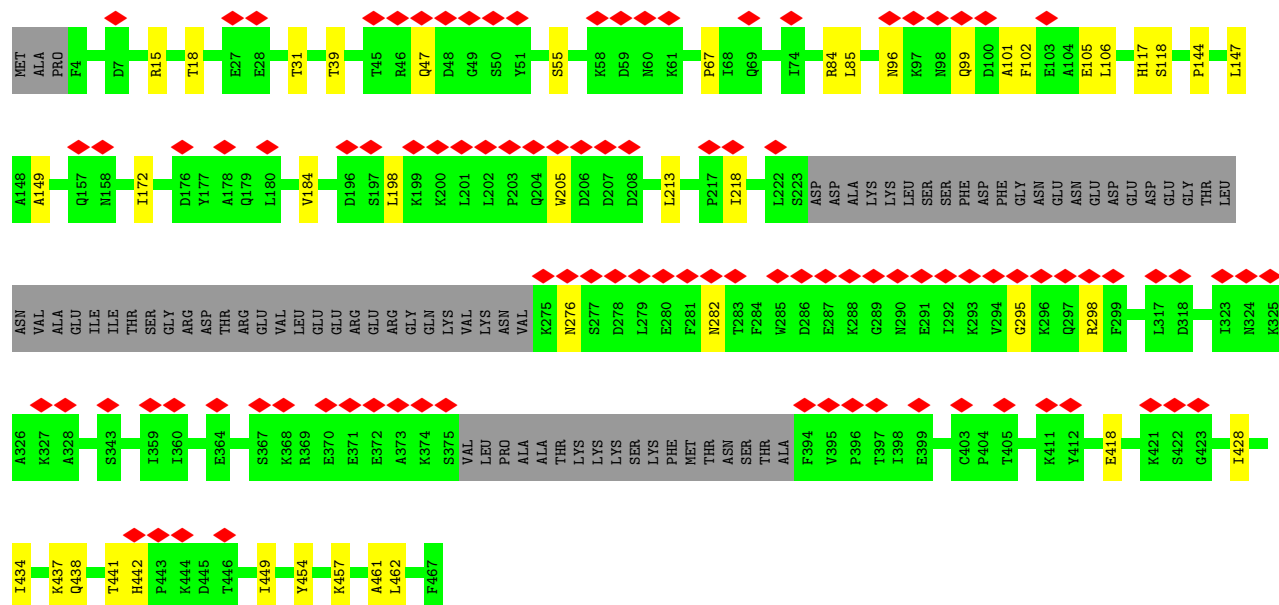


• Molecule 20: Histone H4



• Molecule 21: Actin-like protein ARP9





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45077	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 ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	385.2, 385.2, 385.2	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.14, 2.14, 2.14	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	B	0.18	0/664	0.47	0/889
1	R	0.18	0/711	0.46	0/950
2	N	0.18	0/822	0.42	0/1102
2	Q	0.17	0/794	0.43	0/1064
3	O	0.18	0/833	0.43	0/1124
3	S	0.17	0/833	0.41	0/1124
4	U	0.19	0/3336	0.44	0/5142
5	V	0.20	0/3378	0.40	0/5216
6	J	0.18	0/1836	0.47	0/2480
6	W	0.18	0/598	0.45	0/789
6	Y	0.17	0/4580	0.45	0/6167
7	f	0.16	0/3295	0.41	0/4454
8	h	0.13	0/501	0.37	0/669
9	F	0.18	0/983	0.46	0/1337
10	D	0.15	0/2557	0.39	0/3442
10	H	0.17	0/3275	0.42	0/4409
11	M	0.19	0/3113	0.48	0/4215
12	I	0.16	0/1976	0.41	0/2685
13	G	0.19	0/2039	0.52	0/2769
14	A	0.17	0/3077	0.42	0/4169
15	E	0.18	0/480	0.47	0/643
16	C	0.14	0/272	0.34	0/366
17	K	0.12	0/356	0.35	0/483
18	X	0.14	0/1243	0.41	0/1672
19	L	0.17	0/681	0.47	0/921
20	P	0.15	0/728	0.41	0/983
20	T	0.16	0/736	0.42	0/991
21	g	0.17	0/3261	0.44	2/4421 (0.0%)
All	All	0.17	0/46958	0.43	2/64676 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	g	47	GLN	CA-C-N	5.96	136.69	126.32
21	g	47	GLN	C-N-CA	5.96	136.69	126.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	657	0	706	6	0
1	R	703	0	757	11	0
2	N	810	0	851	8	0
2	Q	784	0	824	7	0
3	O	823	0	882	7	0
3	S	823	0	882	8	0
4	U	2977	0	1639	14	0
5	V	3009	0	1640	10	0
6	J	1814	0	1777	20	0
6	W	592	0	610	9	0
6	Y	4503	0	4573	47	0
7	f	3219	0	3240	38	0
8	h	490	0	467	8	0
9	F	964	0	919	12	0
10	D	2510	0	2542	25	0
10	H	3215	0	3196	38	0
11	M	3058	0	3127	20	0
12	I	1944	0	1964	15	0
13	G	1996	0	1948	19	0
14	A	3007	0	3045	22	0
15	E	477	0	491	8	0
16	C	269	0	279	3	0
17	K	347	0	342	3	0
18	X	1220	0	1192	13	0
19	L	669	0	693	10	0
20	P	717	0	723	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	T	725	0	745	3	0
21	g	3191	0	3179	27	0
22	H	1	0	0	0	0
All	All	45514	0	43233	319	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 4.

