



## Full wwPDB EM Validation Report ⓘ

Oct 29, 2024 – 08:23 PM JST

PDB ID : 8YQV  
EMDB ID : EMD-39507  
Title : African swine fever virus RNA Polymerase core  
Authors : Feng, X.Y.  
Deposited on : 2024-03-20  
Resolution : 2.67 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

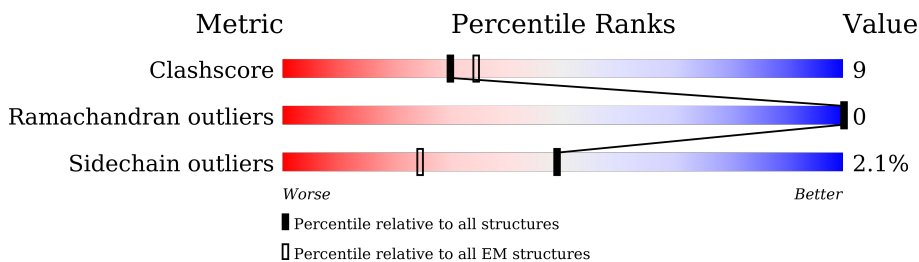
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.67 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1450	<div> <div>20%</div> <div>75%</div> <div>19%</div> <div>• 5%</div> </div>
2	E	147	<div> <div>6%</div> <div>55%</div> <div>16%</div> <div>• 28%</div> </div>
3	B	1242	<div> <div>45%</div> <div>69%</div> <div>26%</div> <div>•</div> </div>
4	C	359	<div> <div>•</div> <div>84%</div> <div>15%</div> <div>••</div> </div>
5	D	205	<div> <div>18%</div> <div>72%</div> <div>27%</div> <div>•</div> </div>
6	H	80	<div> <div>14%</div> <div>72%</div> <div>26%</div> <div>•</div> </div>
7	G	105	<div> <div>10%</div> <div>40%</div> <div>16%</div> <div>44%</div> </div>
8	F	339	<div> <div>80%</div> <div>74%</div> <div>24%</div> <div>•</div> </div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 29637 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1375	Total	C	N	O	S	0	0
			10954	6958	1906	2030	60		

- Molecule 2 is a protein called C147L.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	106	Total	C	N	O	S	0	0
			829	528	143	153	5		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	1196	Total	C	N	O	S	0	0
			9459	5983	1653	1773	50		

- Molecule 4 is a protein called DNA-directed RNA polymerase RPB3-11 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	357	Total	C	N	O	S	0	0
			2897	1880	480	525	12		

- Molecule 5 is a protein called DNA-directed RNA polymerase RPB5 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	205	Total	C	N	O	S	0	0
			1668	1088	278	294	8		

- Molecule 6 is a protein called DNA-directed RNA polymerase RPB10 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	80	Total	C	N	O	S	0	0
			630	411	102	110	7		

- Molecule 7 is a protein called C122R.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	59	Total	C	N	O	S	0	0
			468	295	80	85	8		

- Molecule 8 is a protein called D339L.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	339	Total	C	N	O	S	0	0
			2727	1753	451	509	14		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	Mg	0
			1	1	

