



Full wwPDB EM Validation Report ⓘ

Dec 8, 2025 – 08:44 AM EST

PDB ID : 9YNU / pdb_00009ynu
EMDB ID : EMD-73233
Title : Tra1 and core modules including core tip of ctSAGA complex
Authors : Mattoo, R.U.H.; Chen, D.H.; Bushnell, D.A.; Tamir, S.; Kornberg, R.D.
Deposited on : 2025-10-12
Resolution : 3.20 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:

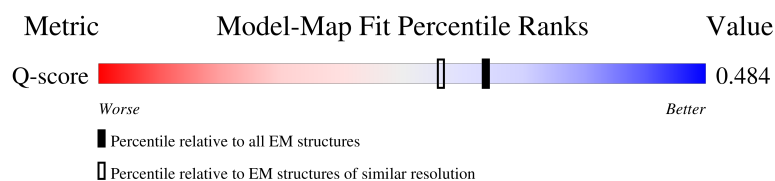
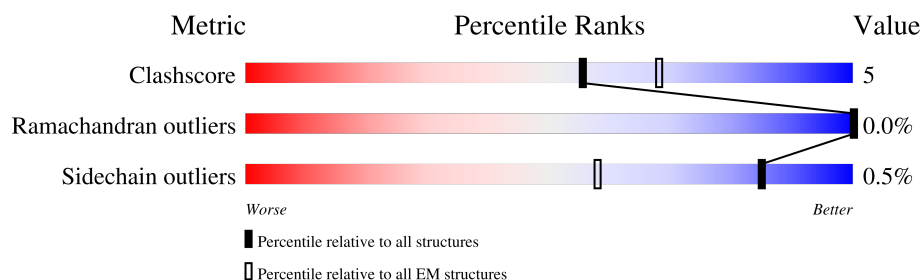
EMDB validation analysis : 0.0.1.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.47

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	Q	1273	95%
2	B	1192	19% 62% 79%
3	C	433	6% 38% 8% 55%
4	D	767	19% 62% 6% 32%

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Mol	Chain	Length	Quality of chain
5	E	480	<div><div></div><div>10%</div><div>80%</div><div>12%</div><div>8%</div></div>
6	F	277	<div><div></div><div>36%</div><div>7%</div><div>56%</div></div>
7	G	204	<div><div></div><div>51%</div><div>44%</div></div>
8	H	485	<div><div></div><div>47%</div><div>5%</div><div>48%</div></div>
9	I	770	<div><div></div><div>16%</div><div>80%</div></div>
10	K	1224	<div><div></div><div>10%</div><div>41%</div><div>7%</div><div>52%</div></div>
11	A	3893	<div><div></div><div>11%</div><div>83%</div><div>10%</div><div>7%</div></div>

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 100918 atoms, of which 50157 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 SCA7 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	Q	62	Total	C	H	N	O	S	0	0
			950	303	472	86	88	1		

- Molecule 2 is a protein called Spt20-like SEP domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	245	Total	C	H	N	O	S	0	0
			3987	1319	1952	341	368	7		

- Molecule 3 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	197	Total	C	H	N	O	S	0	0
			3225	1022	1607	287	303	6		

- Molecule 4 is a protein called Transcription initiation factor TFIID subunit 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	523	Total	C	H	N	O	S	0	0
			8240	2632	4096	730	762	20		

- Molecule 5 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	443	Total	C	H	N	O	S	0	0
			6959	2193	3519	598	639	10		

- Molecule 6 is a protein called Putative transcription initiation factor.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	121	Total	C	H	N	O	S	0	0
			1461	578	546	170	166	1		

- Molecule 7 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	114	Total	C	H	N	O	S	0	0
			1762	556	879	157	166	4		

- Molecule 8 is a protein called Putative transcriptional coactivator HFI1 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	254	Total	C	H	N	O	S	0	0
			3898	1238	1920	346	382	12		

- Molecule 9 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	154	Total	C	H	N	O	S	0	0
			2269	744	1084	215	220	6		

- Molecule 10 is a protein called SAGA complex subunit Spt7.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	K	586	Total	C	H	N	O	S	0	0
			9479	2967	4730	857	907	18		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1197	GLY	-	expression tag	UNP G0S267
K	1198	SER	-	expression tag	UNP G0S267
K	1199	ASP	-	expression tag	UNP G0S267
K	1200	TYR	-	expression tag	UNP G0S267
K	1201	LYS	-	expression tag	UNP G0S267
K	1202	ASP	-	expression tag	UNP G0S267
K	1203	HIS	-	expression tag	UNP G0S267
K	1204	ASP	-	expression tag	UNP G0S267
K	1205	GLY	-	expression tag	UNP G0S267
K	1206	ASP	-	expression tag	UNP G0S267
K	1207	TYR	-	expression tag	UNP G0S267
K	1208	LYS	-	expression tag	UNP G0S267
K	1209	ASP	-	expression tag	UNP G0S267
K	1210	ASP	-	expression tag	UNP G0S267
K	1211	ASP	-	expression tag	UNP G0S267
K	1212	ASP	-	expression tag	UNP G0S267
K	1213	LYS	-	expression tag	UNP G0S267

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1214	GLY	-	expression tag	UNP G0S267
K	1215	LEU	-	expression tag	UNP G0S267
K	1216	GLU	-	expression tag	UNP G0S267
K	1217	ALA	-	expression tag	UNP G0S267
K	1218	SER	-	expression tag	UNP G0S267
K	1219	GLU	-	expression tag	UNP G0S267
K	1220	ASN	-	expression tag	UNP G0S267
K	1221	LEU	-	expression tag	UNP G0S267
K	1222	TYR	-	expression tag	UNP G0S267
K	1223	PHE	-	expression tag	UNP G0S267
K	1224	GLN	-	expression tag	UNP G0S267

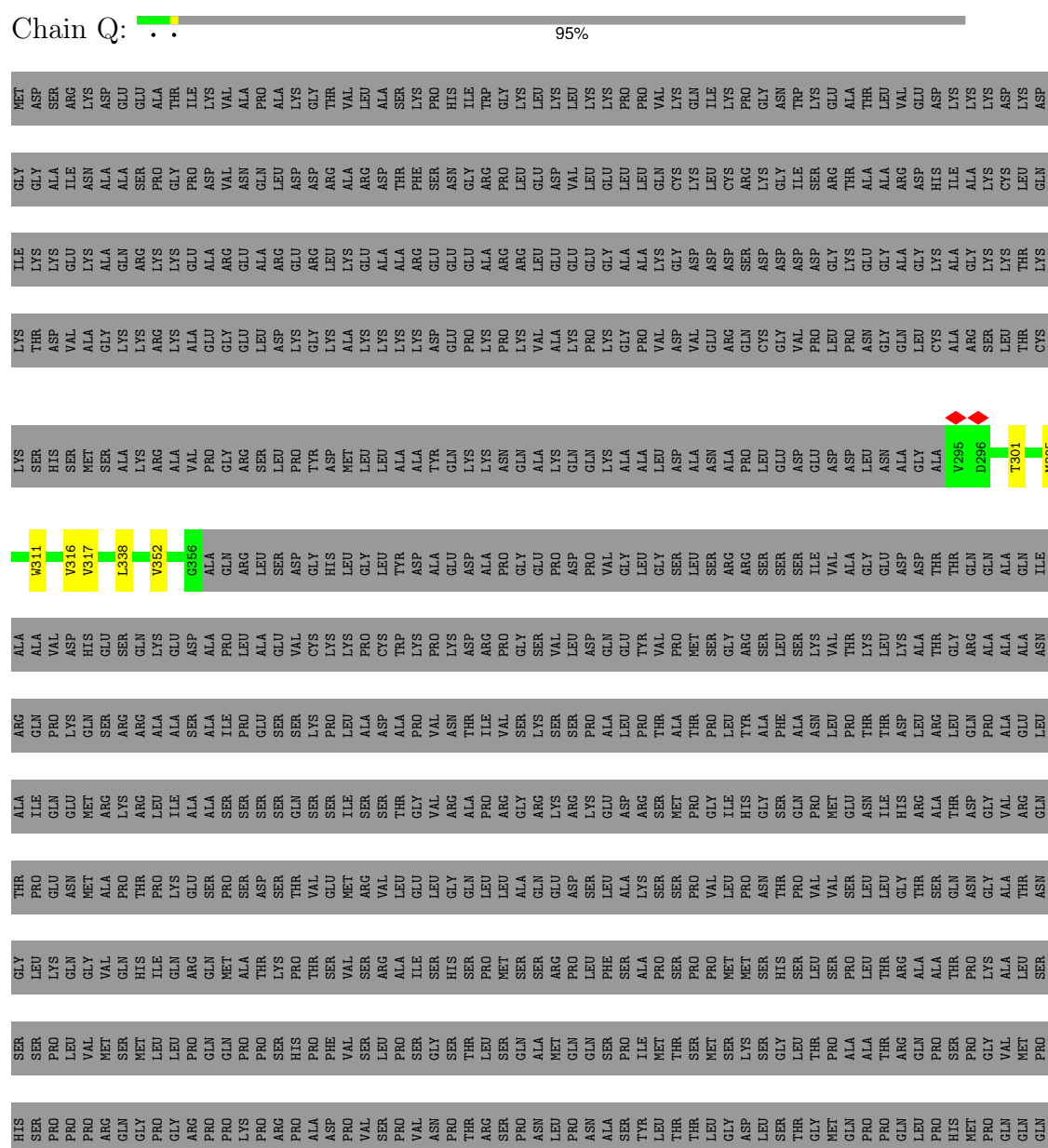
- Molecule 11 is a protein called Non-specific serine/threonine protein kinase.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	A	3619	Total	C	H	N	O	S	0	0
			58688	18811	29352	5111	5270	144		

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: SCA7 domain-containing protein



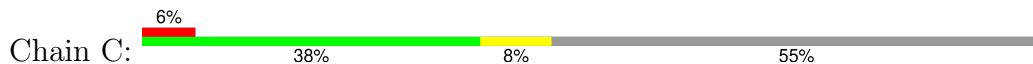
[illegible]

- Molecule 2: Spt20-like SEP domain-containing protein

[illegible]

[illegible]

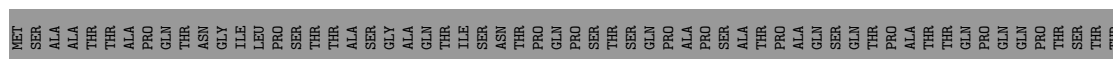
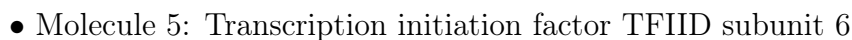
- Molecule 3: Uncharacterized protein

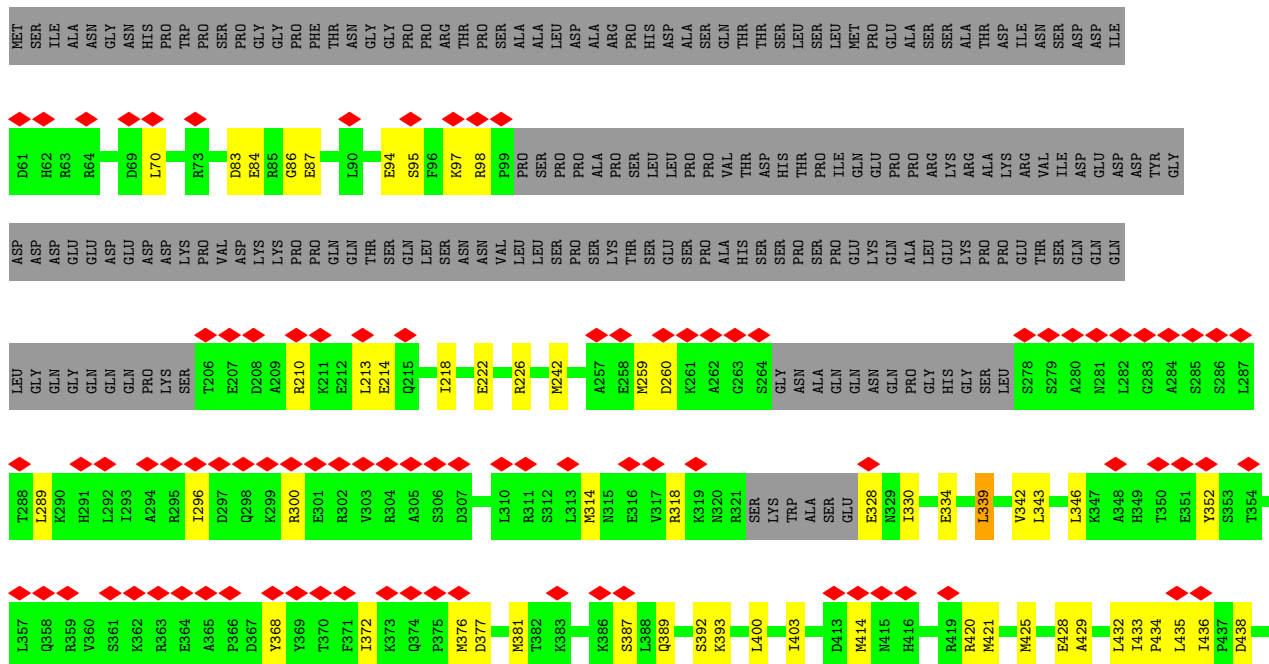
[illegible]