All (319) 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)
18:X:375:GLU:HB2	18:X:514:HIS:HB2	1.79	0.64
6:W:337:ARG:HH22	7:f:447:PRO:HD3	1.62	0.64
6:Y:760:ARG:HH21	6:Y:925:ILE:HD13	1.62	0.63
11:M:521:GLN:HE21	12:I:333:MET:HE2	1.62	0.63
10:D:193:THR:HG22	10:D:195:GLN:H	1.64	0.62
13:G:285:CYS:HB2	13:G:292:PHE:HB3	1.80	0.62
14:A:484:ASN:HD22	18:X:624:LEU:HD13	1.64	0.61
9:F:349:LEU:HB2	9:F:358:HIS:HB2	1.83	0.61
1:R:29:ILE:O	1:R:55:ARG:NH2	2.36	0.59
6:W:337:ARG:NH2	7:f:445:ASN:O	2.36	0.59
6:Y:490:ASN:H	6:Y:645:LEU:HD21	1.69	0.58
1:B:42:GLY:O	2:N:108:ASN:ND2	2.36	0.57
10:H:278:ARG:HB3	10:H:329:MET:HE2	1.87	0.57
6:Y:702:VAL:HG23	6:Y:703:GLU:HG3	1.86	0.57
3:S:88:ARG:NH2	3:S:100:VAL:O	2.38	0.56
11:M:227:GLU:OE2	11:M:268:ARG:NH1	2.37	0.56
18:X:378:LEU:HB2	18:X:484:TYR:HB2	1.88	0.56
21:g:102:PHE:HA	21:g:106:LEU:HB2	1.87	0.56
1:R:38:ALA:HB1	1:R:43:VAL:HB	1.88	0.56
3:O:88:ARG:NH2	3:O:100:VAL:O	2.39	0.56
6:W:359:HIS:HE1	21:g:434:ILE:HD13	1.69	0.56
21:g:295:GLY:O	21:g:298:ARG:NH1	2.39	0.56
6:Y:728:GLN:HE21	6:Y:730:LEU:HD12	1.70	0.55
9:F:365:SER:H	10:H:194:PRO:HB3	1.71	0.55
10:D:357:LEU:O	6:J:123:GLN:NE2	2.39	0.55
2:Q:108:ASN:ND2	1:R:42:GLY:O	2.40	0.55
1:R:18:HIS:HD2	1:R:20:LYS:HB3	1.72	0.55
2:Q:116:ARG:NH1	2:Q:118:THR:O	2.41	0.54
10:D:325:GLU:HG2	10:D:329:MET:HE2	1.88	0.54
7:f:36:ILE:HB	7:f:48:ILE:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:153:SER:HB2	7:f:171:ASP:H	1.73	0.54
6:W:338:GLN:NE2	7:f:148:SER:O	2.40	0.54
6:Y:811:LEU:HB2	6:Y:882:VAL:HG13	1.89	0.54
10:D:119:LYS:HD2	10:D:122:ARG:HD3	1.90	0.54
13:G:20:LEU:HD23	13:G:27:ILE:HD13	1.90	0.54
14:A:14:LEU:HD11	14:A:87:PRO:HG3	1.90	0.54
4:U:100:DG:N2	5:V:49:DC:O2	2.40	0.53
11:M:115:ILE:HG13	11:M:168:LEU:HD21	1.90	0.53
5:V:97:DG:OP1	6:Y:631:GLN:NE2	2.41	0.53
7:f:31:ILE:HD11	7:f:86:GLN:HE21	1.74	0.53
13:G:15:ASN:HD22	13:G:174:THR:HA	1.73	0.53
14:A:399:SER:O	14:A:454:ARG:NH2	2.42	0.53
6:Y:635:PRO:HG2	6:Y:636:GLU:HG3	1.89	0.53
11:M:170:GLN:HB2	6:J:292:ARG:HH12	1.73	0.53
21:g:205:TRP:HZ3	21:g:213:LEU:HD22	1.72	0.53
10:H:272:TYR:HB2	10:H:282:LEU:HB2	1.91	0.53
6:Y:644:VAL:HG12	6:Y:645:LEU:HG	1.91	0.53
10:H:180:GLY:O	12:I:468:ARG:NH1	2.41	0.53
18:X:504:PRO:HD3	18:X:624:LEU:HB2	1.91	0.53
1:R:39:ARG:NH1	1:R:43:VAL:O	2.41	0.53
4:U:52:DA:H5'	6:Y:754:ASN:HD22	1.74	0.52
11:M:110:LYS:HG3	17:K:164:ILE:HG23	1.91	0.52
6:W:362:MET:SD	21:g:437:LYS:NZ	2.81	0.52
10:H:311:VAL:O	10:H:314:ASN:ND2	2.41	0.52
6:J:260:LYS:O	6:J:264:ASN:ND2	2.42	0.52
14:A:88:ILE:HG13	14:A:91:GLY:H	1.74	0.52
10:H:285:ARG:NH2	14:A:208:ILE:O	2.42	0.52
10:H:131:LEU:HD11	10:D:182:SER:H	1.75	0.52
10:H:83:PRO:HA	10:D:192:ASP:HB3	1.91	0.52
21:g:55:SER:HB2	21:g:85:LEU:HD11	1.92	0.51
14:A:37:ALA:O	14:A:79:ARG:NH2	2.44	0.51
2:N:62:ILE:O	2:N:93:GLN:NE2	2.44	0.51
1:B:22:LEU:HD12	1:B:25:ASN:HD21	1.74	0.51
6:W:331:ILE:HD11	7:f:152:SER:HB3	1.91	0.51
10:H:454:LEU:HB3	10:D:454:LEU:HD11	1.92	0.51
14:A:176:ILE:HD13	18:X:446:LYS:HD2	1.93	0.51
6:Y:1000:LYS:HA	6:Y:1004:ASN:HD22	1.76	0.51
1:R:75:HIS:HE1	20:P:93:GLU:HG3	1.76	0.51
6:J:46:ILE:HD11	6:J:82:THR:HG21	1.93	0.51
10:H:154:VAL:HG11	13:G:230:ILE:HD12	1.93	0.51
10:H:272:TYR:OH	10:H:303:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:112:GLN:NE2	14:A:215:ASP:OD2	2.44	0.50
21:g:15:ARG:NH2	21:g:18:THR:OG1	2.45	0.50
7:f:197:LEU:HD21	7:f:301:LEU:HD11	1.91	0.50
10:H:435:LEU:O	12:I:398:LYS:NZ	2.44	0.50
6:Y:395:GLN:O	6:Y:399:THR:OG1	2.29	0.50
1:B:36:ARG:NH1	5:V:61:DA:OP2	2.38	0.50
10:D:480:LEU:HD11	12:I:318:LEU:HD11	1.93	0.50
6:Y:880:ASP:HB3	6:Y:908:ASN:HB3	1.94	0.50
2:N:94:GLU:HG2	3:S:103:ALA:HA	1.93	0.50
3:S:85:LEU:O	3:S:89:ASN:ND2	2.45	0.50
10:H:325:GLU:OE2	6:J:246:LYS:NZ	2.39	0.50
16:C:214:ASP:O	16:C:218:ASN:ND2	2.44	0.50
18:X:370:ARG:NH2	18:X:496:ASN:OD1	2.41	0.50
7:f:36:ILE:HG12	7:f:67:VAL:HG22	1.94	0.50
7:f:73:SER:HA	7:f:162:SER:HB3	1.94	0.50
10:H:424:GLU:HA	15:E:53:ILE:HD11	1.92	0.50
18:X:600:ASN:HB2	18:X:621:ILE:HB	1.93	0.50
21:g:96:ASN:O	21:g:99:GLN:NE2	2.45	0.50
3:O:85:LEU:O	3:O:89:ASN:ND2	2.45	0.50
2:N:83:ARG:HB3	5:V:50:DT:H4'	1.94	0.49
7:f:159:ILE:HB	7:f:399:SER:HB3	1.94	0.49
6:Y:941:GLN:HA	6:Y:944:LYS:HE3	1.93	0.49
19:L:764:ARG:NH2	19:L:766:ASP:OD1	2.46	0.49
10:H:439:LYS:NZ	12:I:40:ASP:OD2	2.44	0.49
6:J:219:ASP:OD1	19:L:878:ARG:NH1	2.42	0.49
16:C:216:LEU:HB3	17:K:189:LEU:HD11	1.94	0.49
6:Y:528:LEU:O	6:Y:846:ARG:NH1	2.44	0.49
7:f:91:TYR:HA	7:f:95:LEU:HB2	1.93	0.49
7:f:214:GLN:HB2	7:f:217:SER:HB3	1.95	0.49
14:A:107:ILE:HG23	14:A:117:TYR:HE1	1.77	0.49
10:H:275:LEU:HB2	10:H:300:ASP:HB2	1.93	0.49
13:G:315:VAL:HG13	13:G:320:LEU:HB2	1.95	0.49
14:A:193:GLN:NE2	18:X:495:GLU:OE2	2.45	0.49
6:Y:630:LEU:HD11	6:Y:640:LEU:HD12	1.94	0.49
10:D:469:LEU:HD22	12:I:258:LYS:HD3	1.94	0.49
2:Q:61:LEU:HD13	1:R:36:ARG:HB3	1.95	0.49
7:f:61:LYS:NZ	7:f:219:ASP:OD1	2.46	0.49
10:D:143:ARG:HH12	13:G:314:ILE:HD11	1.78	0.49
8:h:2:ASP:HB3	8:h:5:THR:HG22	1.93	0.49
10:H:407:LEU:HD22	12:I:426:PRO:HB2	1.94	0.49
13:G:268:ILE:HD11	13:G:341:LYS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:62:ILE:O	2:Q:93:GLN:NE2	2.46	0.48
10:D:227:ASN:ND2	6:J:244:GLU:OE2	2.43	0.48
11:M:128:LYS:HG2	11:M:184:ILE:HD11	1.95	0.48
1:B:39:ARG:NH1	1:B:43:VAL:O	2.46	0.48
7:f:5:ARG:NH2	7:f:446:LEU:O	2.45	0.48
6:W:341:GLN:NE2	7:f:25:GLU:OE1	2.46	0.48
9:F:374:SER:HB2	10:H:186:HIS:HB2	1.94	0.48
10:H:180:GLY:HA3	10:D:198:LYS:HE2	1.94	0.48
10:D:455:GLU:OE2	11:M:552:ARG:NH1	2.46	0.48
18:X:430:MET:HB2	19:L:813:LEU:HD11	1.96	0.48
3:O:79:ILE:HG13	3:O:82:HIS:H	1.79	0.48
10:H:321:LEU:HD22	6:J:239:ILE:HG23	1.95	0.48
6:Y:911:ARG:NH1	6:Y:984:THR:O	2.46	0.48
7:f:148:SER:HB3	7:f:439:GLY:HA2	1.95	0.48
10:H:98:GLU:OE1	10:H:122:ARG:NH1	2.47	0.48
11:M:65:PHE:HB2	11:M:68:PHE:HD2	1.78	0.48
7:f:196:ARG:NH2	7:f:312:TYR:OH	2.47	0.48
10:H:406:LYS:NZ	10:D:396:ALA:O	2.43	0.48
14:A:490:VAL:HG23	19:L:742:MET:HB2	1.96	0.48
7:f:224:ALA:HA	7:f:228:ILE:HB	1.95	0.48
10:H:288:GLN:HA	19:L:802:ARG:HH22	1.78	0.48
21:g:449:ILE:HD11	21:g:462:LEU:HA	1.96	0.48
13:G:321:THR:HG23	13:G:323:GLU:H	1.77	0.48
8:h:31:GLN:NE2	8:h:56:TYR:O	2.42	0.47
9:F:383:SER:HA	10:H:235:TYR:O	2.14	0.47
4:U:128:DG:H1'	4:U:129:DT:H5'	1.96	0.47
13:G:276:ASP:OD1	13:G:301:ASN:ND2	2.46	0.47
1:R:74:GLU:O	20:P:92:ARG:NH2	2.47	0.47
11:M:176:GLN:NE2	11:M:232:TYR:OH	2.46	0.47
2:Q:68:GLN:HE21	2:Q:72:ARG:HH21	1.63	0.47
6:Y:647:LYS:HG2	6:Y:648:ILE:HG23	1.95	0.47
1:B:64:ASN:OD1	1:B:67:ARG:NH1	2.47	0.47
11:M:540:ASP:O	11:M:547:SER:OG	2.32	0.47
6:Y:916:ILE:HG13	6:Y:926:LEU:HD22	1.96	0.47
8:h:30:TYR:HB2	8:h:64:LEU:HD11	1.95	0.47
6:J:128:ASP:OD2	6:J:198:ARG:NH2	2.48	0.47
9:F:387:GLU:O	10:H:188:GLN:HA	2.15	0.47
21:g:218:ILE:O	21:g:276:ASN:ND2	2.48	0.47
6:Y:576:TYR:OH	6:Y:597:ASP:O	2.33	0.47
4:U:54:DC:OP2	6:Y:817:THR:OG1	2.30	0.47
21:g:39:THR:HG22	21:g:67:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:50:DG:H1'	4:U:51:DC:H5'	1.97	0.47
10:D:113:LYS:NZ	10:D:152:SER:OG	2.48	0.47
9:F:394:ASP:O	10:H:224:PHE:N	2.48	0.46
21:g:31:THR:HG22	21:g:418:GLU:HG3	1.97	0.46
12:I:444:LEU:HD12	15:E:29:LEU:HD13	1.97	0.46
21:g:438:GLN:O	21:g:442:HIS:ND1	2.48	0.46
7:f:96:LYS:NZ	21:g:118:SER:O	2.43	0.46
7:f:151:LYS:HD2	7:f:393:ILE:HD11	1.96	0.46
11:M:300:CYS:SG	11:M:301:ASP:N	2.88	0.46
6:J:21:ALA:HB1	6:J:66:GLN:HE21	1.80	0.46
6:Y:731:LYS:HA	6:Y:735:LEU:HD12	1.98	0.46
7:f:16[A]:ARG:NH2	7:f:397:SER:OG	2.48	0.46
14:A:44:PRO:HA	14:A:47:ILE:HB	1.98	0.46
21:g:457:LYS:HB2	21:g:461:ALA:HB2	1.96	0.46
3:S:79:ILE:HG13	3:S:82:HIS:H	1.80	0.46
7:f:196:ARG:NH1	7:f:305:GLU:OE1	2.49	0.46
2:N:102:GLY:O	2:N:131:ARG:NH2	2.49	0.46
13:G:205:PRO:HB2	13:G:220:GLN:HE21	1.80	0.46
21:g:437:LYS:O	21:g:441:THR:OG1	2.32	0.46
2:Q:128:ARG:HB3	2:Q:133:GLU:HB2	1.97	0.46
14:A:129:GLU:OE2	19:L:869:ARG:NE	2.44	0.46
10:D:428:ILE:HG23	15:E:69:LEU:HD11	1.98	0.46
10:D:222:LYS:HG3	12:I:463:ASN:HD21	1.81	0.46
1:R:30:THR:HG21	4:U:61:DA:H5''	1.98	0.46
11:M:167:ASN:O	6:J:292:ARG:NH1	2.43	0.46
11:M:543:ASP:HA	11:M:547:SER:HB2	1.99	0.46
13:G:273:ILE:HD11	13:G:340:LYS:HG2	1.97	0.46
13:G:279:VAL:HG21	13:G:339:ILE:HD13	1.98	0.45
6:J:61:ARG:HD2	19:L:815:LEU:HD13	1.98	0.45
17:K:189:LEU:HA	17:K:192:LEU:HG	1.97	0.45
4:U:137:DA:OP2	6:Y:565:ARG:NH1	2.49	0.45
10:D:221:LYS:O	10:D:365:ARG:NH2	2.49	0.45
11:M:569:LEU:HD13	12:I:310:LEU:HB2	1.99	0.45
13:G:295:ASN:HB2	13:G:376:TRP:HB2	1.98	0.45
14:A:244:LEU:HD22	6:J:242:LEU:HD21	1.98	0.45
18:X:366:ASN:O	18:X:369:ASN:ND2	2.48	0.45