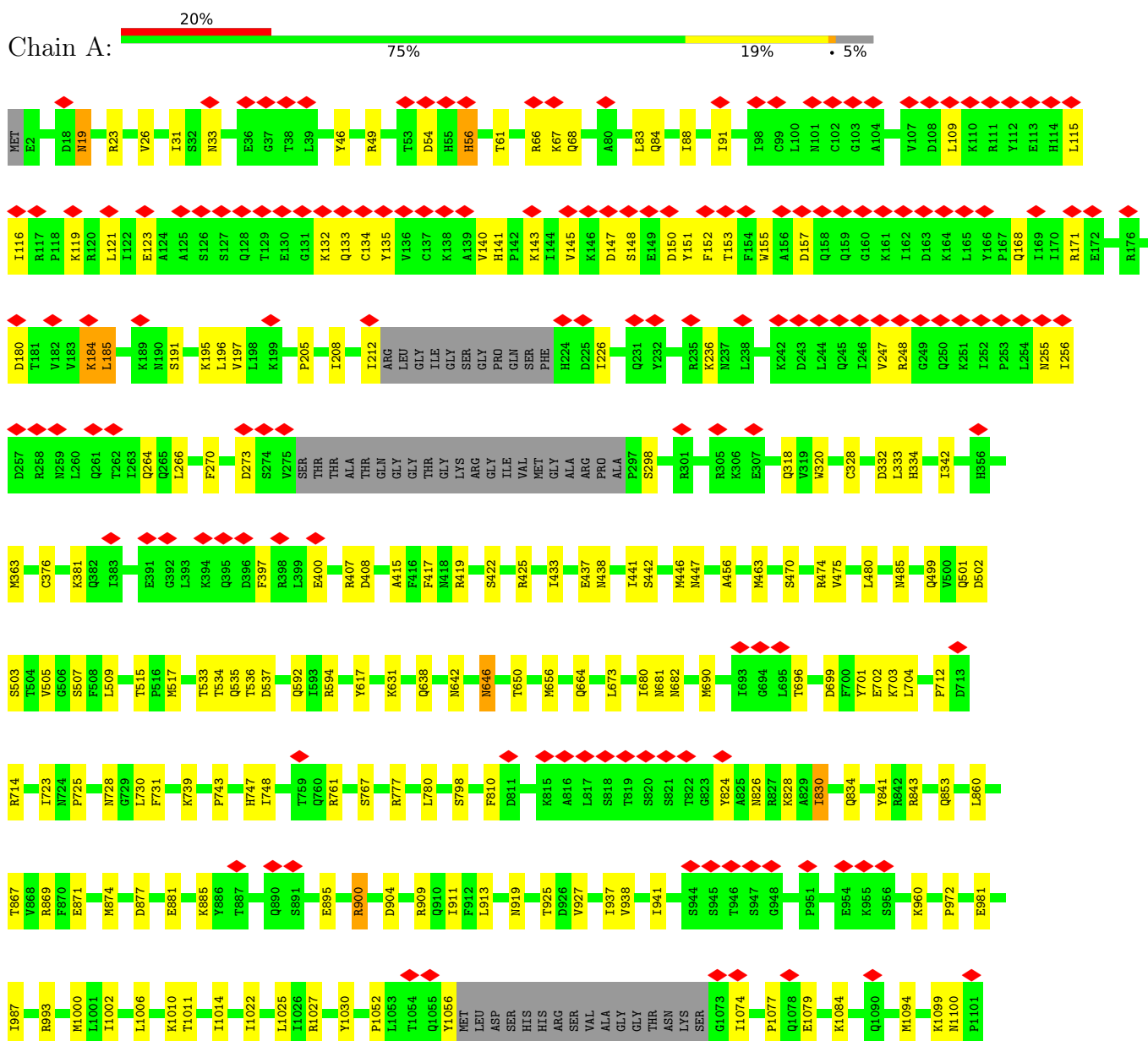
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