- Molecule 4: Transcription initiation factor TFIID subunit 5

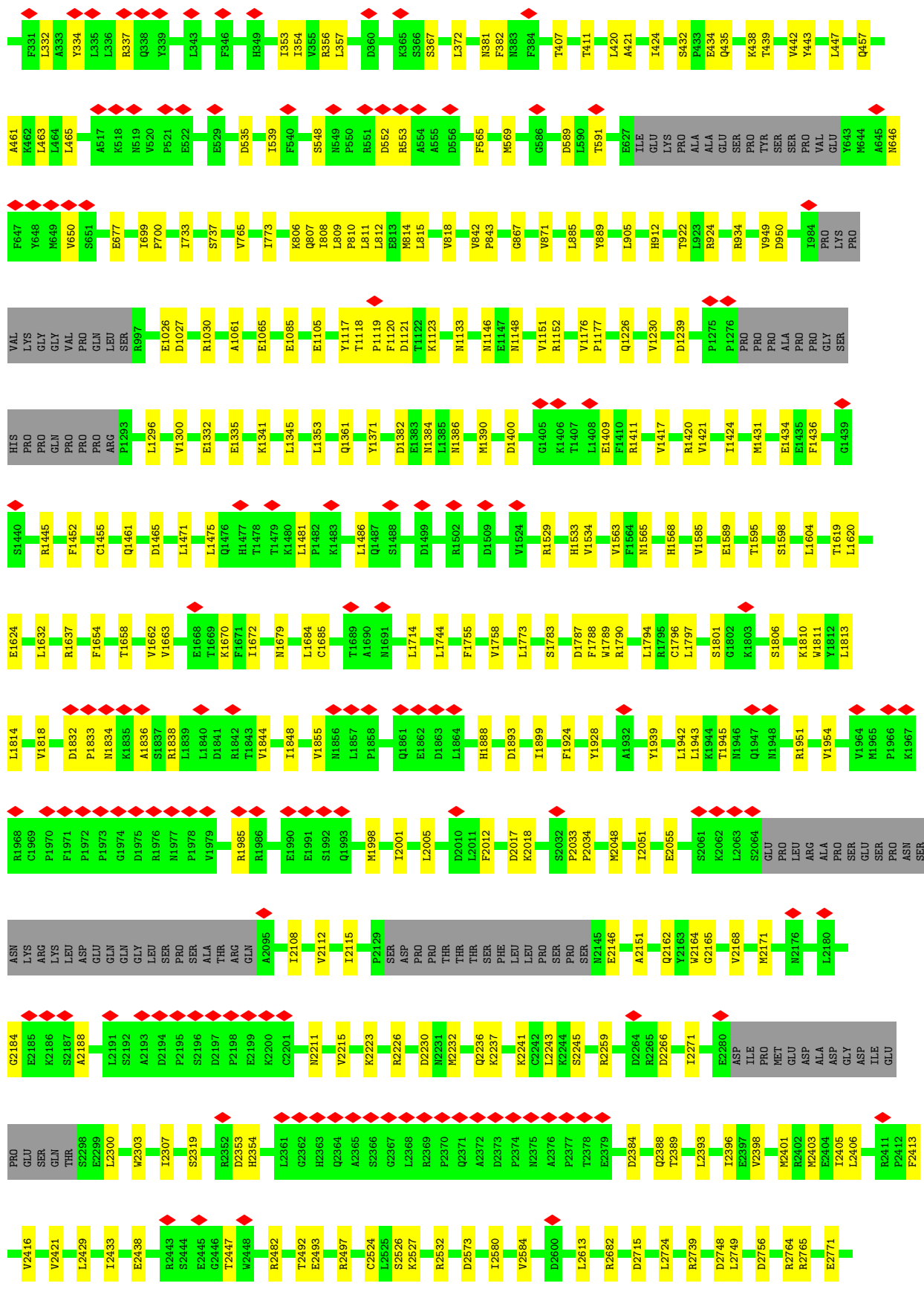


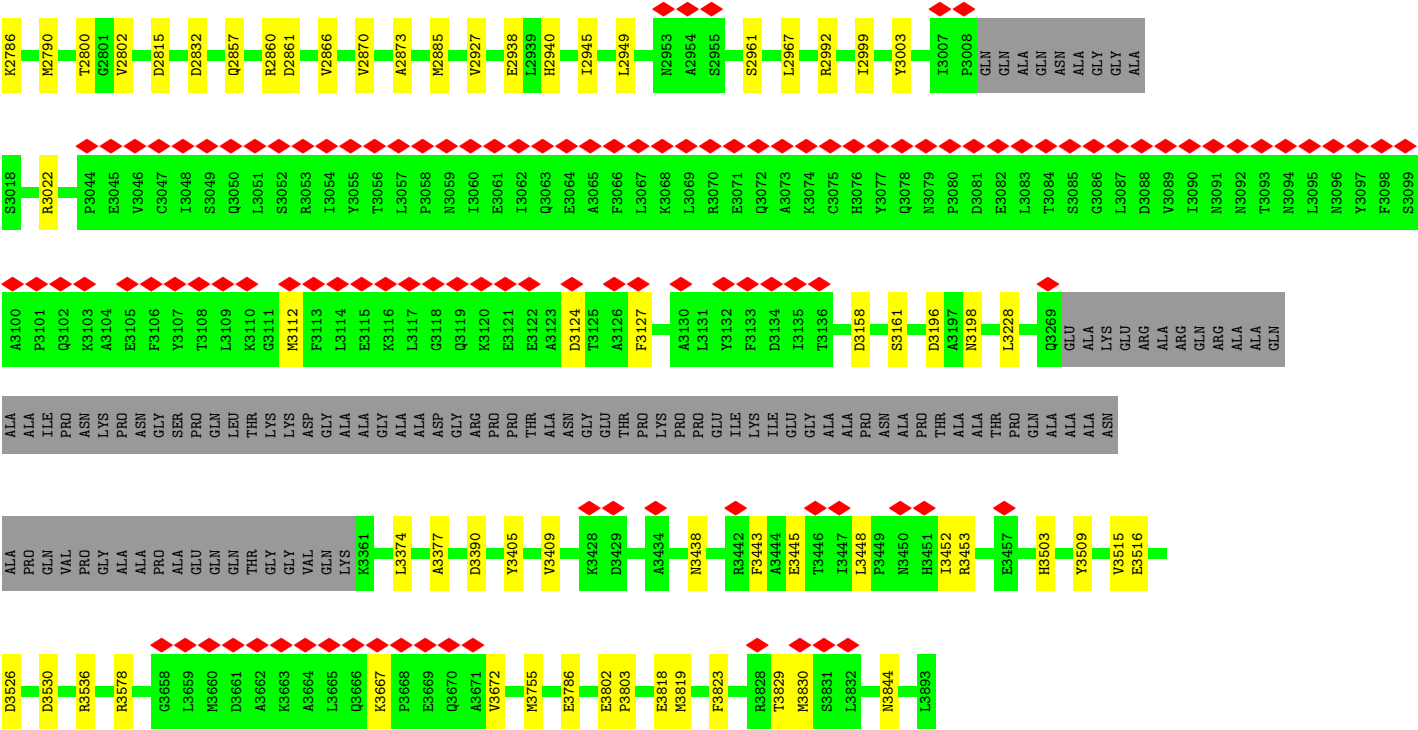
MET	SER	ASN	PRO	ALA	PRO	GLN	ALA	GLY	GLY	ALA	GLY	THR	PRO	PRO	PRO	PRO	SER	ALA	GLY	GLY	GLY	GLY	SER	GLY	SER	SER	ALA	GLY	GLY	SER	ALA	ALA	SER	ALA	PRO	THR	THR	PRO	GLN	ARG	GLN	GLU	THR	ALA	HTS	FEU
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171646	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	68.9	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.428	Depositor
Minimum map value	-2.344	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.5	Depositor
Map size (\AA)	499.68, 499.68, 499.68	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.041, 1.041, 1.041	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	Q	0.11	0/489	0.22	0/667
2	B	0.11	0/2094	0.25	0/2842
3	C	0.10	0/1649	0.24	0/2214
4	D	0.10	0/4235	0.23	0/5730
5	E	0.10	0/3505	0.23	0/4767
6	F	0.11	0/932	0.26	0/1259
7	G	0.11	0/899	0.24	0/1213
8	H	0.10	0/2018	0.22	0/2721
9	I	0.10	0/1203	0.26	0/1624
10	K	0.11	0/4824	0.24	0/6484
11	A	0.10	0/30011	0.26	0/40686
All	All	0.10	0/51859	0.25	0/70207

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	478	472	471	8	0
2	B	2035	1952	2013	17	0
3	C	1618	1607	1602	25	0
4	D	4144	4096	4088	35	0
5	E	3440	3519	3515	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	915	546	922	25	0
7	G	883	879	877	7	0
8	H	1978	1920	1917	22	0
9	I	1185	1084	1220	32	0
10	K	4749	4730	4729	71	0
11	A	29336	29352	29619	257	0
All	All	50761	50157	50973	491	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 5.