9:F:382:THR:HA	10:H:183:PHE:HB3	1.97	0.45
10:H:260:CYS:SG	10:H:267:SER:OG	2.74	0.45
6:Y:763:CYS:SG	6:Y:920:SER:OG	2.68	0.45
7:f:145:ILE:HG21	7:f:395:THR:HG21	1.98	0.45
21:g:101:ALA:HB1	21:g:105:GLU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:330:ILE:HD11	7:f:451:LEU:HB3	1.98	0.45
10:D:432:LEU:HD13	15:E:69:LEU:HD23	1.97	0.45
15:E:36:ILE:HD12	15:E:39:LEU:HD12	1.99	0.45
6:Y:474:GLN:NE2	6:Y:499:LEU:O	2.50	0.45
11:M:568:THR:HG21	12:I:332:LEU:HD13	1.98	0.45
13:G:15:ASN:HB2	13:G:178:GLY:HA2	1.98	0.45
6:J:206:LEU:HB3	6:J:245:LEU:HD12	1.98	0.45
6:J:226:THR:H	6:J:229:ASP:HB2	1.83	0.45
18:X:431:GLN:HE22	18:X:433:GLU:HB2	1.81	0.45
5:V:59:DA:H2"	5:V:60:DA:C8	2.52	0.44
10:D:148:MET:HE1	10:D:156:ILE:HD12	1.99	0.44
10:H:150:VAL:HA	10:H:153:ILE:HG22	1.99	0.44
7:f:292:PHE:O	7:f:296:ASN:N	2.50	0.44
21:g:101:ALA:O	21:g:106:LEU:N	2.48	0.44
8:h:79:GLU:OE1	21:g:84:ARG:NH1	2.51	0.44
10:H:181:PRO:HG3	10:D:201:LEU:HB2	1.99	0.44
18:X:374:THR:OG1	18:X:514:HIS:O	2.31	0.44
21:g:282:ASN:OD1	21:g:298:ARG:NH2	2.51	0.44
6:Y:809:ARG:HH22	6:Y:853:PHE:HA	1.83	0.44
4:U:94:DG:H1	5:V:54:DC:H42	1.65	0.44
7:f:7:CYS:SG	7:f:8:VAL:N	2.91	0.44
9:F:371:TRP:O	9:F:434:TYR:OH	2.35	0.44
6:J:223:GLU:OE1	6:J:231:SER:OG	2.32	0.44
20:T:90:THR:OG1	20:T:93:GLU:OE1	2.33	0.44
3:S:63:LEU:HD13	20:P:45:LEU:HB2	2.00	0.44
6:Y:537:GLU:HG2	6:Y:540:LYS:HE2	1.99	0.44
10:H:145:ASN:HB3	13:G:322:ARG:HE	1.83	0.44
10:H:149:ASP:OD1	10:H:149:ASP:N	2.50	0.44
6:Y:841:THR:OG1	6:Y:842:LYS:N	2.51	0.44
4:U:98:DA:H2"	4:U:99:DG:C8	2.53	0.44
9:F:362:SER:OG	10:H:195:GLN:O	2.29	0.44
21:g:198:LEU:HD13	21:g:213:LEU:HD23	1.98	0.44
19:L:805:ASN:ND2	19:L:808:ASP:OD2	2.51	0.43
10:D:325:GLU:OE2	19:L:871:SER:OG	2.31	0.43
13:G:165:ILE:HG12	13:G:171:ILE:HG21	1.99	0.43
7:f:392:VAL:HB	7:f:423:THR:HG22	1.99	0.43
11:M:341:PRO:HG2	11:M:556:LEU:HD23	1.99	0.43
2:N:40:ARG:HH12	4:U:83:DG:H21	1.66	0.43
7:f:232:LYS:HA	7:f:236:LEU:HD12	2.00	0.43
13:G:169:PRO:HA	13:G:172:ARG:HG2	2.00	0.43
3:O:75:LYS:HB2	3:O:82:HIS:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:20:ILE:HG23	6:J:224:PHE:HE1	1.82	0.43
5:V:94:DG:H3'	6:Y:608:LYS:HD2	2.00	0.43
8:h:31:GLN:HB2	8:h:59:ARG:HG2	1.99	0.43
6:Y:459:ASP:HB3	6:Y:475:LEU:HD13	2.00	0.43
6:Y:994:LEU:O	6:Y:997:LYS:NZ	2.51	0.43
9:F:340:LYS:HA	9:F:344:VAL:HB	2.00	0.43
6:Y:529:SER:OG	6:Y:870:GLY:O	2.37	0.43
6:Y:537:GLU:HA	6:Y:540:LYS:HG2	2.00	0.43
12:I:312:GLU:HB3	12:I:329:HIS:HB3	2.01	0.43
7:f:284:LEU:HA	7:f:303:LEU:HB3	2.01	0.42
1:R:36:ARG:NH1	4:U:61:DA:OP2	2.39	0.42
10:H:283:CYS:SG	10:H:284:SER:N	2.92	0.42
10:H:310:SER:OG	10:H:314:ASN:ND2	2.52	0.42
14:A:177:SER:OG	14:A:182:LYS:NZ	2.50	0.42
6:Y:465:LEU:HD22	6:Y:541:TRP:HE3	1.84	0.42
4:U:17:DC:H2''	4:U:18:DC:C5	2.54	0.42
8:h:26:ARG:O	8:h:63:TRP:HA	2.20	0.42
7:f:188:PHE:HE2	7:f:312:TYR:HB3	1.84	0.42
3:O:68:ASN:OD1	3:O:71:ARG:NH2	2.53	0.42
1:R:51:TYR:O	1:R:55:ARG:NH1	2.52	0.42
7:f:105:VAL:HG22	7:f:137:GLN:HB3	2.02	0.42
6:Y:479:GLU:HA	6:Y:482:VAL:HB	2.01	0.42
6:Y:524:VAL:HB	6:Y:573:LEU:HD23	2.02	0.42
3:S:76:THR:O	20:P:53:GLY:N	2.47	0.42
4:U:135:DA:H4'	6:Y:584:SER:HB3	2.02	0.42
7:f:18:VAL:HG21	7:f:434:ILE:HG22	2.01	0.42
8:h:25:TRP:NE1	21:g:454:TYR:O	2.50	0.42
14:A:209:ILE:HG22	14:A:211:LYS:H	1.85	0.42
14:A:313:ARG:HD3	15:E:16:TYR:HB3	2.00	0.42
5:V:54:DC:N4	5:V:55:DG:O6	2.52	0.42
11:M:107:TYR:OH	16:C:197:ASP:OD2	2.38	0.42
3:O:13:LYS:HG3	3:O:15:LYS:HG3	2.02	0.42
5:V:129:DC:H2''	5:V:130:DG:C8	2.54	0.42
8:h:82:LEU:HD23	21:g:85:LEU:HG	2.01	0.42
10:H:330:TYR:HB2	10:H:337:ILE:HD11	2.01	0.42
7:f:112:ASN:HA	7:f:176:LYS:HB3	2.02	0.42
13:G:158:GLN:HE22	13:G:165:ILE:HG13	1.83	0.42
5:V:26:DC:H4'	5:V:27:DC:H5'	2.02	0.41
6:Y:630:LEU:O	6:Y:892:HIS:NE2	2.53	0.41
7:f:18:VAL:HG22	7:f:30:ILE:HG12	2.02	0.41
14:A:306:ARG:NH1	15:E:17:ASN:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:862:GLY:HA2	19:L:863:PRO:HD3	1.94	0.41
7:f:164:CYS:H	7:f:182:SER:HB3	1.85	0.41
11:M:141:LEU:HD21	11:M:215:PHE:HB2	2.01	0.41
15:E:56:GLU:HA	15:E:59:ARG:HG2	2.01	0.41
6:Y:583:LYS:HG2	6:Y:616:TYR:HE1	1.86	0.41
6:Y:885:PHE:HE1	6:Y:915:LEU:HB2	1.86	0.41
3:S:13:LYS:HG3	3:S:15:LYS:HG3	2.01	0.41
6:Y:684:ARG:HA	6:Y:687:HIS:HD2	1.85	0.41
6:Y:760:ARG:HH12	6:Y:889:TRP:NE1	2.18	0.41
4:U:131:DA:H2''	4:U:132:DG:H5''	2.02	0.41
6:W:333:PHE:HB3	6:W:337:ARG:HH12	1.85	0.41
7:f:38:ARG:HB3	7:f:46:GLU:HB3	2.03	0.41
20:T:36:SER:OG	20:T:63:ASN:ND2	2.54	0.41
6:Y:448:TYR:OH	6:Y:948:LYS:O	2.38	0.41
10:H:276:ARG:HB2	10:H:296:PHE:HE1	1.85	0.41
21:g:144:PRO:HG2	21:g:147:LEU:HD12	2.02	0.41
6:Y:938:LYS:HG2	6:Y:961:LEU:HD21	2.03	0.41
6:Y:975:GLU:HG2	6:Y:980:GLU:HB3	2.02	0.41
6:Y:979:ASP:OD1	6:Y:979:ASP:N	2.54	0.41
2:N:110:CYS:SG	2:Q:113:HIS:NE2	2.94	0.41
14:A:269:LEU:HG	14:A:274:TYR:HE1	1.86	0.41
21:g:117:HIS:CD2	21:g:172:ILE:HD11	2.56	0.41
6:Y:472:GLU:OE2	6:Y:476:ARG:NE	2.54	0.41
9:F:320:LEU:HB2	10:D:68:LYS:HE3	2.01	0.41
10:H:178:LEU:HD21	12:I:476:LEU:HB2	2.01	0.41
11:M:192:LEU:HB3	11:M:245:THR:HG21	2.02	0.41
11:M:561:LEU:HD11	11:M:571:LEU:HD12	2.03	0.41
6:J:48:LYS:HE2	6:J:82:THR:HG23	2.03	0.41
21:g:172:ILE:HG12	21:g:184:VAL:HG13	2.01	0.41
1:B:36:ARG:HB3	2:N:61:LEU:HD13	2.03	0.41
12:I:7:PRO:HB2	14:A:282:LEU:HB3	2.01	0.41
3:O:32:ARG:NH2	20:T:35:GLU:OE2	2.45	0.40
7:f:389:LEU:HD12	7:f:419:TYR:HD2	1.84	0.40
14:A:395:ASN:O	6:J:90:GLN:NE2	2.54	0.40
9:F:330:PHE:HB2	10:D:144:ARG:HH11	1.87	0.40
13:G:19:ARG:HA	13:G:22:ASN:HB2	2.02	0.40
21:g:149:ALA:HB2	21:g:428:ILE:HG12	2.04	0.40
6:Y:470:LEU:HD13	6:Y:475:LEU:HD21	2.02	0.40
10:D:72:PHE:HE2	10:D:127:ASN:HB3	1.84	0.40
18:X:602:LEU:HD23	18:X:619:PHE:HB2	2.02	0.40
12:I:322:VAL:HG23	12:I:323:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:24:ALA:HB3	6:J:73:LYS:HD2	2.03	0.40
3:S:68:ASN:OD1	3:S:71:ARG:NH2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	80/103 (78%)	78 (98%)	2 (2%)	0	100	100
1	R	85/103 (82%)	83 (98%)	2 (2%)	0	100	100
2	N	96/136 (71%)	94 (98%)	2 (2%)	0	100	100
2	Q	93/136 (68%)	93 (100%)	0	0	100	100
3	O	105/130 (81%)	105 (100%)	0	0	100	100
3	S	105/130 (81%)	105 (100%)	0	0	100	100
6	J	229/1359 (17%)	210 (92%)	19 (8%)	0	100	100
6	W	67/1359 (5%)	67 (100%)	0	0	100	100
6	Y	536/1359 (39%)	497 (93%)	39 (7%)	0	100	100
7	f	391/477 (82%)	383 (98%)	8 (2%)	0	100	100
8	h	46/157 (29%)	44 (96%)	2 (4%)	0	100	100
9	F	116/435 (27%)	108 (93%)	8 (7%)	0	100	100
10	D	295/557 (53%)	283 (96%)	12 (4%)	0	100	100
10	H	387/557 (70%)	369 (95%)	18 (5%)	0	100	100
11	M	378/581 (65%)	362 (96%)	16 (4%)	0	100	100
12	I	236/483 (49%)	223 (94%)	13 (6%)	0	100	100
13	G	238/426 (56%)	221 (93%)	17 (7%)	0	100	100
14	A	357/502 (71%)	331 (93%)	26 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	E	56/78 (72%)	55 (98%)	1 (2%)	0	100	100
16	C	31/883 (4%)	31 (100%)	0	0	100	100
17	K	40/885 (4%)	40 (100%)	0	0	100	100
18	X	139/625 (22%)	127 (91%)	12 (9%)	0	100	100
19	L	79/889 (9%)	70 (89%)	9 (11%)	0	100	100
20	P	91/126 (72%)	91 (100%)	0	0	100	100
20	T	91/126 (72%)	91 (100%)	0	0	100	100
21	g	390/467 (84%)	381 (98%)	9 (2%)	0	100	100
All	All	4757/13069 (36%)	4542 (96%)	215 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	68/79 (86%)	68 (100%)	0	100	100
1	R	72/79 (91%)	72 (100%)	0	100	100
2	N	86/111 (78%)	86 (100%)	0	100	100
2	Q	83/111 (75%)	83 (100%)	0	100	100
3	O	84/102 (82%)	84 (100%)	0	100	100
3	S	84/102 (82%)	84 (100%)	0	100	100
6	J	187/1228 (15%)	187 (100%)	0	100	100
6	W	63/1228 (5%)	63 (100%)	0	100	100
6	Y	502/1228 (41%)	502 (100%)	0	100	100
7	f	356/420 (85%)	356 (100%)	0	100	100
8	h	53/140 (38%)	53 (100%)	0	100	100
9	F	111/388 (29%)	111 (100%)	0	100	100
10	D	285/500 (57%)	285 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	H	363/500 (73%)	363 (100%)	0	100	100
11	M	349/521 (67%)	349 (100%)	0	100	100
12	I	223/435 (51%)	223 (100%)	0	100	100
13	G	226/384 (59%)	225 (100%)	1 (0%)	84	84
14	A	343/462 (74%)	343 (100%)	0	100	100
15	E	56/75 (75%)	56 (100%)	0	100	100
16	C	32/824 (4%)	32 (100%)	0	100	100
17	K	39/832 (5%)	39 (100%)	0	100	100
18	X	141/578 (24%)	141 (100%)	0	100	100
19	L	77/810 (10%)	77 (100%)	0	100	100
20	P	77/105 (73%)	77 (100%)	0	100	100
20	T	79/105 (75%)	79 (100%)	0	100	100
21	g	362/423 (86%)	362 (100%)	0	100	100
All	All	4401/11770 (37%)	4400 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
13	G	300	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	25	ASN
2	N	68	GLN
3	O	31	HIS
3	O	82	HIS
3	O	84	GLN
2	Q	68	GLN
2	Q	93	GLN
1	R	18	HIS
1	R	27	GLN
1	R	75	HIS
3	S	31	HIS
3	S	73	ASN
3	S	82	HIS