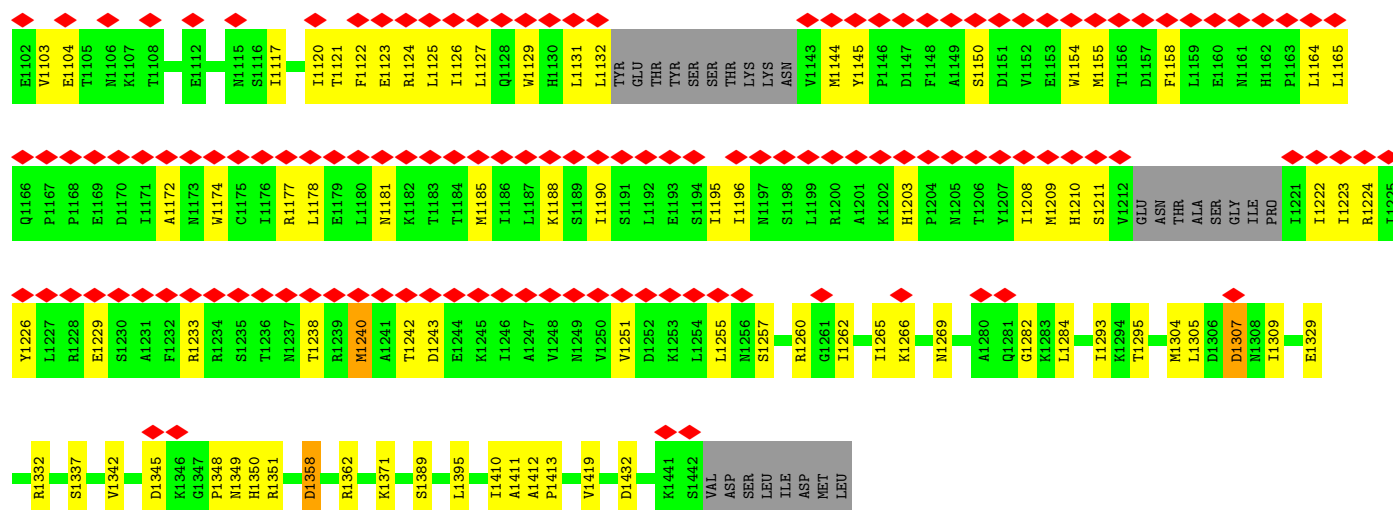
Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Zn	0
			1	1	
10	B	1	Total	Zn	0
			1	1	
10	H	1	Total	Zn	0
			1	1	
10	G	1	Total	Zn	0
			1	1	

### 3 Residue-property plots

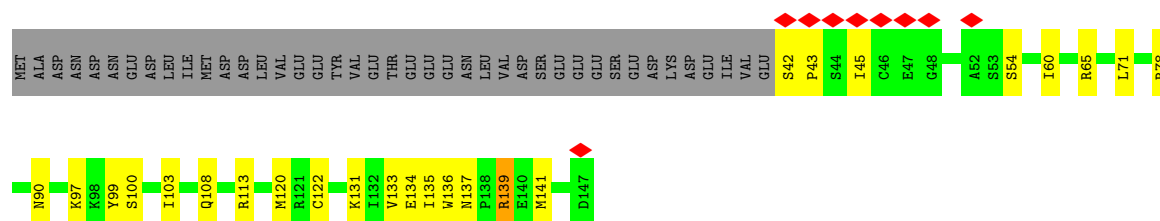
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: DNA-directed RNA polymerase subunit