All (491) 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)
4:D:472:SER:OG	4:D:474:ASP:OD1	1.93	0.86
9:I:628:TYR:OH	11:A:2756:ASP:OD1	1.93	0.85
11:A:435:GLN:O	11:A:439:THR:HG23	1.79	0.83
2:B:400:ARG:NH2	9:I:684:GLU:OE1	2.14	0.81
2:B:220:ILE:O	11:A:2765:ARG:NH1	2.13	0.81
1:Q:338:LEU:HD21	2:B:157:MET:HE2	1.63	0.81
5:E:10:LEU:HD13	8:H:181:LEU:HD11	1.62	0.80
11:A:1888:HIS:O	11:A:1928:TYR:OH	1.99	0.80
4:D:546:HIS:ND1	4:D:548:ASN:OD1	2.14	0.80
11:A:1436:PHE:O	11:A:1445:ARG:NH1	2.16	0.79
11:A:2526:SER:O	11:A:2532:ARG:NH1	2.15	0.79
3:C:246:VAL:HG23	10:K:897:MET:HE1	1.64	0.79
11:A:1589:GLU:OE2	11:A:1598:SER:OG	2.00	0.78
5:E:203:ASP:O	5:E:214:ARG:NH1	2.16	0.78
11:A:1400:ASP:OD1	11:A:1420:ARG:NH2	2.17	0.77
11:A:1146:ASN:O	11:A:1152:ARG:NH1	2.18	0.77
5:E:466:ASN:O	5:E:470:ASN:ND2	2.17	0.77
9:I:746:GLN:N	9:I:746:GLN:OE1	2.18	0.77
11:A:1148:ASN:O	11:A:1152:ARG:NH1	2.18	0.76
10:K:428:GLU:O	10:K:432:LEU:HD12	1.85	0.76
8:H:170:LEU:O	8:H:175:ARG:NH1	2.19	0.76
11:A:773:ILE:HD13	11:A:814:MET:HE3	1.68	0.76
5:E:203:ASP:OD2	5:E:210:LYS:NZ	2.17	0.74
6:F:203:GLU:O	10:K:837:LYS:NZ	2.20	0.74
2:B:143:ARG:NH1	2:B:144:PHE:O	2.21	0.74
4:D:645:ASP:OD1	4:D:647:THR:OG1	2.05	0.73
10:K:414:MET:O	10:K:420:ARG:NH2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1585:VAL:HG21	11:A:1604:LEU:HD13	1.71	0.73
11:A:2438:GLU:OE2	11:A:2482:ARG:NH1	2.21	0.73
10:K:210:ARG:NH2	10:K:435:LEU:O	2.21	0.73
9:I:647:GLU:N	9:I:647:GLU:OE1	2.21	0.73
5:E:263:VAL:HG21	5:E:328:MET:HE1	1.70	0.72
11:A:1026:GLU:OE1	11:A:1026:GLU:N	2.22	0.72
5:E:341:ARG:NH1	10:K:86:GLY:O	2.22	0.72
10:K:222:GLU:OE2	10:K:226:ARG:NH1	2.22	0.72
11:A:2493:GLU:OE2	11:A:2497:ARG:NH1	2.22	0.72
4:D:353:ARG:O	4:D:353:ARG:NH1	2.22	0.72
6:F:68:ASP:HA	6:F:71:THR:HG22	1.70	0.72
11:A:548:SER:O	11:A:553:ARG:NH2	2.22	0.71
4:D:338:ARG:NH2	4:D:343:GLU:OE2	2.24	0.71
4:D:365:ILE:HD11	5:E:228:HIS:HB2	1.72	0.71
10:K:352:TYR:OH	10:K:577:GLN:OE1	2.08	0.71
3:C:144:VAL:O	3:C:276:ARG:NH2	2.24	0.71
5:E:476:VAL:HG13	5:E:479:LEU:HD12	1.74	0.70
11:A:126:GLU:N	11:A:126:GLU:OE1	2.24	0.70
3:C:347:GLN:NE2	8:H:300:SER:O	2.25	0.70
11:A:1758:VAL:HG13	11:A:1813:LEU:HD22	1.72	0.70
8:H:276:GLU:OE2	9:I:662:LEU:HD22	1.92	0.69
3:C:137:GLU:N	3:C:137:GLU:OE1	2.25	0.69
4:D:499:PHE:O	4:D:500:ARG:NH1	2.26	0.69
11:A:1529:ARG:O	11:A:1533:HIS:ND1	2.26	0.69
11:A:2162:GLN:N	11:A:2162:GLN:OE1	2.25	0.69
4:D:189:GLN:NE2	5:E:211:MET:SD	2.65	0.69
11:A:2303:TRP:CE2	11:A:2307:ILE:HD11	2.28	0.68
11:A:3445:GLU:O	11:A:3453:ARG:NH1	2.25	0.68
11:A:589:ASP:OD1	11:A:591:THR:HG23	1.92	0.68
11:A:2764:ARG:NH1	11:A:3786:GLU:OE2	2.25	0.68
10:K:392:SER:OG	10:K:438:ASP:OD1	2.11	0.68
3:C:413:LYS:NZ	10:K:867:GLU:OE1	2.26	0.68
11:A:270:THR:O	11:A:274:LYS:NZ	2.24	0.68
11:A:421:ALA:HB1	11:A:463:LEU:HD22	1.76	0.68
10:K:387:SER:O	10:K:389:GLN:NE2	2.27	0.67
5:E:189:GLU:N	5:E:189:GLU:OE1	2.27	0.67
10:K:882:GLU:OE1	10:K:882:GLU:N	2.27	0.67
11:A:1085:GLU:OE1	11:A:1085:GLU:N	2.27	0.67
11:A:2171:MET:O	11:A:2223:LYS:NZ	2.27	0.67
2:B:387:HIS:O	2:B:391:SER:OG	2.13	0.66
11:A:326:VAL:HG23	11:A:372:LEU:HD23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1899:ILE:HD11	11:A:1924:PHE:CD1	2.31	0.66
4:D:346:LYS:O	4:D:350:ASN:ND2	2.29	0.66
11:A:2146:GLU:N	11:A:2146:GLU:OE1	2.28	0.65
11:A:2771:GLU:N	11:A:2771:GLU:OE1	2.29	0.65
5:E:385:ASN:CG	10:K:70:LEU:HD21	2.22	0.65
10:K:377:ASP:O	10:K:381:MET:HE2	1.97	0.65
4:D:201:ARG:NH1	5:E:219:GLU:OE2	2.30	0.65
8:H:467:GLU:O	8:H:471:SER:OG	2.09	0.65
11:A:1382:ASP:OD2	11:A:1384:ASN:ND2	2.29	0.65
10:K:429:ALA:O	10:K:433:ILE:HG23	1.97	0.64
4:D:388:ASN:ND2	4:D:443:ASP:O	2.30	0.64
5:E:108:GLU:N	5:E:108:GLU:OE1	2.31	0.63
3:C:250:GLU:OE2	3:C:250:GLU:N	2.32	0.63
5:E:186:ILE:HD11	5:E:233:TYR:CE2	2.34	0.63
9:I:651:GLU:OE1	9:I:655:ASN:ND2	2.32	0.63
9:I:625:ARG:NH1	11:A:2815:ASP:OD1	2.31	0.63
11:A:1783:SER:OG	11:A:1789:TRP:NE1	2.31	0.63
11:A:2211:ASN:O	11:A:2215:VAL:HG23	1.99	0.62
5:E:183:LYS:HB3	10:K:613:VAL:HG22	1.82	0.62
10:K:871:ASP:OD1	10:K:872:ILE:N	2.33	0.62
11:A:2949:LEU:HD11	11:A:3003:TYR:CE1	2.35	0.62
11:A:1146:ASN:HD22	11:A:1151:VAL:HG11	1.65	0.61
1:Q:311:TRP:CZ3	6:F:75:LEU:HD21	2.36	0.61
11:A:1814:LEU:O	11:A:1818:VAL:HG23	2.01	0.61
8:H:160:GLU:OE1	8:H:160:GLU:N	2.33	0.61
11:A:1475:LEU:CD2	11:A:1481:LEU:HD21	2.31	0.61
11:A:57:LEU:O	11:A:61:THR:HG23	2.01	0.61
9:I:597:LYS:O	9:I:598:LEU:HD12	2.01	0.60
4:D:388:ASN:ND2	4:D:442:SER:O	2.35	0.60
10:K:586:ILE:O	10:K:590:VAL:HG23	2.02	0.60
11:A:180:ASP:OD1	11:A:181:LYS:N	2.35	0.60
11:A:1461:GLN:NE2	11:A:1465:ASP:OD1	2.34	0.60
11:A:806:LYS:O	11:A:806:LYS:HG2	2.02	0.60
3:C:268:GLN:NE2	8:H:298:SER:O	2.34	0.60
10:K:433:ILE:O	10:K:436:ILE:HG22	2.02	0.59
6:F:76:LEU:HB2	6:F:84:PHE:HZ	1.66	0.59
11:A:166:GLN:N	11:A:166:GLN:OE1	2.34	0.59
11:A:1813:LEU:O	11:A:1813:LEU:HD23	2.02	0.59
6:F:68:ASP:O	6:F:71:THR:HG22	2.02	0.59
2:B:235:TYR:CG	2:B:236:PRO:HD2	2.37	0.59
6:F:68:ASP:HA	6:F:71:THR:CG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:421:ALA:CB	11:A:463:LEU:HD22	2.33	0.59
11:A:535:ASP:OD1	11:A:535:ASP:N	2.35	0.59
11:A:1434:GLU:N	11:A:1434:GLU:OE1	2.35	0.59
10:K:566:GLY:O	10:K:570:VAL:HG23	2.03	0.59
11:A:1998:MET:SD	11:A:1998:MET:N	2.76	0.59
11:A:1714:LEU:HD12	11:A:1714:LEU:O	2.04	0.58
11:A:286:CYS:O	11:A:356:ARG:NH2	2.35	0.58
11:A:1899:ILE:HD11	11:A:1924:PHE:CE1	2.38	0.58
11:A:183:VAL:HG22	11:A:248:PHE:CZ	2.38	0.58
11:A:1758:VAL:CG1	11:A:1813:LEU:HD22	2.33	0.58
2:B:229:PRO:O	2:B:230:SER:HB3	2.03	0.58
11:A:1353:LEU:O	11:A:1361:GLN:NE2	2.35	0.58
11:A:1836:ALA:O	11:A:1838:ARG:NH2	2.37	0.58
11:A:1985:ARG:O	11:A:1985:ARG:NH1	2.36	0.58
4:D:548:ASN:ND2	4:D:550:THR:OG1	2.36	0.57
9:I:715:GLU:OE1	9:I:715:GLU:N	2.37	0.57
11:A:3448:LEU:HD22	11:A:3452:ILE:HD11	1.85	0.57
4:D:185:ILE:O	4:D:220:VAL:HG13	2.04	0.57
9:I:697:ASN:OD1	9:I:727:TYR:OH	2.22	0.57
5:E:394:LEU:O	5:E:398:ARG:N	2.36	0.57
10:K:381:MET:HE3	10:K:403:ILE:HD11	1.85	0.57
9:I:610:GLN:OE1	9:I:610:GLN:HA	2.04	0.57
11:A:3829:THR:OG1	11:A:3830:MET:N	2.37	0.57
3:C:348:GLU:OE1	3:C:400:HIS:NE2	2.38	0.57
4:D:98:LEU:HD23	4:D:98:LEU:C	2.30	0.57
8:H:298:SER:OG	8:H:333:ARG:NH2	2.37	0.57
11:A:334:TYR:O	11:A:337:ARG:NE	2.38	0.57
11:A:1844:VAL:O	11:A:1848:ILE:HG13	2.04	0.57
3:C:246:VAL:CG2	10:K:897:MET:HE1	2.34	0.57
11:A:733:ILE:O	11:A:737:SER:OG	2.15	0.57
5:E:348:CYS:HB3	5:E:369:VAL:HG23	1.88	0.56
6:F:68:ASP:CA	6:F:71:THR:HG22	2.35	0.56
11:A:773:ILE:HD11	11:A:815:LEU:HD23	1.87	0.56
5:E:476:VAL:HG12	5:E:476:VAL:O	2.05	0.56
11:A:3158:ASP:O	11:A:3161:SER:OG	2.22	0.56
11:A:2384:ASP:O	11:A:2388:GLN:NE2	2.39	0.55
11:A:443:TYR:CE2	11:A:463:LEU:HD23	2.41	0.55
11:A:2938:GLU:OE2	11:A:2992:ARG:NH2	2.37	0.55
1:Q:352:VAL:HG22	2:B:134:ILE:HD12	1.88	0.55
3:C:248:VAL:HG13	10:K:897:MET:HE2	1.88	0.55
11:A:1797:LEU:O	11:A:1801:SER:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:353:GLU:OE1	3:C:354:ARG:N	2.39	0.55
11:A:434:GLU:N	11:A:434:GLU:OE1	2.39	0.55
10:K:433:ILE:HD12	10:K:434:PRO:N	2.22	0.55
10:K:760:GLN:N	10:K:760:GLN:OE1	2.37	0.55
11:A:1105:GLU:OE1	11:A:1133:ASN:ND2	2.36	0.55
11:A:124:ALA:O	11:A:128:VAL:HG22	2.05	0.55
9:I:598:LEU:HD13	11:A:924:ARG:HG3	1.89	0.55
11:A:3755:MET:HE1	11:A:3819:MET:SD	2.47	0.55
11:A:2232:MET:HE1	11:A:2300:LEU:HD22	1.89	0.55
11:A:179:LEU:O	11:A:183:VAL:HG23	2.07	0.54
11:A:1226:GLN:O	11:A:1230:VAL:HG23	2.07	0.54
1:Q:305:MET:HE1	6:F:74:LEU:HD22	1.88	0.54
6:F:86:PRO:C	6:F:87:ARG:HG3	2.33	0.54
11:A:152:ASP:OD1	11:A:153:ILE:N	2.41	0.54
10:K:368:TYR:O	10:K:372:ILE:N	2.41	0.54
1:Q:311:TRP:CE3	6:F:75:LEU:HD21	2.43	0.54
11:A:1475:LEU:HD22	11:A:1481:LEU:HD21	1.90	0.54
11:A:3112:MET:HA	11:A:3112:MET:HE2	1.90	0.54
3:C:147:GLU:OE1	3:C:393:ARG:NH2	2.41	0.54
3:C:135:TRP:CD1	3:C:156:THR:HG21	2.43	0.53
11:A:2226:ARG:NH2	11:A:2230:ASP:OD1	2.40	0.53
11:A:3228:LEU:HD12	11:A:3228:LEU:O	2.08	0.53
5:E:442:LEU:HD12	5:E:443:THR:N	2.22	0.53
11:A:2492:THR:HG22	11:A:2493:GLU:H	1.73	0.53
11:A:2748:ASP:OD2	11:A:2748:ASP:C	2.51	0.53
3:C:329:LEU:O	3:C:333:MET:HG3	2.07	0.53
6:F:89:SER:O	6:F:93:LEU:HG	2.08	0.53
4:D:107:LEU:HD11	5:E:260:GLU:CD	2.33	0.53
11:A:1332:GLU:N	11:A:1335:GLU:OE1	2.40	0.53
11:A:2786:LYS:O	11:A:2790:MET:HG2	2.09	0.53
3:C:247:GLU:OE1	3:C:247:GLU:N	2.36	0.53
8:H:228:ARG:NH2	8:H:256:GLU:OE2	2.39	0.53
10:K:387:SER:OG	10:K:389:GLN:OE1	2.07	0.53
11:A:809:LEU:N	11:A:810:PRO:HD2	2.24	0.53
11:A:1118:THR:O	11:A:1118:THR:OG1	2.27	0.52
11:A:1998:MET:HE3	11:A:2001:ILE:HD11	1.90	0.52
11:A:100:ARG:O	11:A:104:LEU:HD13	2.08	0.52
5:E:287:SER:O	5:E:319:ARG:NH2	2.40	0.52
9:I:599:PRO:HD3	11:A:2940:HIS:NE2	2.24	0.52
11:A:3196:ASP:OD1	11:A:3198:ASN:N	2.41	0.52
11:A:842:VAL:HG22	11:A:843:PRO:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:609:ILE:HG13	9:I:609:ILE:O	2.10	0.52
11:A:814:MET:O	11:A:818:VAL:HG12	2.09	0.52
5:E:39:VAL:HG21	6:F:100:THR:CG2	2.40	0.52
9:I:675:ASP:N	9:I:675:ASP:OD1	2.42	0.52
11:A:548:SER:OG	11:A:553:ARG:NH2	2.38	0.52
9:I:599:PRO:O	9:I:601:PRO:HD3	2.10	0.52
5:E:385:ASN:ND2	10:K:70:LEU:HD21	2.25	0.52
10:K:328:GLU:OE2	10:K:444:ARG:N	2.42	0.52
11:A:1239:ASP:OD1	11:A:3509:TYR:OH	2.26	0.52
11:A:1637:ARG:NH2	11:A:1679:ASN:OD1	2.43	0.52
2:B:223:HIS:CD2	2:B:236:PRO:HB3	2.45	0.52
11:A:108:HIS:ND1	11:A:152:ASP:OD2	2.40	0.52
11:A:1390:MET:HE3	11:A:1390:MET:HA	1.91	0.52
11:A:2526:SER:OG	11:A:2527:LYS:N	2.43	0.52
11:A:2800:THR:HG22	11:A:2802:VAL:HG13	1.92	0.52
11:A:14:SER:CB	11:A:46:LYS:HZ3	2.24	0.51
11:A:2421:VAL:CG1	11:A:2433:ILE:HG21	2.40	0.51
11:A:461:ALA:O	11:A:465:LEU:HD23	2.11	0.51
5:E:59:ARG:NH1	5:E:61:THR:O	2.42	0.51
11:A:353:ILE:O	11:A:357:LEU:HG	2.09	0.51
11:A:2055:GLU:OE1	11:A:2164:TRP:NE1	2.39	0.51
11:A:1619:THR:HG21	11:A:1632:LEU:HD22	1.92	0.51
4:D:105:ASN:OD1	4:D:105:ASN:C	2.53	0.51
11:A:1794:LEU:HD21	11:A:1844:VAL:HG12	1.92	0.51
10:K:334:GLU:OE1	10:K:334:GLU:N	2.44	0.51
11:A:2384:ASP:OD1	11:A:2388:GLN:NE2	2.44	0.51
7:G:69:ILE:HD11	10:K:797:ILE:HG13	1.91	0.51
9:I:663:VAL:HG11	9:I:678:MET:CB	2.41	0.51
11:A:3443:PHE:CZ	11:A:3448:LEU:HD21	2.46	0.51
10:K:214:GLU:O	10:K:218:ILE:HG12	2.11	0.51
11:A:1790:ARG:O	11:A:1794:LEU:HD23	2.11	0.51
6:F:142:ASN:ND2	9:I:708:GLU:OE1	2.41	0.50
11:A:2017:ASP:OD1	11:A:2018:LYS:N	2.43	0.50
10:K:97:LYS:O	10:K:97:LYS:NZ	2.40	0.50
10:K:342:VAL:O	10:K:346:LEU:HG	2.11	0.50
11:A:1619:THR:HG21	11:A:1632:LEU:CD2	2.41	0.50
11:A:69:PHE:O	11:A:73:VAL:HG13	2.12	0.50
11:A:773:ILE:CD1	11:A:814:MET:HE3	2.39	0.50
11:A:1239:ASP:OD2	11:A:3536:ARG:NH2	2.42	0.50
3:C:135:TRP:CD1	3:C:139:CYS:HG	2.30	0.50
4:D:658:ASP:OD1	4:D:660:ASN:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:260:ASP:OD1	10:K:260:ASP:N	2.45	0.50
10:K:84:GLU:OE1	10:K:642:LYS:NZ	2.41	0.50
6:F:68:ASP:C	6:F:71:THR:HG22	2.37	0.49
10:K:400:LEU:HA	10:K:403:ILE:HD12	1.93	0.49
11:A:457:GLN:N	11:A:457:GLN:OE1	2.45	0.49
11:A:1755:PHE:HE1	11:A:1814:LEU:HD11	1.77	0.49
10:K:433:ILE:N	10:K:434:PRO:CD	2.75	0.49
11:A:2492:THR:HG22	11:A:2493:GLU:N	2.27	0.49
8:H:464:GLU:OE1	8:H:464:GLU:N	2.45	0.49
11:A:179:LEU:C	11:A:179:LEU:HD12	2.37	0.49
11:A:2866:VAL:O	11:A:2870:VAL:HG22	2.12	0.49
11:A:1386:ASN:O	11:A:1390:MET:HG2	2.12	0.49
5:E:255:MET:HE2	5:E:255:MET:HA	1.94	0.49
11:A:677:GLU:OE1	11:A:1595:THR:N	2.45	0.49
2:B:234:PRO:O	2:B:235:TYR:HB2	2.11	0.49
11:A:47:ALA:HB2	11:A:99:LEU:CD1	2.43	0.49
11:A:447:LEU:HD23	11:A:447:LEU:O	2.13	0.49
11:A:2108:ILE:O	11:A:2112:VAL:HG23	2.13	0.49
5:E:244:HIS:NE2	10:K:242:MET:HE1	2.28	0.49
10:K:702:ASP:OD1	10:K:704:GLU:N	2.45	0.49
11:A:1796:CYS:SG	11:A:1814:LEU:HD12	2.53	0.49