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Mol	Chain	Res	Type
7	f	86	GLN
7	f	253	GLN
9	F	358	HIS
10	H	127	ASN
10	H	145	ASN
10	H	245	GLN
10	H	255	HIS
10	H	261	HIS
10	H	265	ASN
10	H	314	ASN
10	H	483	ASN
10	D	76	GLN
10	D	318	GLN
10	D	344	HIS
11	M	69	GLN
11	M	241	HIS
11	M	521	GLN
12	I	432	HIS
12	I	463	ASN
12	I	480	GLN
13	G	10	GLN
13	G	156	GLN
13	G	220	GLN
13	G	278	HIS
13	G	299	ASN
14	A	193	GLN
14	A	219	HIS
14	A	272	ASN
14	A	297	ASN
14	A	392	ASN
14	A	484	ASN
6	J	66	GLN
6	J	72	ASN
6	J	90	GLN
6	J	123	GLN
6	J	254	GLN
15	E	23	ASN
18	X	380	ASN
18	X	431	GLN
18	X	487	ASN
18	X	489	ASN
18	X	503	GLN

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Mol	Chain	Res	Type
18	X	529	ASN
18	X	622	ASN
20	T	63	ASN
20	P	49	HIS
20	P	63	ASN
21	g	70	ASN
21	g	81	GLN
21	g	99	GLN
21	g	209	GLN
21	g	433	GLN
6	Y	452	HIS
6	Y	488	HIS
6	Y	490	ASN
6	Y	556	GLN
6	Y	615	HIS
6	Y	621	ASN
6	Y	687	HIS
6	Y	728	GLN
6	Y	753	ASN
6	Y	754	ASN
6	Y	808	HIS
6	Y	898	GLN
6	Y	982	ASN
6	Y	1004	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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](#)