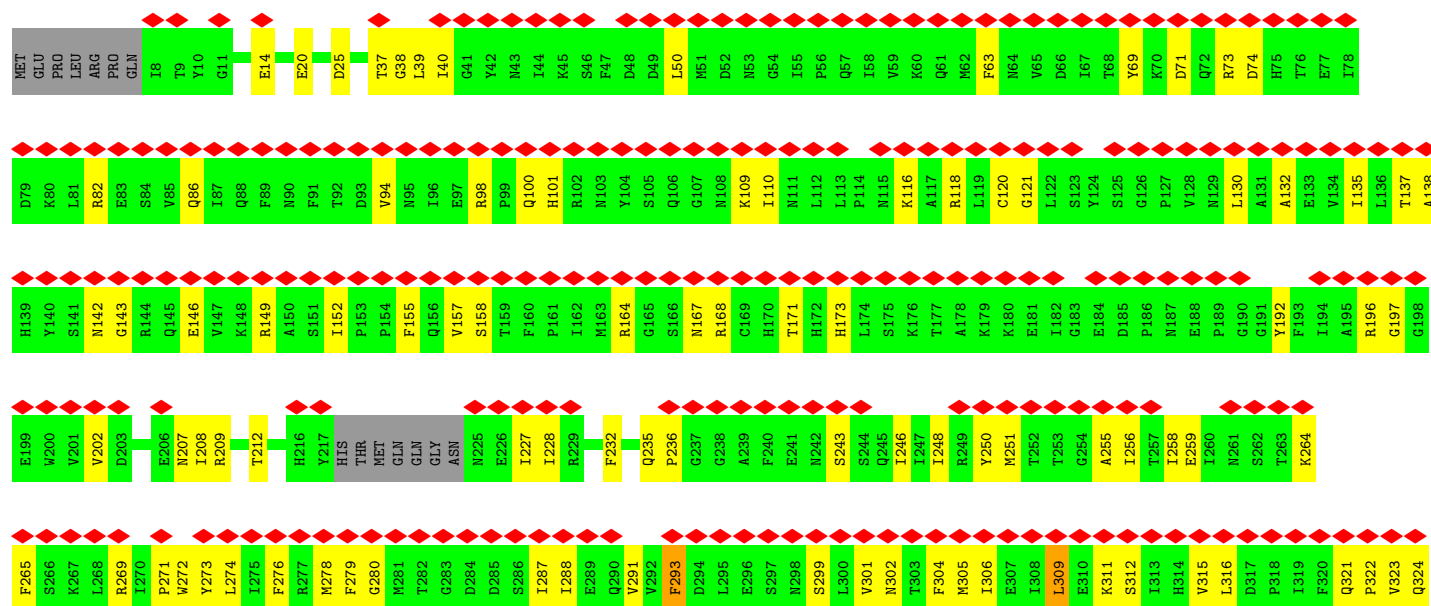


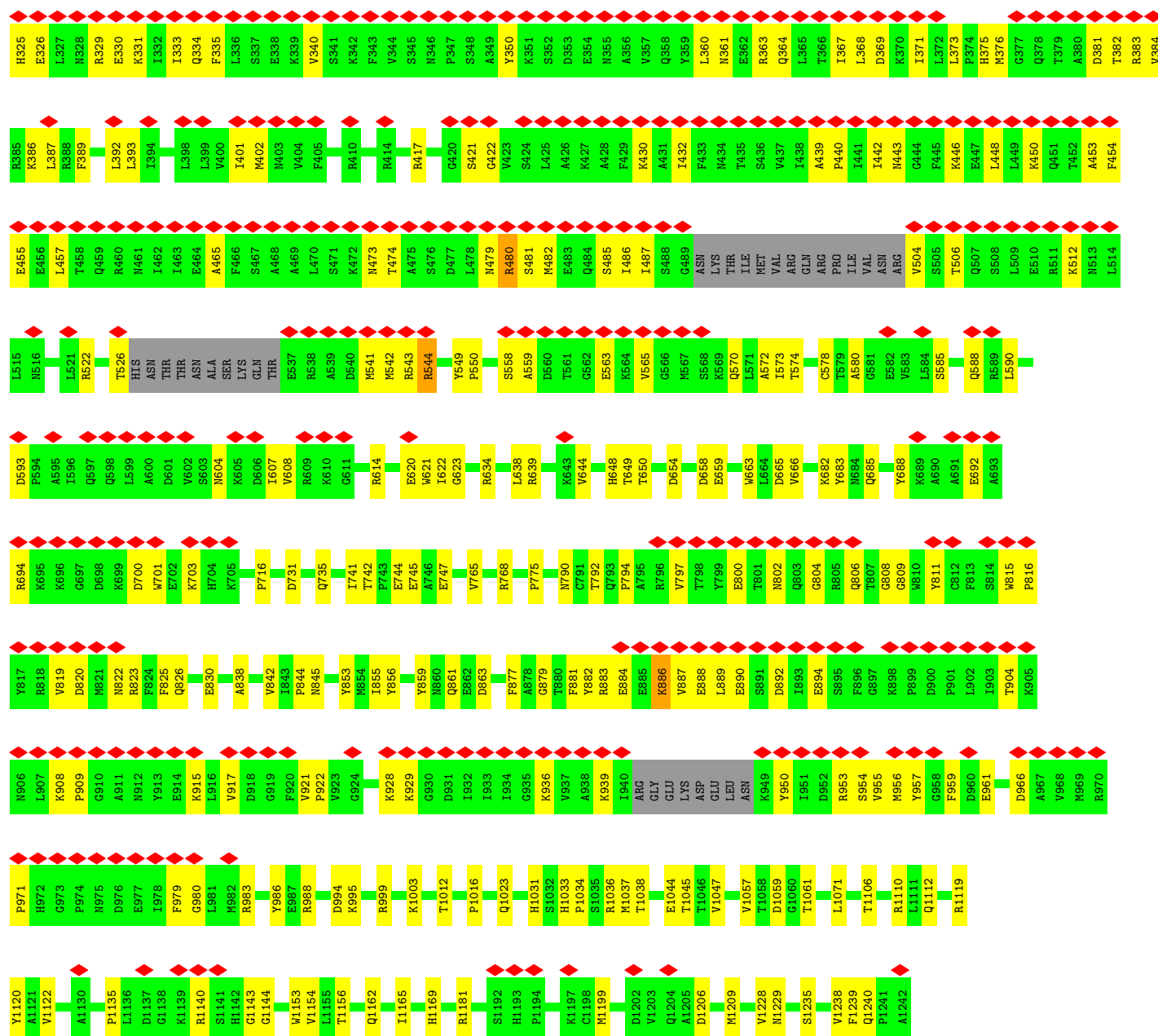


• Molecule 2: C147L



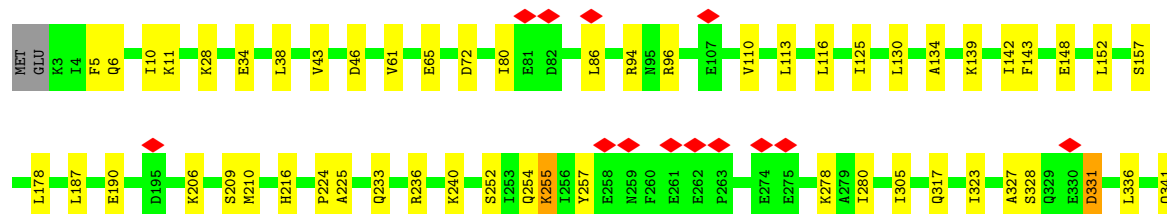