11:A:2724:LEU:CD1	11:A:2749:LEU:HD12	2.42	0.49
11:A:332:LEU:C	11:A:332:LEU:HD23	2.37	0.49
10:K:732:ARG:O	10:K:733:ARG:HB3	2.13	0.49
11:A:1121:ASP:O	11:A:1123:LYS:NZ	2.35	0.49
11:A:3823:PHE:HB3	11:A:3829:THR:HG22	1.95	0.48
3:C:346:GLU:OE2	3:C:347:GLN:N	2.47	0.48
11:A:438:LYS:O	11:A:442:VAL:HG23	2.13	0.48
5:E:279:ALA:HB3	5:E:280:PRO:HD3	1.96	0.48
11:A:2393:LEU:HD12	11:A:2429:LEU:HD13	1.96	0.48
2:B:466:ILE:HD11	11:A:2832:ASP:HB2	1.96	0.48
11:A:78:ILE:HG23	11:A:130:LEU:HD13	1.94	0.48
1:Q:301:THR:OG1	8:H:167:VAL:HG21	2.14	0.48
4:D:136:ASP:OD1	4:D:136:ASP:N	2.45	0.48
5:E:223:SER:O	5:E:223:SER:OG	2.28	0.48
9:I:663:VAL:HG11	9:I:678:MET:HB3	1.96	0.48
11:A:1855:VAL:O	11:A:1855:VAL:HG13	2.12	0.48
9:I:600:ILE:HD11	11:A:924:ARG:NH2	2.28	0.48
11:A:57:LEU:O	11:A:61:THR:N	2.46	0.48
11:A:2115:ILE:HD13	11:A:2151:ALA:CB	2.43	0.48
11:A:2165:GLY:O	11:A:2168:VAL:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:183:VAL:HG22	11:A:248:PHE:HZ	1.77	0.48
11:A:1951:ARG:HH21	11:A:1954:VAL:HG11	1.79	0.48
11:A:3530:ASP:OD1	11:A:3530:ASP:N	2.43	0.48
4:D:629:SER:OG	4:D:749:VAL:HG22	2.13	0.48
7:G:186:LEU:O	7:G:190:VAL:HG22	2.14	0.48
11:A:134:LEU:O	11:A:138:ASP:N	2.38	0.48
11:A:140:GLU:HA	11:A:143:VAL:HG22	1.95	0.48
11:A:1027:ASP:OD2	11:A:1030:ARG:NH1	2.47	0.48
11:A:2961:SER:O	11:A:3022:ARG:NH1	2.47	0.48
1:Q:305:MET:HE3	8:H:163:LEU:HD11	1.95	0.47
11:A:1744:LEU:O	11:A:1744:LEU:HD12	2.14	0.47
11:A:179:LEU:HD21	11:A:283:ALA:HB2	1.96	0.47
11:A:905:LEU:HD22	11:A:922:THR:HG23	1.95	0.47
6:F:85:GLU:O	6:F:88:VAL:HG23	2.14	0.47
9:I:709:ARG:NH2	9:I:715:GLU:OE2	2.47	0.47
11:A:2860:ARG:HB2	11:A:2885:MET:HE1	1.95	0.47
10:K:296:ILE:O	10:K:300:ARG:N	2.47	0.47
5:E:183:LYS:CB	10:K:613:VAL:HG22	2.44	0.47
4:D:200:GLU:OE1	4:D:351:ARG:NH1	2.48	0.47
5:E:90:TYR:CG	6:F:66:PRO:HD3	2.49	0.47
6:F:76:LEU:CB	6:F:84:PHE:HZ	2.27	0.47
11:A:3405:TYR:O	11:A:3409:VAL:HG23	2.15	0.47
5:E:285:LEU:O	5:E:319:ARG:NH1	2.48	0.47
10:K:594:ASP:OD2	10:K:679:ALA:N	2.47	0.47
4:D:195:LEU:HD23	4:D:199:LEU:HD23	1.97	0.47
5:E:449:VAL:O	5:E:453:LEU:N	2.42	0.47
10:K:421:MET:O	10:K:425:MET:HG3	2.15	0.47
11:A:1998:MET:HE3	11:A:1998:MET:HA	1.97	0.47
11:A:3667:LYS:HE3	11:A:3672:VAL:HG13	1.96	0.46
4:D:104:ASP:OD2	4:D:104:ASP:N	2.48	0.46
5:E:409:TYR:O	5:E:413:VAL:HG23	2.15	0.46
3:C:141:MET:HE1	3:C:296:PHE:HD1	1.80	0.46
11:A:1534:VAL:CG2	11:A:1563:VAL:HG11	2.44	0.46
4:D:419:GLU:OE2	4:D:419:GLU:HA	2.14	0.46
5:E:207:ASP:OD1	5:E:208:GLU:N	2.49	0.46
5:E:270:ILE:O	5:E:270:ILE:HG22	2.16	0.46
4:D:221:GLU:N	4:D:221:GLU:OE1	2.49	0.46
10:K:580:GLU:OE1	10:K:580:GLU:HA	2.15	0.46
11:A:69:PHE:O	11:A:73:VAL:HG22	2.15	0.46
1:Q:316:VAL:HG12	1:Q:317:VAL:HG13	1.97	0.46
11:A:2048:MET:O	11:A:2051:ILE:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:504:GLY:N	4:D:509:TYR:O	2.49	0.46
11:A:2405:ILE:HD12	11:A:2405:ILE:O	2.15	0.46
11:A:2353:ASP:OD1	11:A:2354:HIS:N	2.48	0.46
11:A:2580:ILE:O	11:A:2584:VAL:HG22	2.16	0.46
9:I:658:LYS:O	9:I:662:LEU:HG	2.16	0.46
11:A:1061:ALA:O	11:A:1065:GLU:HG2	2.16	0.45
11:A:1119:PRO:C	11:A:1120:PHE:HD1	2.24	0.45
11:A:2184:GLY:O	11:A:2188:ALA:N	2.43	0.45
11:A:2682:ARG:HA	11:A:2682:ARG:NE	2.31	0.45
11:A:3802:GLU:CB	11:A:3803:PRO:HD3	2.46	0.45
10:K:83:ASP:OD1	10:K:87:GLU:N	2.42	0.45
11:A:2115:ILE:HD13	11:A:2151:ALA:HB3	1.98	0.45
11:A:2245:SER:O	11:A:2319:SER:OG	2.34	0.45
11:A:2398:VAL:HA	11:A:2401:MET:HE2	1.98	0.45
3:C:345:LYS:NZ	3:C:395:PRO:O	2.50	0.45
11:A:1942:LEU:HD22	11:A:1954:VAL:HG13	1.98	0.45
11:A:2403:MET:SD	11:A:2406:LEU:HD12	2.56	0.45
10:K:343:LEU:HD12	10:K:343:LEU:O	2.17	0.45
11:A:1893:ASP:N	11:A:1893:ASP:OD1	2.48	0.45
9:I:609:ILE:HG22	11:A:912:HIS:CG	2.51	0.45
11:A:1431:MET:HA	11:A:1431:MET:HE2	1.99	0.45
6:F:67:ARG:C	6:F:69:ALA:H	2.25	0.45
11:A:812:LEU:O	11:A:812:LEU:HG	2.17	0.45
9:I:615:VAL:HG11	11:A:2873:ALA:HA	1.99	0.45
10:K:87:GLU:OE1	10:K:87:GLU:HA	2.16	0.45
11:A:178:GLN:NE2	11:A:245:MET:O	2.44	0.45
11:A:3578:ARG:NH1	11:A:3818:GLU:OE1	2.49	0.45
5:E:442:LEU:HD12	5:E:443:THR:HG23	1.99	0.45
11:A:139:ASN:O	11:A:143:VAL:HG22	2.16	0.45
8:H:259:LEU:HD21	9:I:707:LYS:HB2	1.99	0.44
10:K:259:MET:SD	10:K:260:ASP:N	2.90	0.44
10:K:328:GLU:O	10:K:444:ARG:N	2.48	0.44
2:B:349:PRO:O	2:B:352:ILE:HG22	2.18	0.44
11:A:177:GLU:HG3	11:A:279:LEU:HD21	2.00	0.44
11:A:2005:LEU:HD11	11:A:2012:PHE:CD2	2.51	0.44
4:D:107:LEU:HD11	5:E:260:GLU:OE1	2.18	0.44
11:A:811:LEU:O	11:A:811:LEU:HD12	2.17	0.44
11:A:432:SER:N	11:A:435:GLN:OE1	2.41	0.44
11:A:934:ARG:HD2	11:A:2927:VAL:HG13	1.99	0.44
6:F:67:ARG:C	6:F:68:ASP:OD1	2.61	0.44
5:E:10:LEU:CD1	8:H:181:LEU:HD11	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:597:LYS:C	9:I:598:LEU:HD12	2.43	0.44
11:A:552:ASP:N	11:A:552:ASP:OD1	2.51	0.44
5:E:276:ALA:HB2	10:K:686:PRO:HG3	1.99	0.44
11:A:97:GLN:O	11:A:101:ASN:ND2	2.43	0.44
11:A:2682:ARG:NH1	11:A:2715:ASP:OD2	2.51	0.44
11:A:1481:LEU:HD22	11:A:1486:LEU:HD21	1.99	0.44
4:D:592:ASN:OD1	4:D:593:GLY:N	2.51	0.43
5:E:393:VAL:HG23	5:E:394:LEU:N	2.33	0.43
9:I:610:GLN:O	9:I:611:MET:HB3	2.17	0.43
2:B:235:TYR:CD2	2:B:236:PRO:HD2	2.53	0.43
2:B:351:ASN:O	2:B:355:VAL:HG23	2.19	0.43
4:D:98:LEU:HD23	4:D:98:LEU:O	2.19	0.43
5:E:327:SER:HB2	5:E:371:ALA:HB1	2.01	0.43
11:A:1565:ASN:O	11:A:1568:HIS:ND1	2.52	0.43
11:A:2033:PRO:N	11:A:2034:PRO:CD	2.81	0.43
11:A:407:THR:O	11:A:411:THR:OG1	2.28	0.43
5:E:138:VAL:HG21	10:K:620:ARG:HB3	2.00	0.43
8:H:467:GLU:N	8:H:468:PRO:HD2	2.33	0.43
11:A:765:VAL:CG1	11:A:807:GLN:HG2	2.49	0.43
11:A:3526:ASP:OD1	11:A:3526:ASP:N	2.52	0.43
4:D:442:SER:OG	4:D:443:ASP:N	2.51	0.43
11:A:420:LEU:HD23	11:A:424:ILE:HD12	2.00	0.43
11:A:539:ILE:HD13	11:A:1773:LEU:HD22	2.01	0.43
11:A:1417:VAL:O	11:A:1421:VAL:HG23	2.19	0.43
11:A:1624:GLU:O	11:A:1672:ILE:HG21	2.19	0.43
3:C:354:ARG:NH2	8:H:336:MET:SD	2.92	0.42
5:E:185:VAL:HG23	5:E:186:ILE:N	2.34	0.42
7:G:69:ILE:HG22	10:K:731:THR:HG22	2.00	0.42
11:A:1341:LYS:HG3	11:A:1345:LEU:HD12	2.01	0.42
11:A:2389:THR:O	11:A:2393:LEU:HD13	2.17	0.42
11:A:3390:ASP:OD2	11:A:3390:ASP:C	2.60	0.42
3:C:283:GLU:OE2	11:A:2447:THR:OG1	2.25	0.42
11:A:47:ALA:HB2	11:A:99:LEU:HD12	2.00	0.42
11:A:1411:ARG:NH1	11:A:1411:ARG:HG2	2.33	0.42
10:K:613:VAL:O	10:K:613:VAL:HG13	2.18	0.42
11:A:565:PHE:CE1	11:A:569:MET:HE3	2.55	0.42
11:A:1684:LEU:O	11:A:1685:CYS:SG	2.77	0.42
4:D:340:VAL:O	4:D:341:VAL:HB	2.19	0.42
11:A:1832:ASP:O	11:A:1834:ASN:N	2.46	0.42
11:A:2413:PHE:O	11:A:2416:VAL:HG12	2.19	0.42
10:K:95:SER:OG	10:K:98:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:806:LYS:HB2	11:A:806:LYS:HE3	1.84	0.42
11:A:1658:THR:O	11:A:1662:VAL:HG23	2.18	0.42
11:A:1663:VAL:HG23	11:A:1670:LYS:HB2	2.02	0.42
4:D:187:LEU:HD12	4:D:220:VAL:HG11	2.01	0.42
4:D:649:ARG:NH1	4:D:735:GLN:OE1	2.53	0.42
11:A:144:ILE:HG23	11:A:145:LEU:N	2.33	0.42
11:A:57:LEU:C	11:A:61:THR:HG23	2.45	0.42
11:A:3124:ASP:HA	11:A:3127:PHE:CZ	2.55	0.42
10:K:747:LEU:HD22	10:K:894:HIS:CE1	2.55	0.42
11:A:2243:LEU:HD21	11:A:2271:ILE:HD11	2.02	0.42
10:K:584:TYR:CD1	10:K:584:TYR:C	2.98	0.42
11:A:151:SER:HB3	11:A:257:ILE:HG23	2.01	0.42
11:A:2945:ILE:CG1	11:A:2967:LEU:HD23	2.50	0.42
2:B:139:GLN:O	2:B:197:ARG:NH1	2.49	0.42
6:F:83:SER:OG	6:F:84:PHE:N	2.53	0.42
7:G:103:GLN:HG3	10:K:797:ILE:HD11	2.02	0.42
8:H:389:ASN:OD1	8:H:389:ASN:N	2.53	0.42
10:K:330:ILE:HD11	10:K:444:ARG:HD3	2.00	0.42
11:A:699:ILE:HB	11:A:700:PRO:HD3	2.02	0.42
11:A:177:GLU:CG	11:A:279:LEU:HD21	2.51	0.41
9:I:649:GLU:OE1	9:I:653:VAL:HG11	2.20	0.41
11:A:166:GLN:O	11:A:169:LEU:HG	2.20	0.41
11:A:867:GLY:O	11:A:871:VAL:HG23	2.20	0.41
11:A:1452:PHE:HB3	11:A:1471:LEU:HD13	2.01	0.41
11:A:1620:LEU:HD13	11:A:1654:PHE:HE1	1.85	0.41
11:A:2259:ARG:NH2	11:A:2266:ASP:OD1	2.53	0.41
3:C:385:LEU:HD12	11:A:2524:CYS:CB	2.50	0.41
5:E:380:VAL:HG12	5:E:380:VAL:O	2.19	0.41
7:G:181:LEU:HD22	10:K:798:PHE:CD2	2.56	0.41
11:A:1787:ASP:O	11:A:1788:PHE:HB3	2.19	0.41
11:A:2232:MET:SD	11:A:2236:GLN:NE2	2.89	0.41
11:A:2857:GLN:NE2	11:A:2861:ASP:OD1	2.53	0.41
2:B:217:PRO:O	11:A:2739:ARG:NH1	2.53	0.41
3:C:330:THR:O	3:C:334:VAL:HG23	2.20	0.41
10:K:339:LEU:O	10:K:342:VAL:HG22	2.20	0.41
11:A:885:LEU:HD22	11:A:889:TYR:CD2	2.56	0.41
11:A:1424:ILE:HD11	11:A:1455:CYS:SG	2.61	0.41
3:C:408:LEU:HD21	8:H:305:LEU:HD13	2.02	0.41
11:A:1296:LEU:O	11:A:1300:VAL:HG23	2.21	0.41
11:A:2300:LEU:HD12	11:A:2300:LEU:O	2.19	0.41
6:F:67:ARG:HD3	8:H:174:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:116:PRO:N	11:A:117:PRO:HD2	2.36	0.41
11:A:169:LEU:HD22	11:A:272:ASN:ND2	2.35	0.41
9:I:600:ILE:HD11	11:A:924:ARG:HH21	1.86	0.41
10:K:213:LEU:HD23	10:K:213:LEU:C	2.46	0.41
10:K:791:GLN:HE21	10:K:811:LEU:HD23	1.86	0.41
11:A:1939:TYR:CZ	11:A:1943:LEU:HD11	2.55	0.41
11:A:3819:MET:SD	11:A:3844:ASN:ND2	2.94	0.41
10:K:376:MET:HB2	10:K:381:MET:HE1	2.03	0.41
10:K:806:LEU:C	10:K:806:LEU:HD12	2.46	0.41
11:A:176:PHE:O	11:A:179:LEU:HD23	2.20	0.41
11:A:2237:LYS:O	11:A:2241:LYS:NZ	2.54	0.41
11:A:2800:THR:CG2	11:A:2802:VAL:HG13	2.51	0.41
4:D:340:VAL:HG12	4:D:341:VAL:N	2.35	0.41
5:E:442:LEU:HD21	5:E:465:ARG:CZ	2.50	0.41
6:F:76:LEU:HD13	6:F:84:PHE:HE1	1.86	0.41
9:I:605:HIS:CD2	9:I:607:LYS:HB3	2.56	0.41
10:K:94:GLU:OE2	10:K:94:GLU:HA	2.21	0.41
10:K:314:MET:O	10:K:318:ARG:N	2.52	0.41
11:A:949:VAL:O	11:A:949:VAL:HG12	2.20	0.41
11:A:1833:PRO:O	11:A:1834:ASN:C	2.64	0.41
11:A:3515:VAL:HG12	11:A:3516:GLU:N	2.36	0.41
7:G:182:THR:HG22	7:G:185:ASP:OD2	2.20	0.41
10:K:381:MET:SD	10:K:381:MET:N	2.94	0.41
11:A:54:ARG:HB2	11:A:106:ILE:HD11	2.02	0.41
11:A:1806:SER:O	11:A:1811:TRP:NE1	2.54	0.41
2:B:235:TYR:CD1	2:B:236:PRO:HD2	2.56	0.40
5:E:446:GLY:O	5:E:450:ILE:HG13	2.21	0.40
6:F:86:PRO:O	6:F:87:ARG:HG3	2.21	0.40
11:A:646:ASN:OD1	11:A:650:VAL:HG13	2.21	0.40
11:A:3667:LYS:CE	11:A:3672:VAL:HG13	2.51	0.40
3:C:346:GLU:C	3:C:346:GLU:CD	2.90	0.40
10:K:393:LYS:HD2	10:K:436:ILE:HG23	2.03	0.40
11:A:1810:LYS:O	11:A:1814:LEU:HD23	2.21	0.40
5:E:39:VAL:HG21	6:F:100:THR:HG23	2.02	0.40
6:F:81:VAL:HG12	6:F:83:SER:O	2.21	0.40
7:G:87:PRO:N	7:G:88:PRO:CD	2.84	0.40
8:H:194:ASN:OD1	8:H:194:ASN:N	2.54	0.40
8:H:466:ALA:O	8:H:470:THR:HG22	2.21	0.40
9:I:598:LEU:HA	9:I:599:PRO:HD3	1.89	0.40
11:A:152:ASP:OD1	11:A:152:ASP:C	2.63	0.40
11:A:934:ARG:CD	11:A:2927:VAL:HG13	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:461:ILE:HA	5:E:464:LEU:HG	2.02	0.40
8:H:246:ILE:O	8:H:250:MET:HG3	2.21	0.40
9:I:674:GLN:OE1	9:I:675:ASP:N	2.54	0.40
11:A:145:LEU:H	11:A:145:LEU:HD12	1.86	0.40
11:A:260:SER:O	11:A:264:VAL:HG23	2.21	0.40
11:A:381:ASN:OD1	11:A:381:ASN:C	2.64	0.40
11:A:381:ASN:OD1	11:A:382:PHE:N	2.55	0.40
11:A:950:ASP:OD1	11:A:950:ASP:N	2.55	0.40
11:A:1176:VAL:N	11:A:1177:PRO:HD2	2.36	0.40
4:D:389:ASP:OD1	4:D:389:ASP:N	2.55	0.40
10:K:579:TYR:O	10:K:579:TYR:CG	2.75	0.40
11:A:183:VAL:HG22	11:A:248:PHE:CE1	2.57	0.40
11:A:3374:LEU:O	11:A:3377:ALA:O	2.39	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	Q	60/1273 (5%)	60 (100%)	0	0	100	100
2	B	233/1192 (20%)	221 (95%)	11 (5%)	1 (0%)	30	64
3	C	189/433 (44%)	184 (97%)	5 (3%)	0	100	100
4	D	509/767 (66%)	488 (96%)	21 (4%)	0	100	100
5	E	435/480 (91%)	428 (98%)	7 (2%)	0	100	100
6	F	117/277 (42%)	110 (94%)	7 (6%)	0	100	100
7	G	110/204 (54%)	107 (97%)	3 (3%)	0	100	100
8	H	248/485 (51%)	243 (98%)	5 (2%)	0	100	100
9	I	148/770 (19%)	140 (95%)	8 (5%)	0	100	100
10	K	572/1224 (47%)	556 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	A	3597/3893 (92%)	3433 (95%)	164 (5%)	0	100	100
All	All	6218/10998 (56%)	5970 (96%)	247 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	230	SER