Of 1 ligands modelled in this entry, 1 is 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.

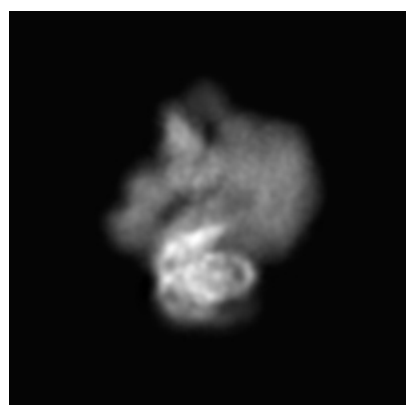
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0777. These allow visual inspection of the internal detail of the map and identification of artifacts.

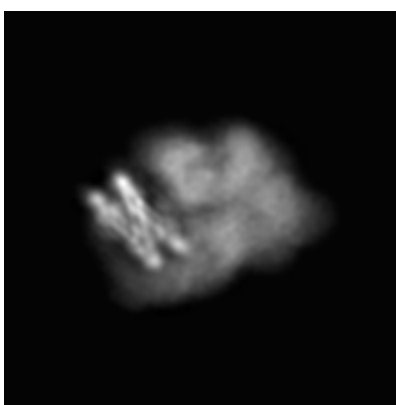
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

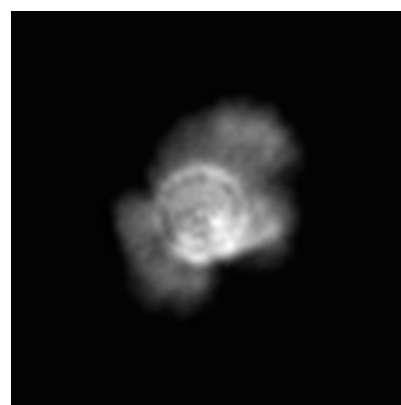
6.1.1 Primary map



X



Y

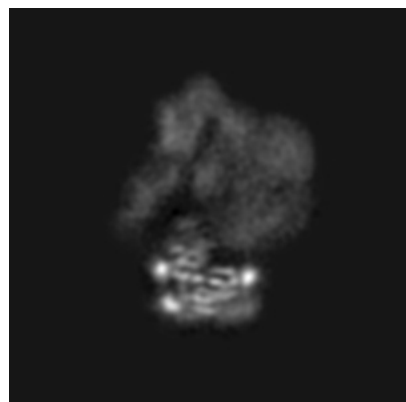


Z

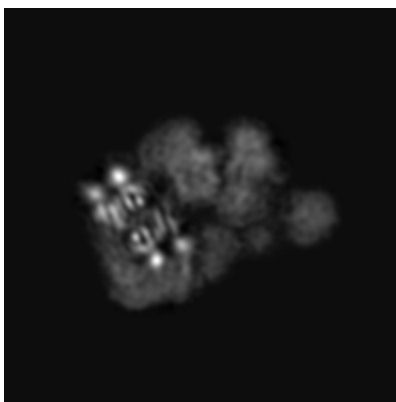
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