• Molecule 3: DNA-directed RNA polymerase subunit beta





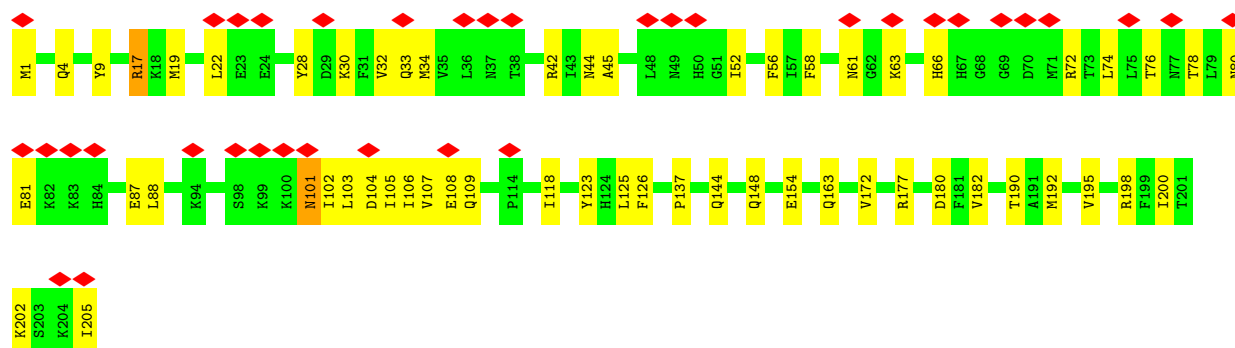
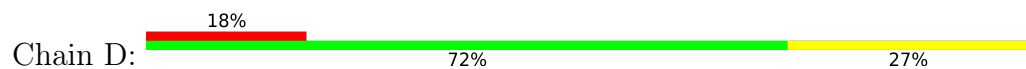
• Molecule 4: DNA-directed RNA polymerase RPB3-11 homolog