5.3.2 Protein sidechains [i](#)

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	Q	50/1047 (5%)	50 (100%)	0	100	100
2	B	227/928 (24%)	227 (100%)	0	100	100
3	C	173/377 (46%)	171 (99%)	2 (1%)	67	85
4	D	450/635 (71%)	449 (100%)	1 (0%)	92	97
5	E	375/401 (94%)	371 (99%)	4 (1%)	70	86
6	F	92/212 (43%)	90 (98%)	2 (2%)	47	73
7	G	90/157 (57%)	90 (100%)	0	100	100
8	H	206/387 (53%)	206 (100%)	0	100	100
9	I	129/620 (21%)	128 (99%)	1 (1%)	79	90
10	K	506/1023 (50%)	502 (99%)	4 (1%)	79	90
11	A	3197/3412 (94%)	3184 (100%)	13 (0%)	89	94
All	All	5495/9199 (60%)	5468 (100%)	27 (0%)	85	93

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	136	PHE
3	C	285	TYR
4	D	751	PHE

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Mol	Chain	Res	Type
5	E	30	GLU
5	E	277	LEU
5	E	450	ILE
5	E	471	ARG
6	F	100	THR
6	F	108	LEU
9	I	623	SER
10	K	289	LEU
10	K	339	LEU
10	K	581	ASP
10	K	747	LEU
11	A	354	ILE
11	A	367	SER
11	A	808	ILE
11	A	1117	TYR
11	A	1371	TYR
11	A	1409	GLU
11	A	1945	THR
11	A	2396	ILE
11	A	2573	ASP
11	A	2613	LEU
11	A	2999	ILE
11	A	3438	ASN
11	A	3503	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	335	HIS
2	B	139	GLN
2	B	196	HIS
2	B	221	HIS
2	B	223	HIS
2	B	293	GLN
2	B	296	HIS
4	D	46	ASN
4	D	148	HIS
4	D	197	HIS
5	E	131	HIS
5	E	470	ASN
8	H	313	HIS
9	I	635	GLN

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Mol	Chain	Res	Type
9	I	701	GLN
10	K	245	GLN
10	K	772	HIS
10	K	868	ASN
10	K	894	HIS
11	A	114	GLN
11	A	349	HIS
11	A	764	HIS
11	A	873	GLN
11	A	1006	GLN
11	A	1554	ASN
11	A	1596	HIS
11	A	1807	GLN
11	A	1927	HIS
11	A	1947	GLN
11	A	1977	ASN
11	A	2105	HIS
11	A	2478	ASN
11	A	2705	HIS
11	A	2822	GLN
11	A	2891	HIS
11	A	2993	GLN
11	A	3223	GLN
11	A	3269	GLN
11	A	3584	GLN
11	A	3588	GLN
11	A	3735	HIS
11	A	3738	ASN
11	A	3745	ASN
11	A	3825	ASN
11	A	3844	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

There are no chain breaks in this entry.

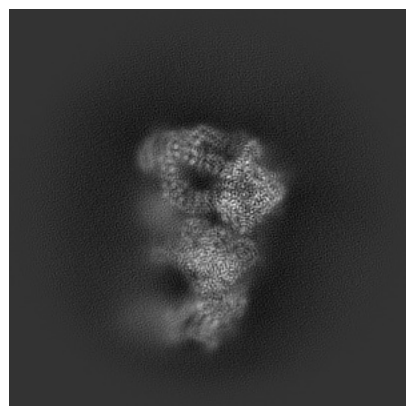
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73233. These allow visual inspection of the internal detail of the map and identification of artifacts.