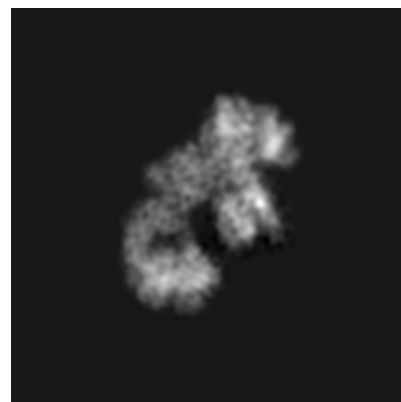
6.2.1 Primary map



X Index: 90



Y Index: 90



Z Index: 90

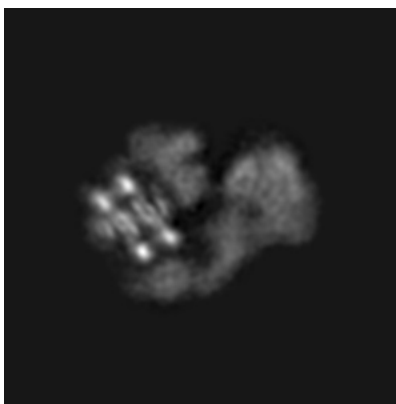
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

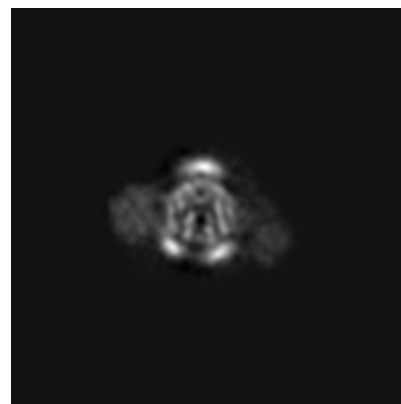
6.3.1 Primary map



X Index: 94



Y Index: 75



Z Index: 60

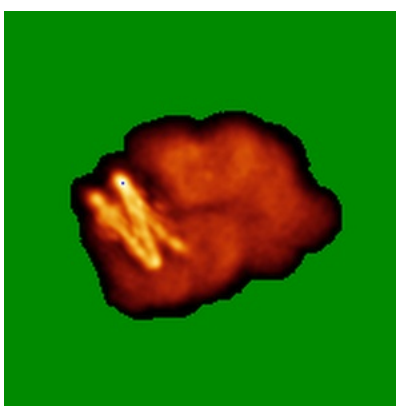
The images above show the largest variance slices of the map in three orthogonal directions.

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

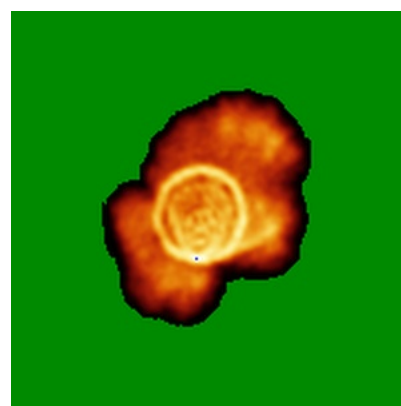
6.4.1 Primary map



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 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

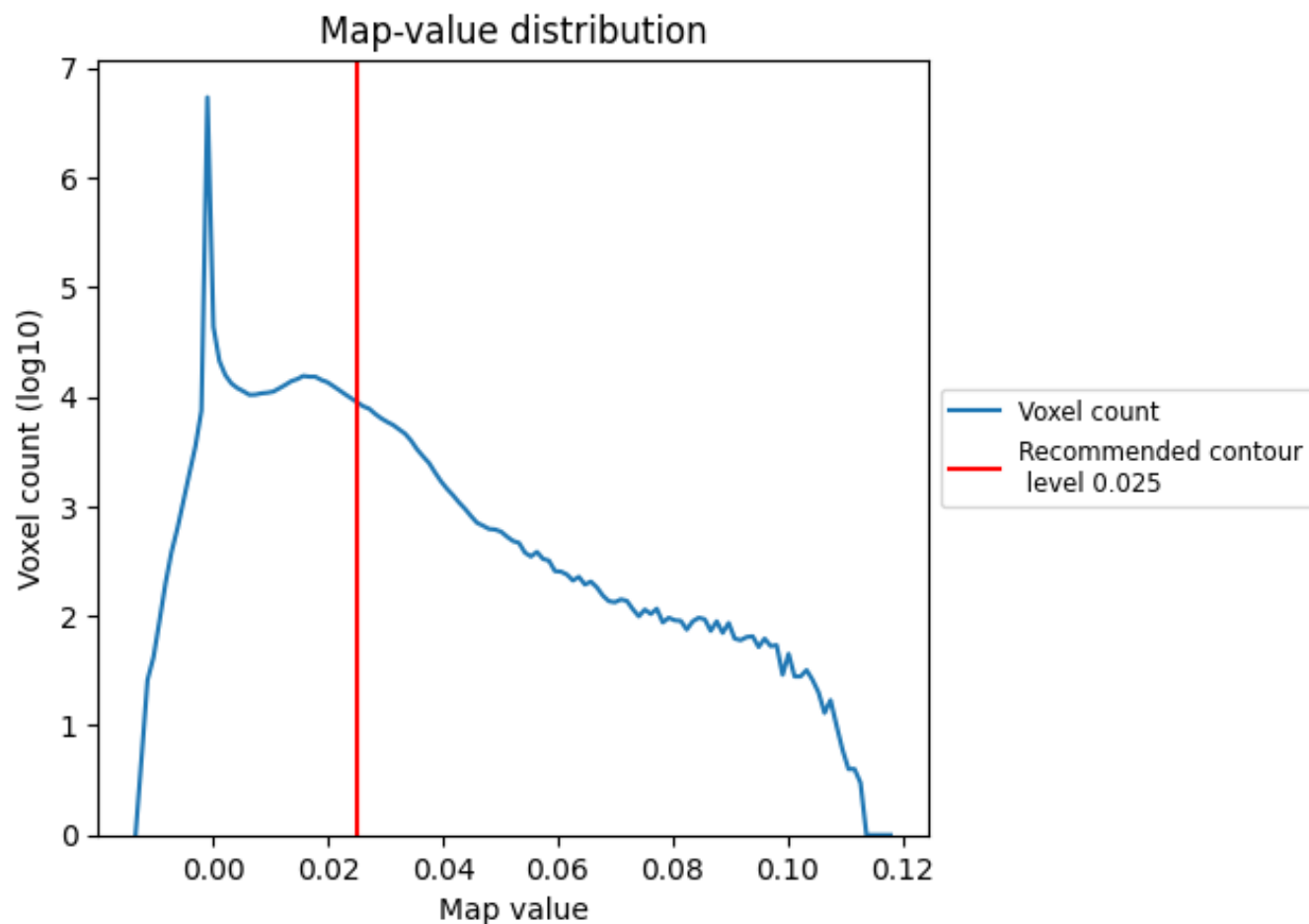
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