Chain C: 84% 15% 99%

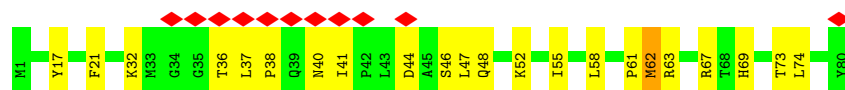
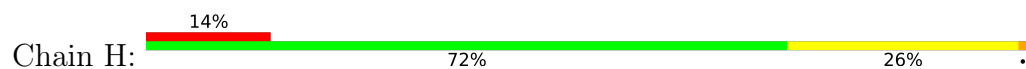




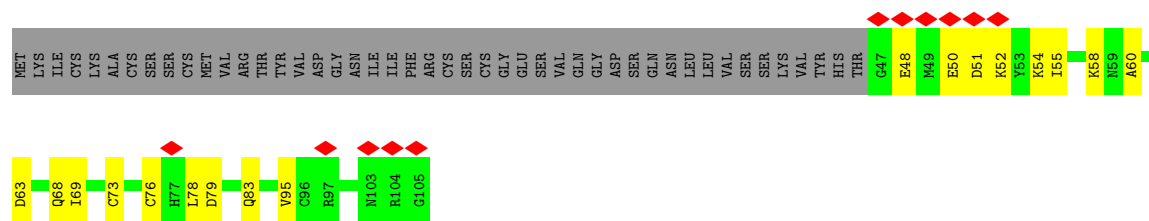
• Molecule 5: DNA-directed RNA polymerase RPB5 homolog



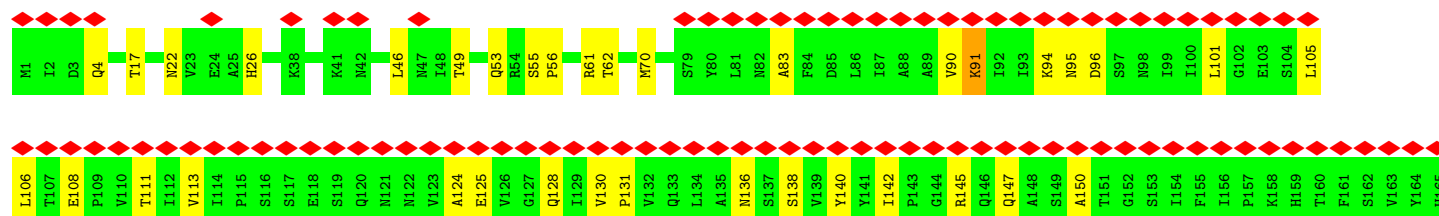
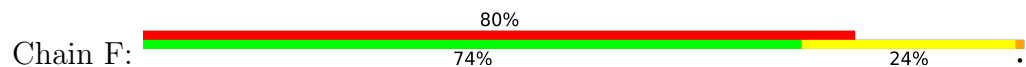
• Molecule 6: DNA-directed RNA polymerase RPB10 homolog



• Molecule 7: C122R



• Molecule 8: D339L



I286	C287	S288	A289	E290	V291	M292	F293	V294	T295	L296	L297	K298	E299	I300	I301	N302	N303	L304	Q305	F306	I307	D309	C311	T313	F314	N315	N316	E317	Q318	L319	I320	K321	R322	H323	E324	N325	L326	V327	M328	L329	I330	E331	Q332	K333	K334	I335	G336	H337	D338	F339									
P226	K227	G228	K229	E230	M231	S232	K233	L234	K235	P236	C237	M238	V239	L240	S241	F242	L243	Y244	D245	A246	L247	K248	N249	K250	N251	S252	S253	L254	G255	F256	W257	R258	R259	P260	P261	N262	L263	L264	K265	S266	Y267	P268	L269	A270	Y271	Q272	Q273	D274	Q275	N276	S277	F278	N279	A280	T281	E282	L283	P284	T285
V166	Q167	E168	E169	L170	T171	Q172	E173	Q174	A175	L176	M177	L178	T179	K180	L181	V182	M183	L184	I185	I186	M187	L188	L189	E190	S191	R192	S193	K194	K195	D196	F197	K198	Q199	I200	C201	F202	F203	E204	K205	L206	Y207	Y208	T209	Y210	S211	I212	S213	S214	D215	E216	L217	L218	D219	L220	K221	I222	W223	K224	G225