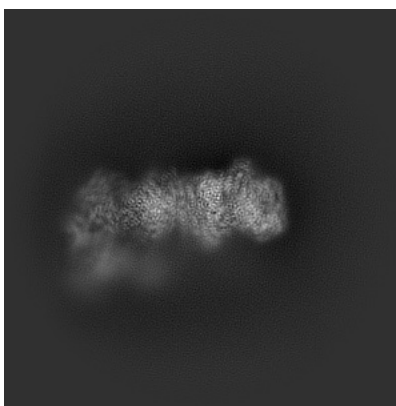
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

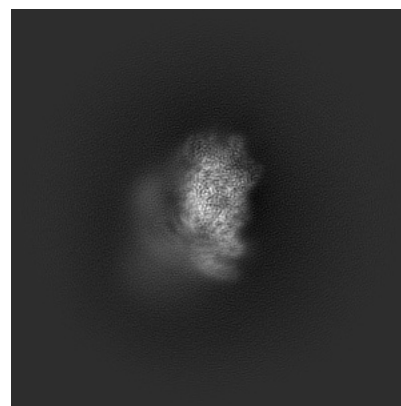
6.1.1 Primary map



X

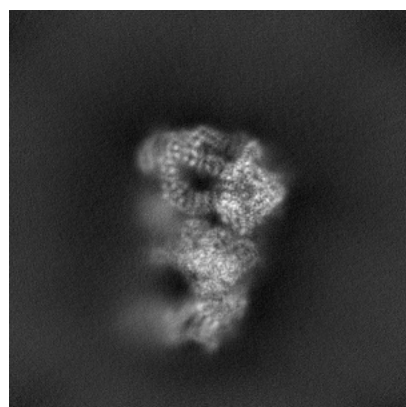


Y

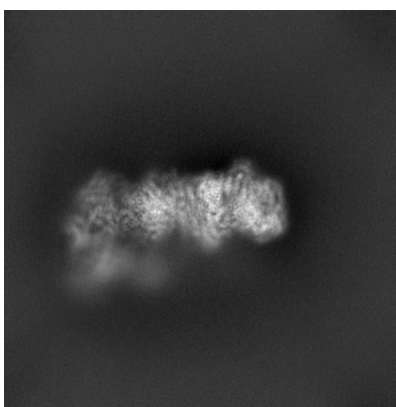


Z

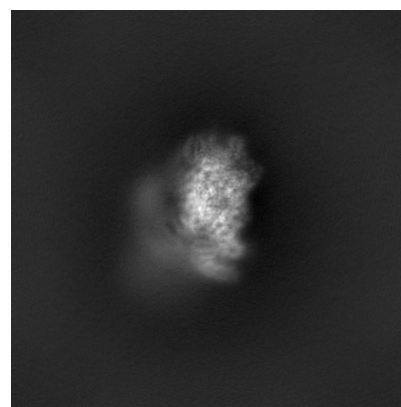
6.1.2 Raw map



X



Y

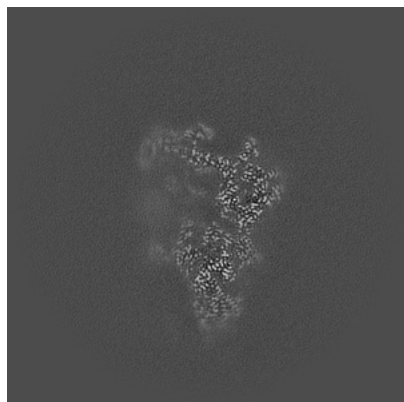


Z

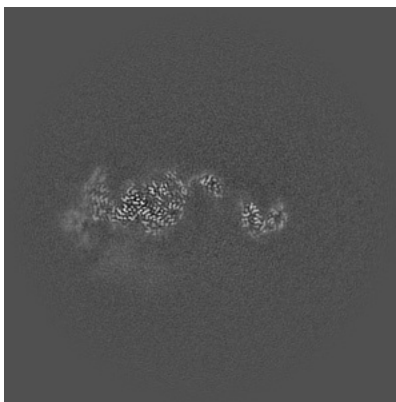
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

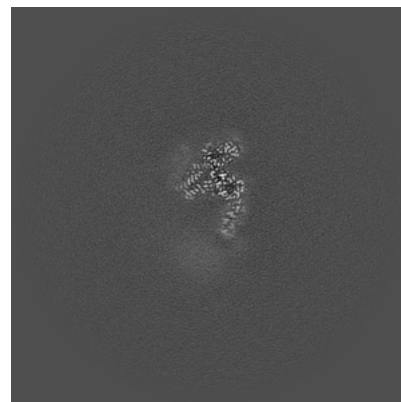
6.2.1 Primary map



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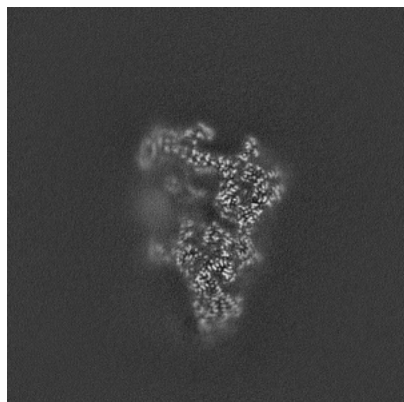


Y Index: 240

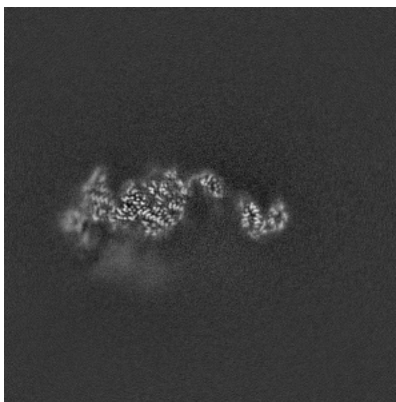


Z Index: 240

6.2.2 Raw map



X Index: 240



Y Index: 240

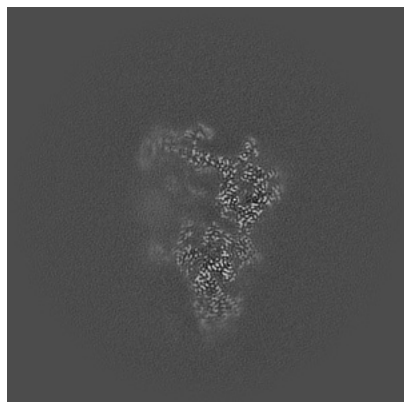


Z Index: 240

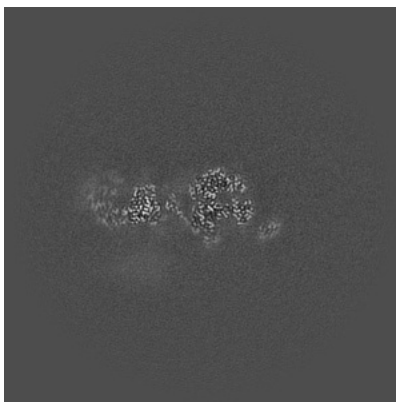
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

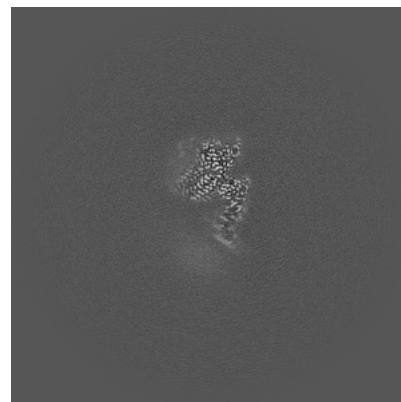
6.3.1 Primary map



X Index: 240

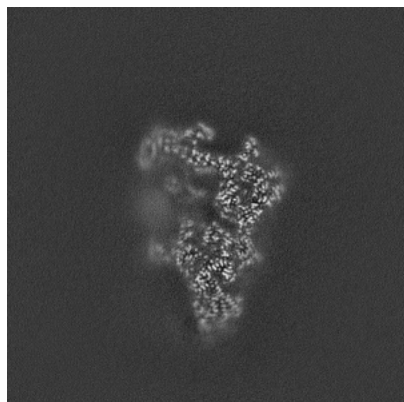


Y Index: 262

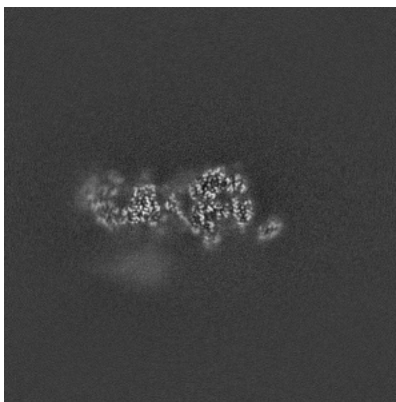


Z Index: 246

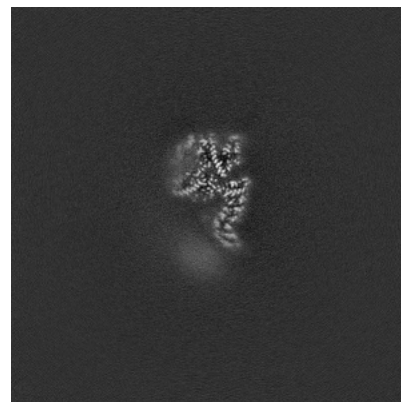
6.3.2 Raw map



X Index: 240



Y Index: 262

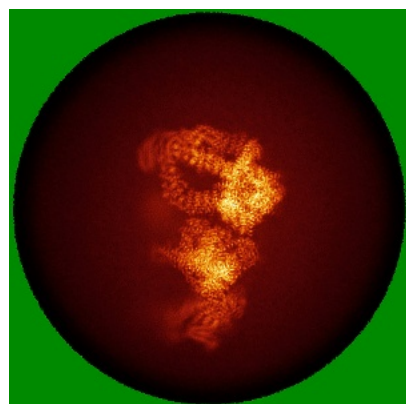


Z Index: 249

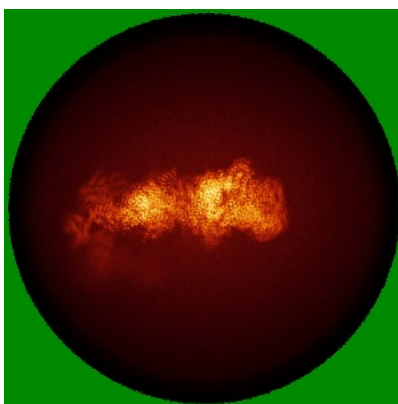
The images above show the largest variance slices of the map in three orthogonal directions.