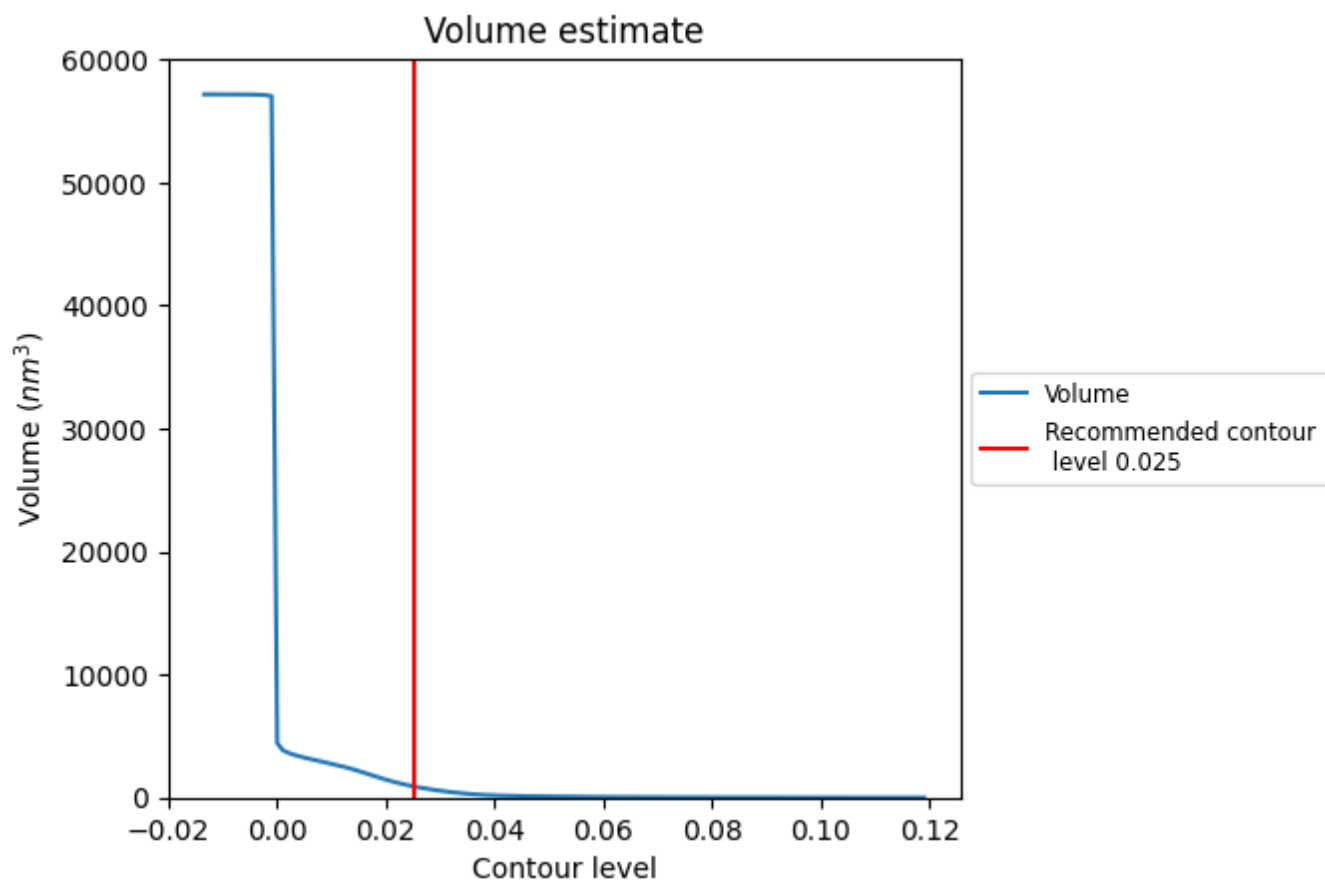
This section contains the results of statistical analysis of the map.

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.

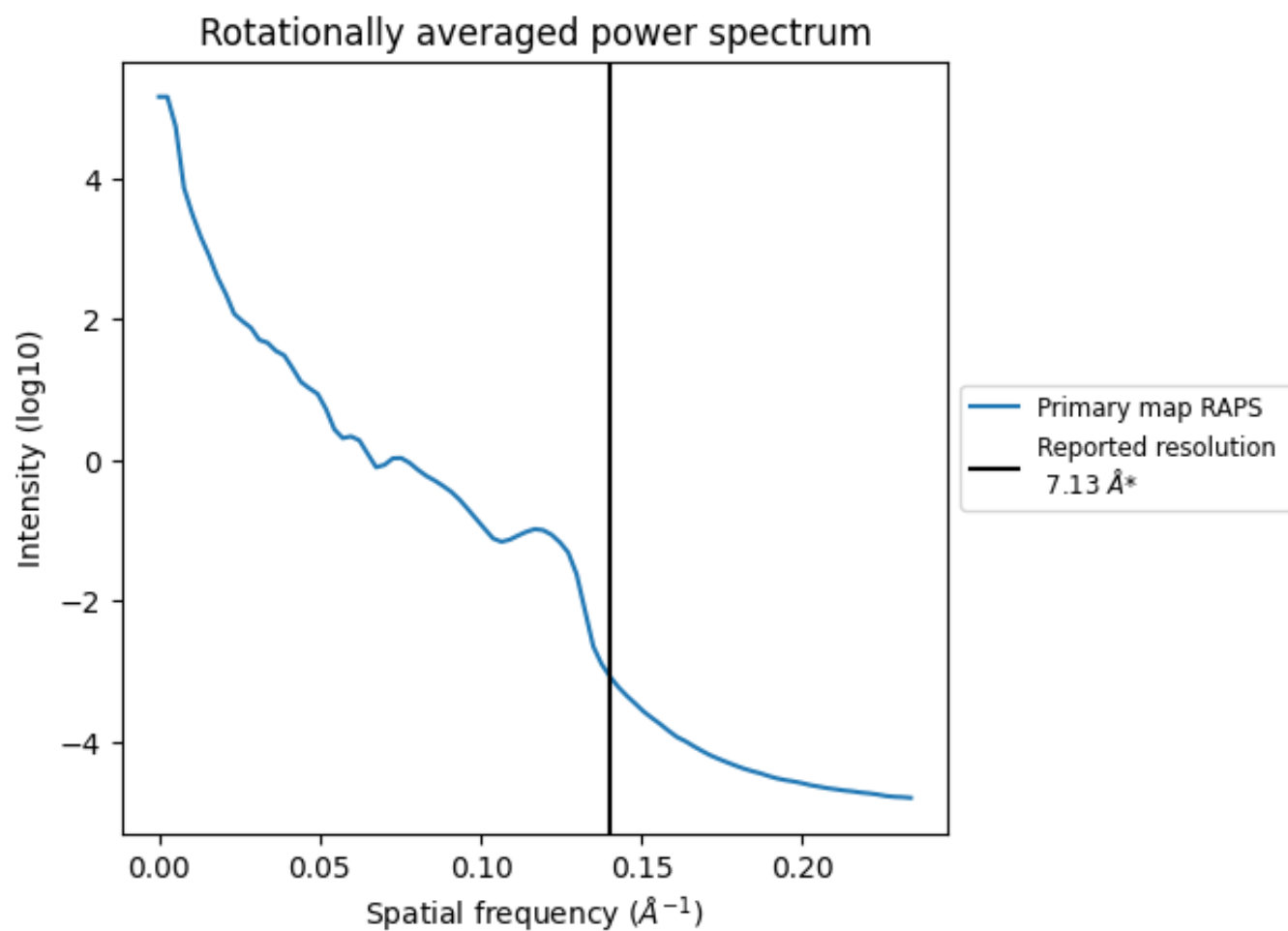
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 915 nm³; this corresponds to an approximate mass of 827 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 0.140 Å⁻¹

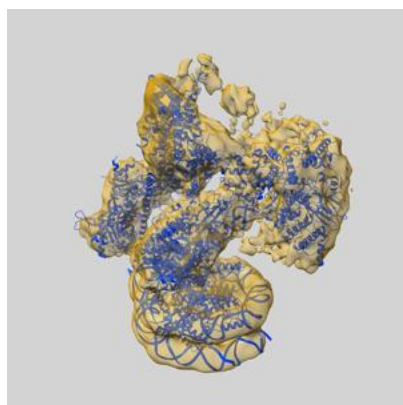
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

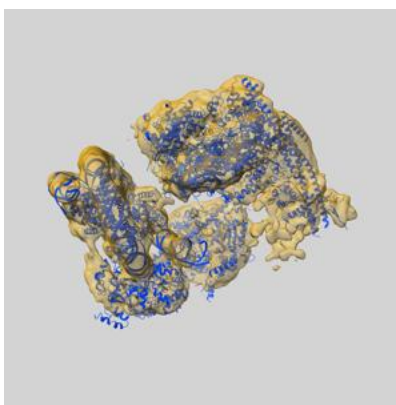
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0777 and PDB model 6KW3. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

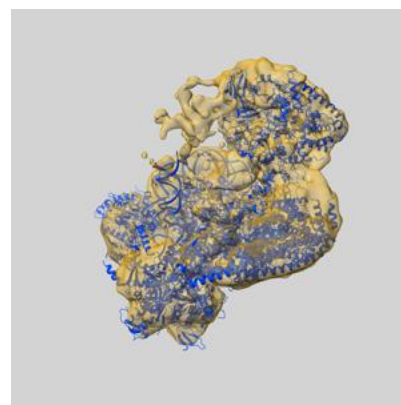
9.1 Map-model overlay [i](#)