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	354548	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 ( $e^-/\text{\AA}^2$ )	1.25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.260	Depositor
Minimum map value	-1.946	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.095	Depositor
Recommended contour level	0.488	Depositor
Map size ( $\text{\AA}$ )	290.88, 290.88, 290.88	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.808, 0.808, 0.808	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, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.36	0/11163	0.52	2/15116 (0.0%)
2	E	0.35	0/841	0.54	0/1139
3	B	0.34	0/9648	0.52	1/13055 (0.0%)
4	C	0.38	0/2959	0.50	0/4000
5	D	0.36	0/1707	0.52	0/2311
6	H	0.41	0/643	0.56	0/872
7	G	0.32	0/476	0.53	0/638
8	F	0.28	0/2782	0.48	0/3767
All	All	0.35	0/30219	0.52	3/40898 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	LEU	CA-CB-CG	8.20	134.16	115.30
3	B	741	ILE	C-N-CA	5.42	135.25	121.70
1	A	121	LEU	CA-CB-CG	5.34	127.58	115.30

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	A	10954	0	11085	177	0
2	E	829	0	877	21	0
3	B	9459	0	9413	217	0
4	C	2897	0	2976	33	0
5	D	1668	0	1713	42	0
6	H	630	0	659	13	0
7	G	468	0	467	11	0
8	F	2727	0	2755	62	0
9	A	1	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	G	1	0	0	0	0
10	H	1	0	0	0	0
All	All	29637	0	29945	529	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 9.