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

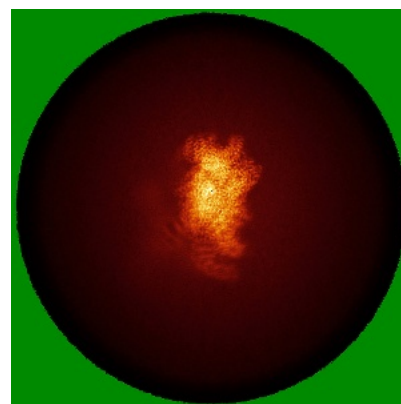
6.4.1 Primary map



X

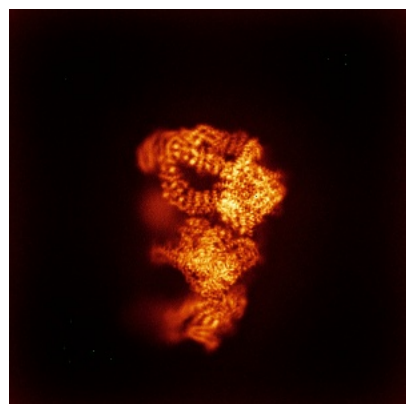


Y

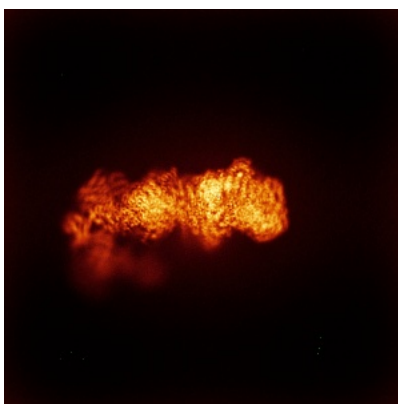


Z

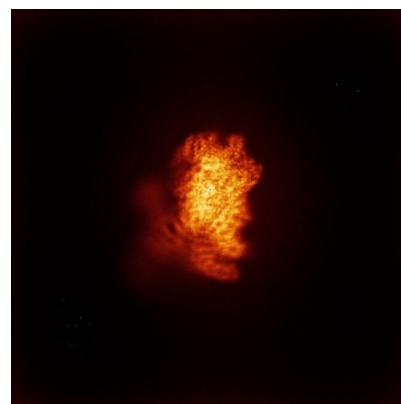
6.4.2 Raw map



X



Y

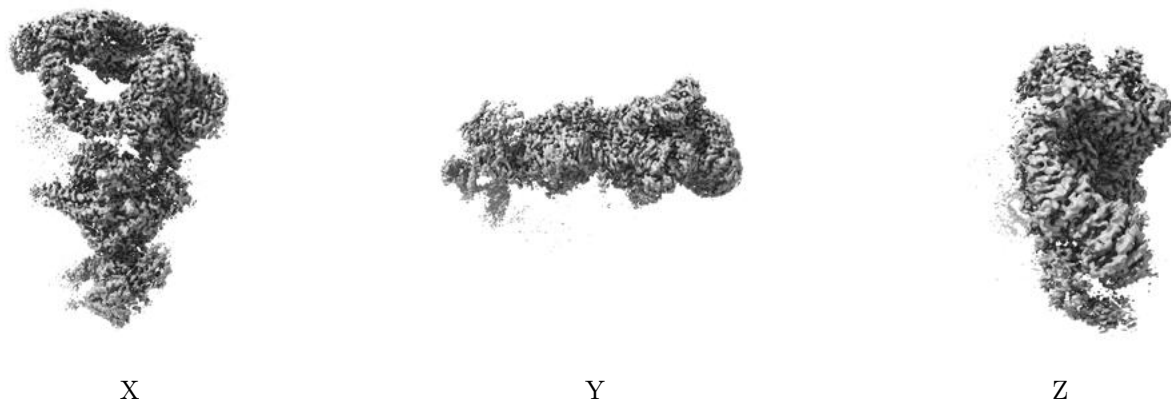


Z

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

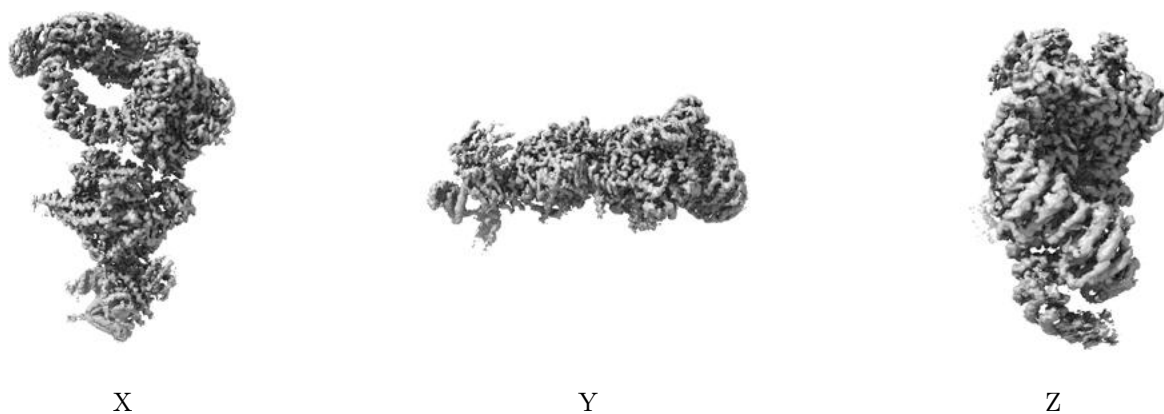
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

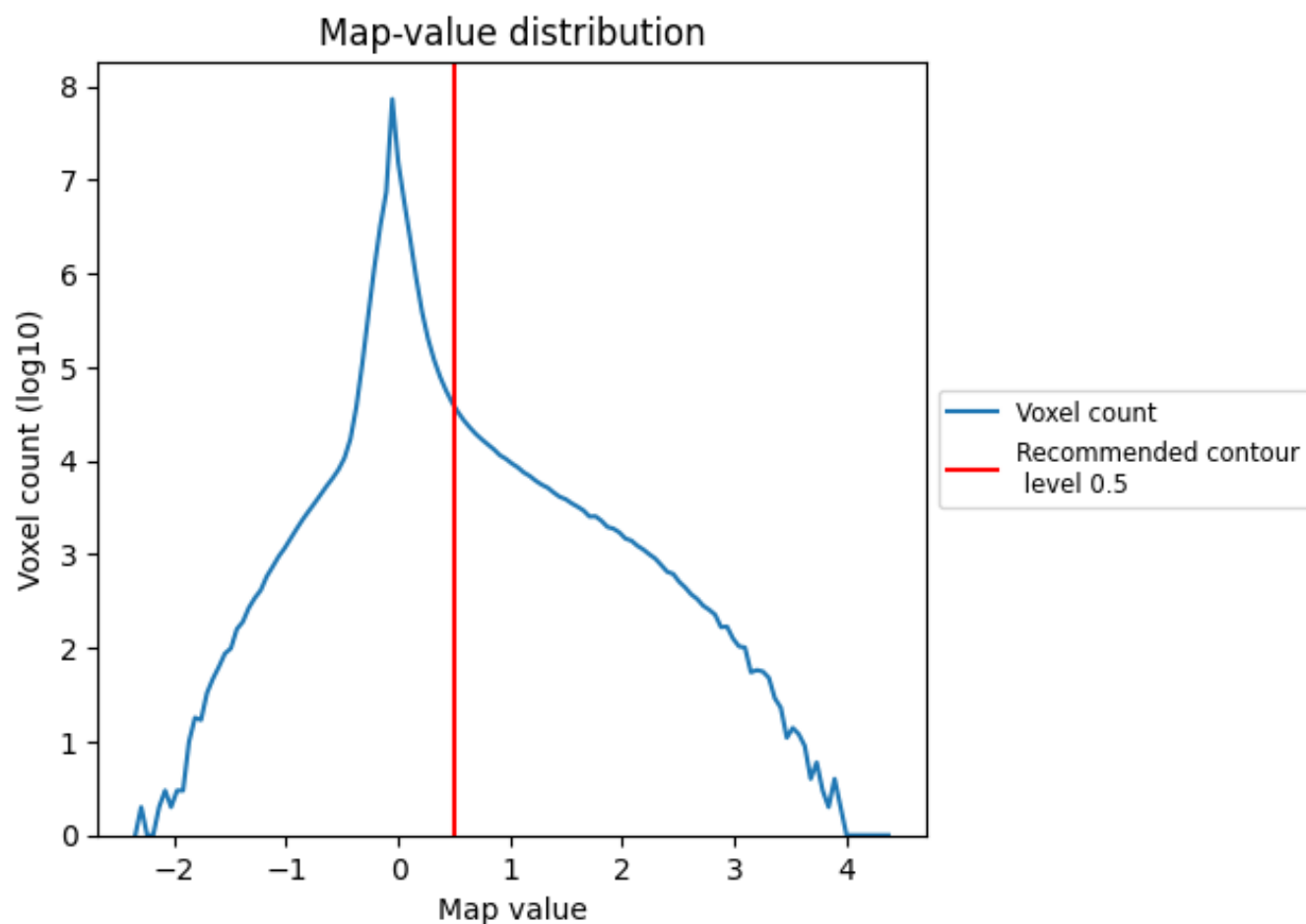
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

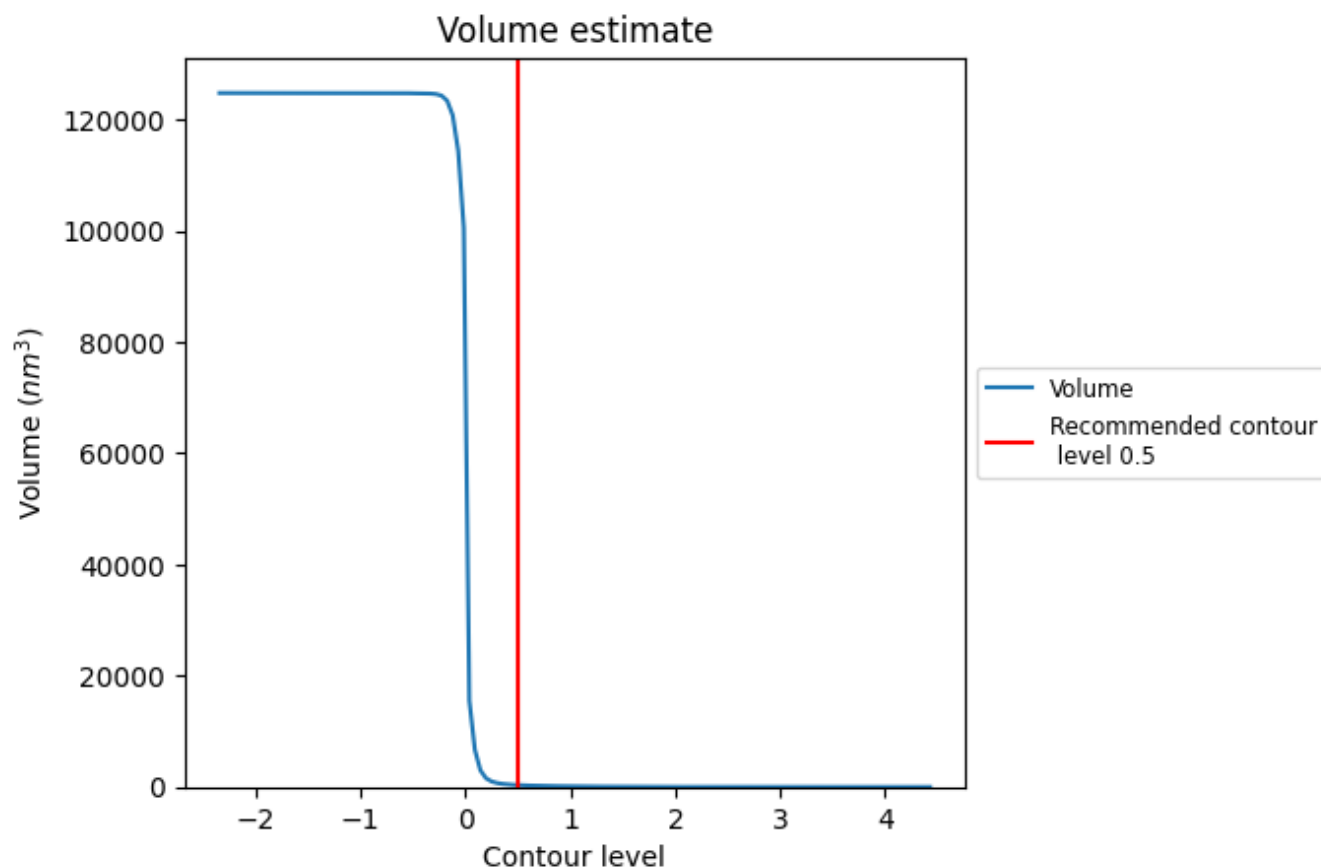
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

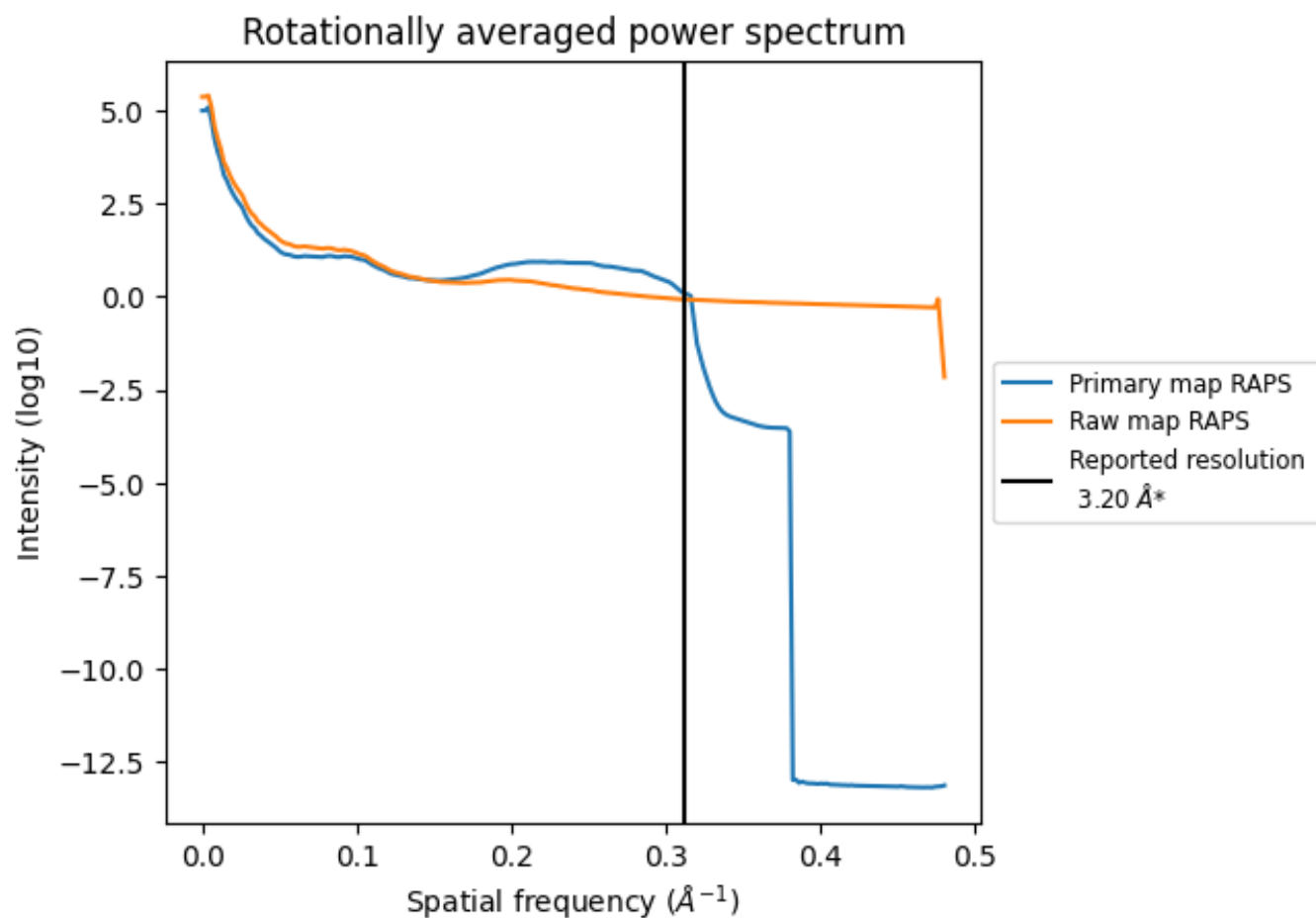
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 331 nm³; this corresponds to an approximate mass of 299 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 ⓘ