X



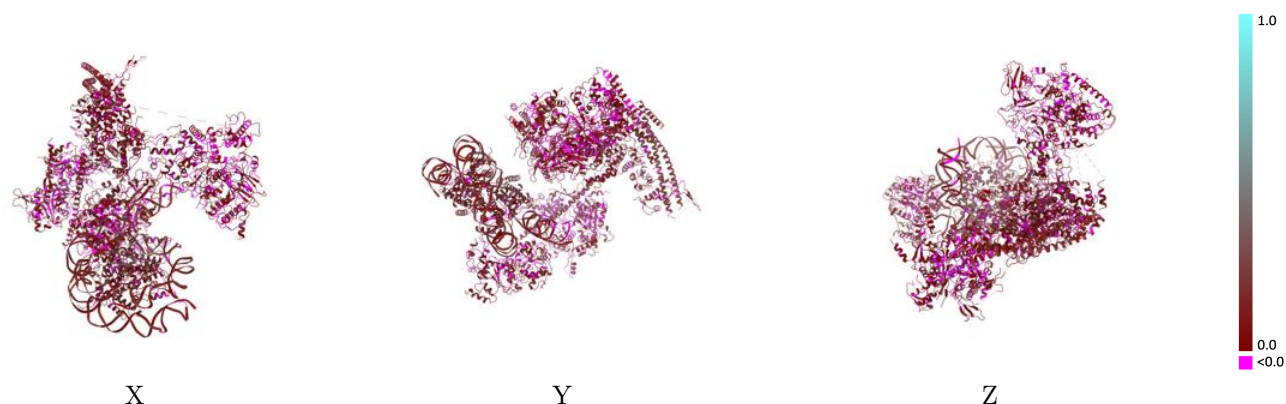
Y



Z

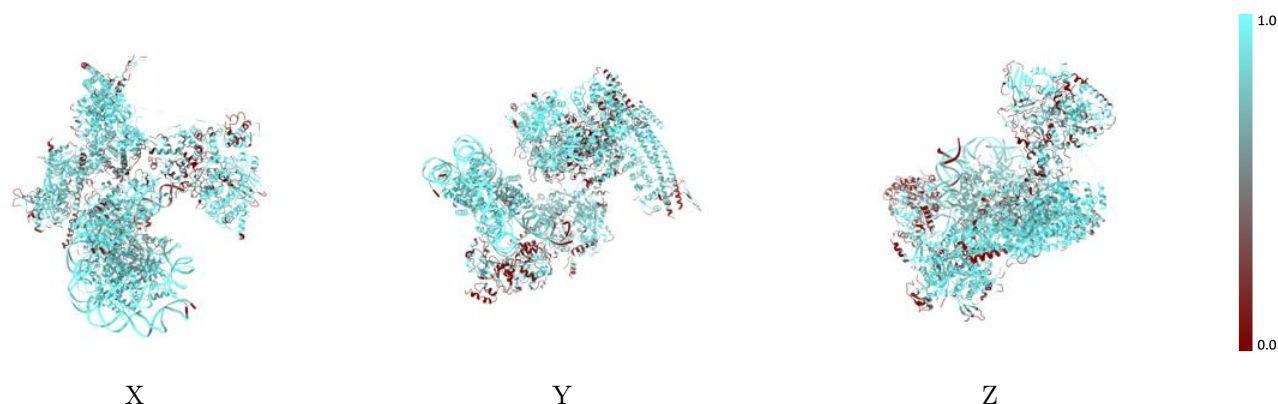
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



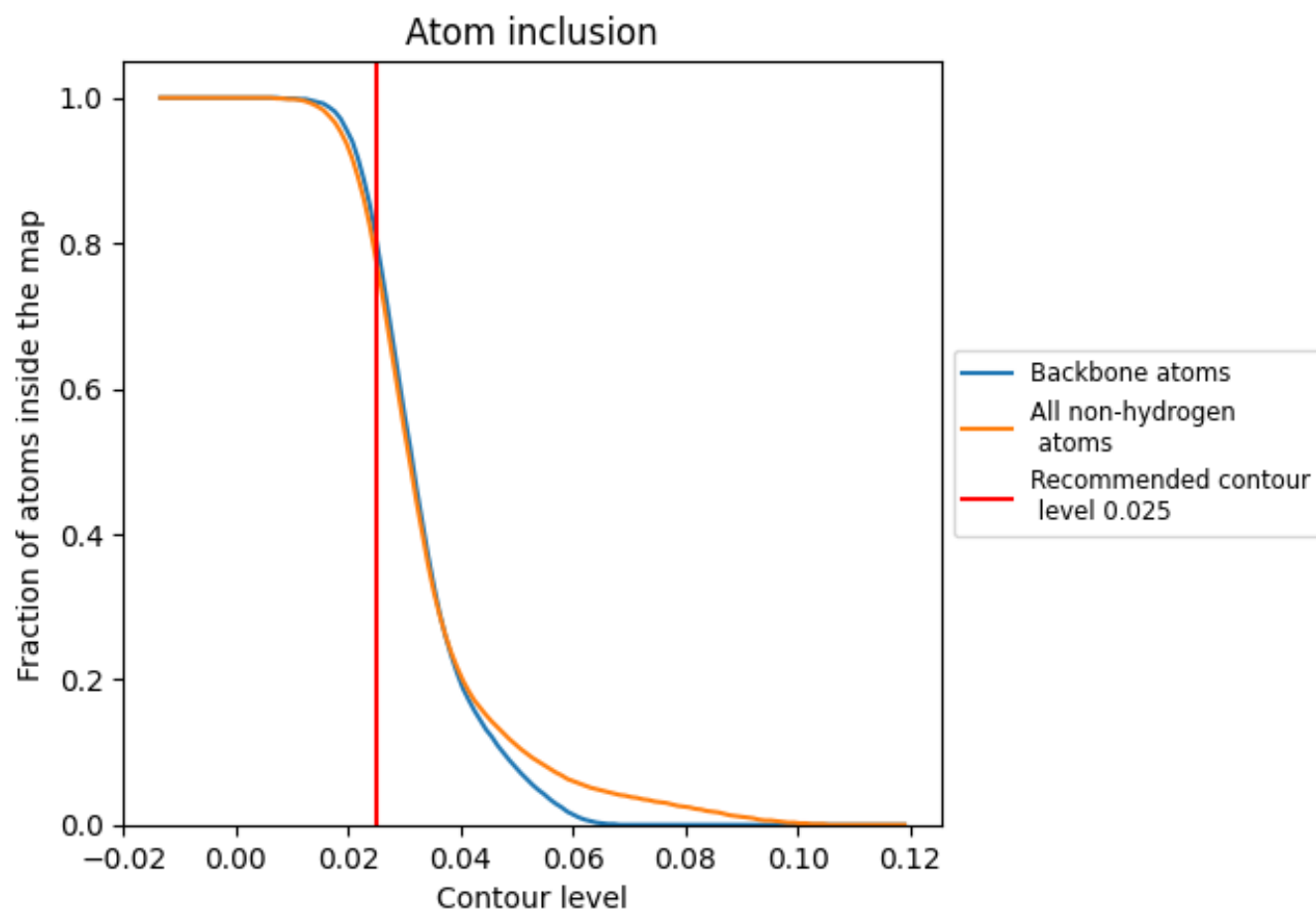
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 77% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7740	 0.0860
A	 0.7840	 0.0650
B	 0.9100	 0.1200
C	 0.5170	 0.0940
D	 0.8260	 0.0890
E	 0.9270	 0.0990
F	 0.8740	 0.0960
G	 0.7560	 0.0770
H	 0.7560	 0.0820
I	 0.7620	 0.0840
J	 0.5730	 0.0520
K	 0.5010	 0.1200
L	 0.6910	 0.0260
M	 0.8140	 0.0970
N	 0.9330	 0.1350
O	 0.8210	 0.1220
P	 0.9530	 0.1470
Q	 0.9340	 0.1330
R	 0.8370	 0.1170
S	 0.9620	 0.1380
T	 0.8840	 0.1460
U	 0.9170	 0.1190
V	 0.9240	 0.1220
W	 0.5010	 0.0830
X	 0.7310	 0.0530
Y	 0.5040	 0.0690
f	 0.8540	 0.0540
g	 0.7070	 0.0420
h	 0.7380	 0.0900