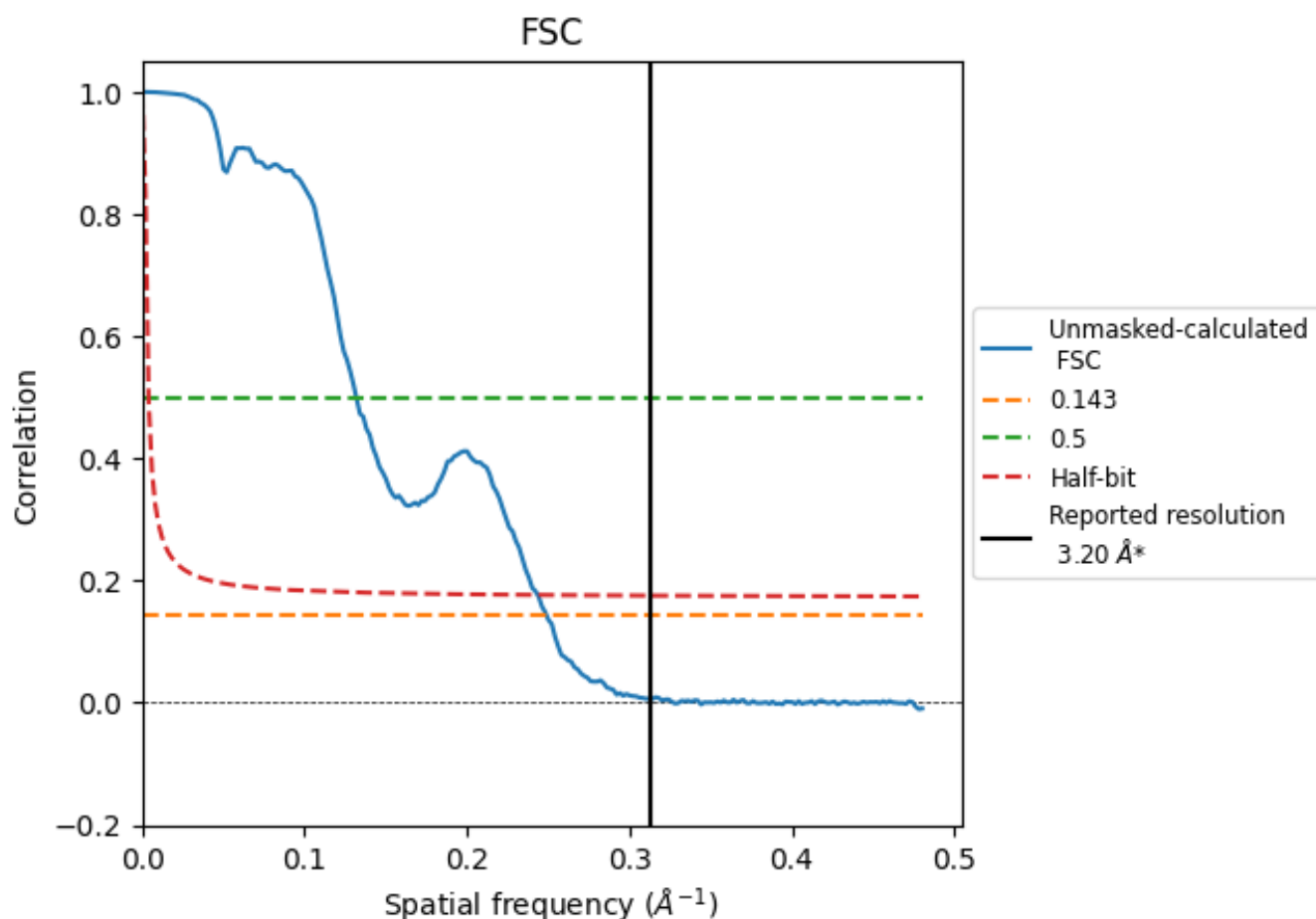


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

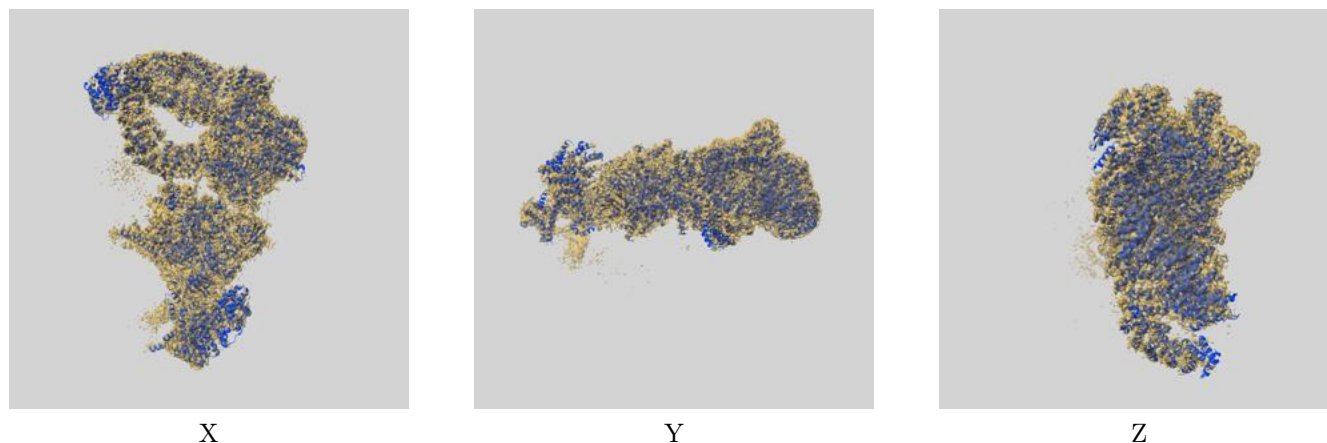
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.02	7.59	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.02 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

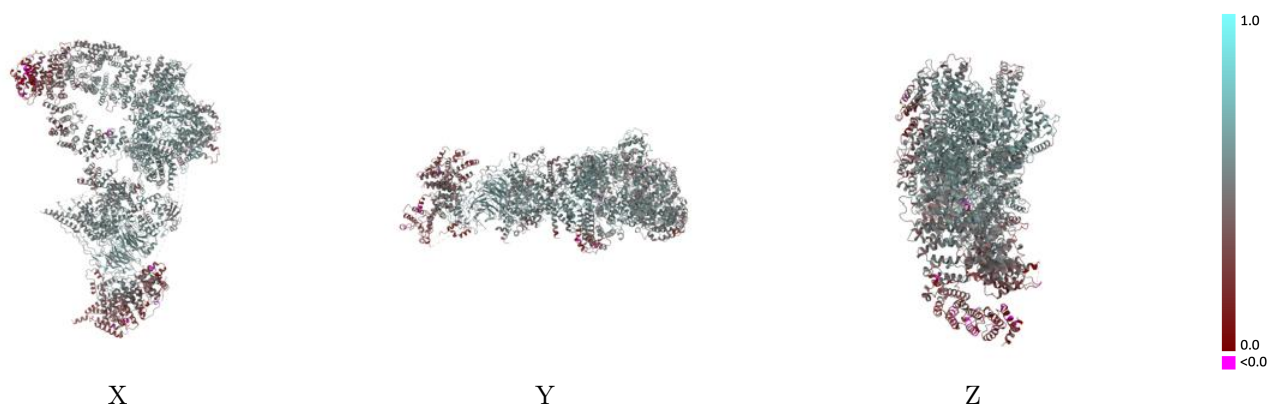
This section contains information regarding the fit between EMDB map EMD-73233 and PDB model 9YNU. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



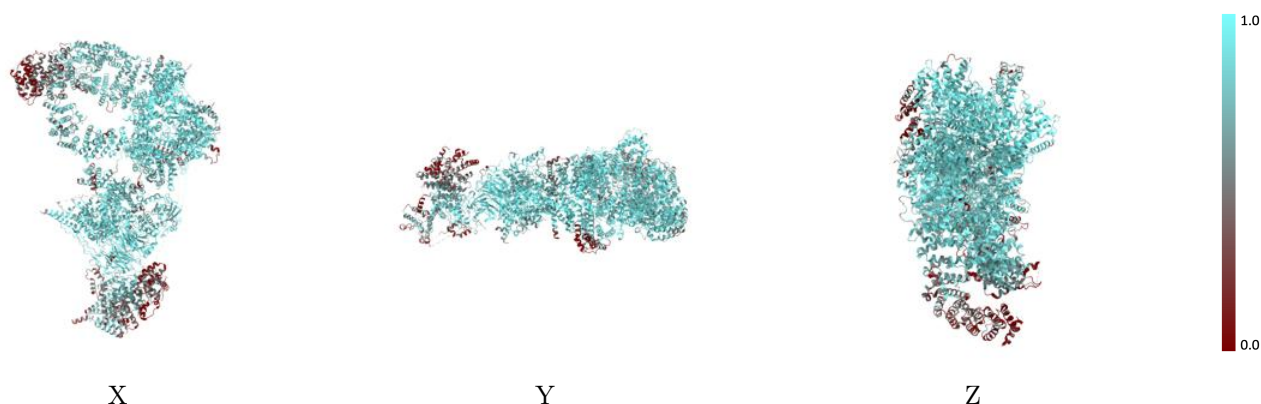
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



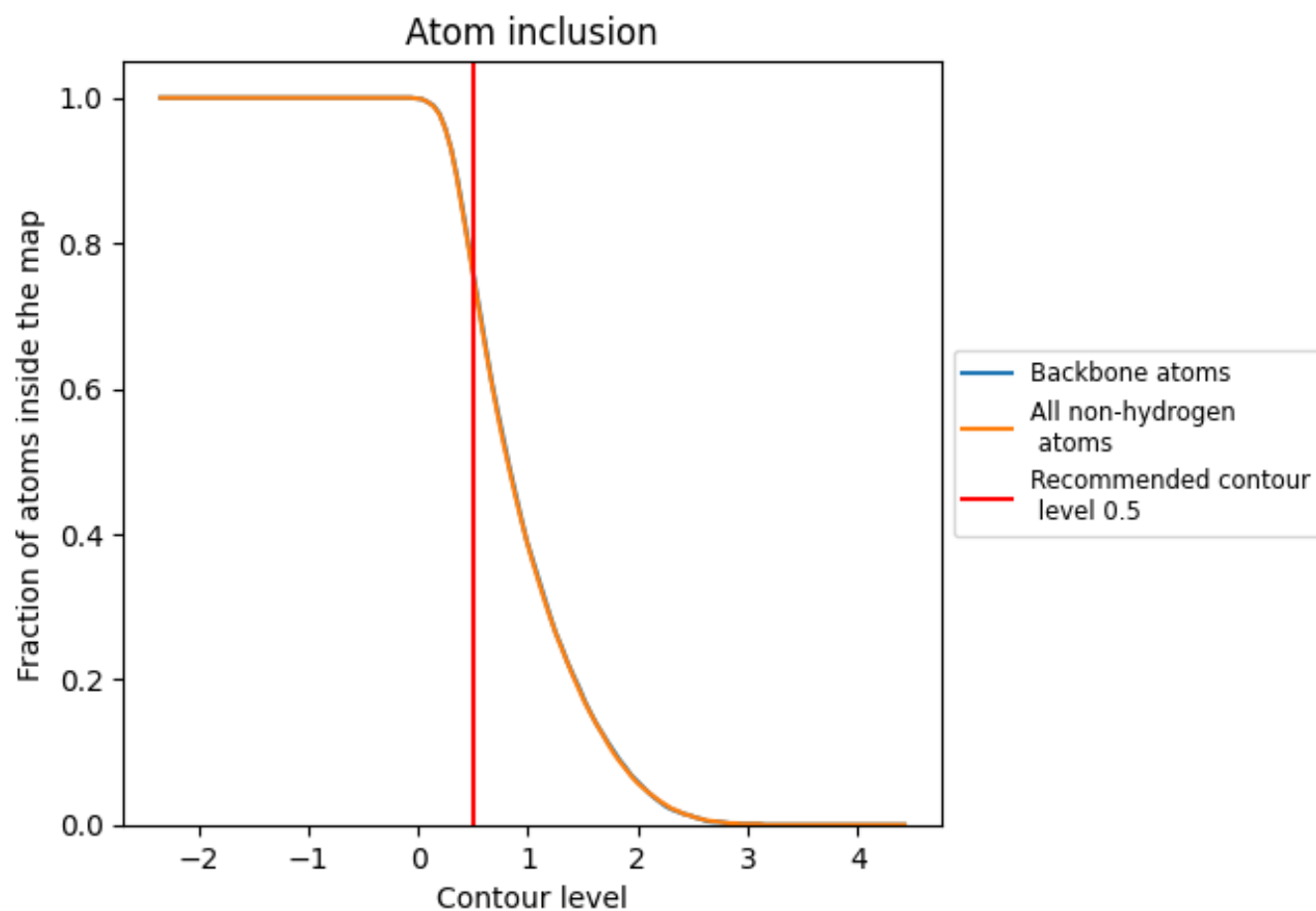
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7570	<div></div> 0.4840
A	<div></div> 0.7740	<div></div> 0.4860
B	<div></div> 0.8340	<div></div> 0.5280
C	<div></div> 0.7500	<div></div> 0.4880
D	<div></div> 0.6890	<div></div> 0.4890
E	<div></div> 0.7400	<div></div> 0.4760
F	<div></div> 0.9100	<div></div> 0.5550
G	<div></div> 0.8800	<div></div> 0.5450
H	<div></div> 0.8240	<div></div> 0.5260
I	<div></div> 0.7930	<div></div> 0.5280
K	<div></div> 0.6520	<div></div> 0.3990
Q	<div></div> 0.8570	<div></div> 0.5220

1.0

0.0

<0.0