All (529) 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)
1:A:1123:GLU:O	1:A:1126:ILE:HG13	1.62	0.97
3:B:522:ARG:HB2	3:B:570:GLN:HE22	1.35	0.89
2:E:42:SER:OG	2:E:43:PRO:HD3	1.72	0.88
6:H:37:LEU:HD12	6:H:38:PRO:HD2	1.59	0.85
4:C:139:LYS:HE3	4:C:139:LYS:HA	1.61	0.83
1:A:54:ASP:OD2	1:A:56:HIS:ND1	2.12	0.82
1:A:1123:GLU:HG3	1:A:1255:LEU:HD12	1.64	0.79
1:A:1432:ASP:OD2	2:E:139:ARG:NH2	2.16	0.79
8:F:46:LEU:HD21	8:F:108:GLU:HG2	1.65	0.78
8:F:91:LYS:HB2	8:F:105:LEU:HD11	1.64	0.77
1:A:1224:ARG:NH1	1:A:1226:TYR:OH	2.18	0.75
2:E:122:CYS:SG	2:E:131:LYS:NZ	2.59	0.75
1:A:109:LEU:HD13	1:A:184:LYS:HD3	1.67	0.74
8:F:267:SER:HB2	8:F:269:LEU:HD22	1.69	0.74
3:B:522:ARG:CB	3:B:570:GLN:HE22	2.00	0.73
1:A:1196:ILE:HD12	1:A:1208:ILE:HG21	1.69	0.73
3:B:578:CYS:SG	3:B:648:HIS:ND1	2.63	0.72
3:B:863:ASP:OD1	3:B:1036:ARG:NH2	2.22	0.71
3:B:167:ASN:OD1	3:B:168:ARG:NH1	2.23	0.71
3:B:522:ARG:HB2	3:B:570:GLN:NE2	2.05	0.71
3:B:73:ARG:NH1	3:B:450:LYS:O	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:GLU:OE1	1:A:1010:LYS:NZ	2.17	0.70
2:E:65:ARG:HG2	2:E:134:GLU:HG2	1.73	0.70
1:A:515:THR:HG22	1:A:517:MET:H	1.56	0.70
3:B:86:GLN:HB3	3:B:137:THR:HB	1.74	0.70
1:A:1079:GLU:HG2	1:A:1084:LYS:HD2	1.74	0.69
3:B:368:LEU:HA	3:B:371:ILE:HG22	1.74	0.69
4:C:34:GLU:N	4:C:34:GLU:OE1	2.25	0.69
8:F:22:ASN:O	8:F:26:HIS:ND1	2.25	0.69
1:A:501:GLN:O	3:B:1031:HIS:NE2	2.25	0.69
3:B:236:PRO:HA	3:B:375:HIS:HA	1.75	0.69
2:E:78:ARG:HH11	3:B:1162:GLN:HE21	1.38	0.69
3:B:302:ASN:O	3:B:306:ILE:HG13	1.92	0.69
3:B:844:PRO:HG2	6:H:74:LEU:HD11	1.74	0.69
4:C:233:GLN:OE1	4:C:236:ARG:NH2	2.26	0.68
3:B:118:ARG:NH2	3:B:192:TYR:OH	2.25	0.68
5:D:87:GLU:OE2	5:D:177:ARG:NH2	2.26	0.68
1:A:1052:PRO:HG2	1:A:1348:PRO:HD3	1.76	0.68
1:A:1177:ARG:HG3	1:A:1224:ARG:HG2	1.74	0.68
1:A:900:ARG:NH2	1:A:904:ASP:OD1	2.27	0.68
3:B:886:LYS:NZ	3:B:888:GLU:OE2	2.26	0.68
1:A:777:ARG:NH1	7:G:63:ASP:OD2	2.26	0.67
3:B:792:THR:HG23	3:B:1038:THR:HA	1.77	0.67
3:B:164:ARG:NH1	3:B:171:THR:OG1	2.27	0.67
1:A:1188:LYS:HB3	1:A:1260:ARG:HH22	1.59	0.66
8:F:4:GLN:NE2	8:F:49:THR:OG1	2.28	0.66
8:F:94:LYS:HB3	8:F:101:LEU:HB3	1.77	0.66
1:A:925:THR:HG22	1:A:927:VAL:H	1.59	0.66
3:B:69:TYR:CZ	3:B:446:LYS:HG2	2.31	0.66
1:A:332:ASP:OD2	3:B:859:TYR:OH	2.13	0.66
3:B:683:TYR:OH	7:G:79:ASP:OD1	2.13	0.65
5:D:72:ARG:O	5:D:76:THR:HG23	1.96	0.65
1:A:1164:LEU:HG	1:A:1165:LEU:HG	1.77	0.65
1:A:1126:ILE:HG21	1:A:1178:LEU:HD23	1.79	0.65
1:A:133:GLN:HA	1:A:140:VAL:HA	1.78	0.65
1:A:1129:TRP:HB2	1:A:1178:LEU:HG	1.78	0.65
1:A:1332:ARG:NH1	1:A:1358:ASP:OD2	2.29	0.65
3:B:248:ILE:HG12	3:B:258:ILE:HG12	1.77	0.64
3:B:808:GLY:HA2	3:B:1112:GLN:HE21	1.62	0.64
3:B:1181:ARG:HB2	3:B:1206:ASP:HB3	1.77	0.64
3:B:995:LYS:HD3	3:B:1003:LYS:HD2	1.79	0.64
3:B:158:SER:OG	3:B:479:ASN:ND2	2.25	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:ASN:ND2	4:C:209:SER:OG	2.30	0.64
5:D:42:ARG:NH1	5:D:44:ASN:OD1	2.31	0.64
3:B:100:GLN:HB3	3:B:109:LYS:HB3	1.79	0.64
3:B:209:ARG:NE	3:B:212:THR:HG21	2.12	0.64
8:F:111:THR:OG1	8:F:147:GLN:HG3	1.98	0.64
3:B:417:ARG:NH1	3:B:665:ASP:OD2	2.31	0.63
6:H:69:HIS:O	6:H:73:THR:OG1	2.15	0.63
2:E:45:ILE:HD13	3:B:1229:ASN:HD22	1.63	0.62
1:A:767:SER:HB3	3:B:747:GLU:OE1	2.00	0.62
3:B:138:ALA:HB2	3:B:454:PHE:HE2	1.65	0.62
1:A:145:VAL:HG13	1:A:155:TRP:HB2	1.82	0.62
3:B:486:ILE:HG13	3:B:487:ILE:HG13	1.81	0.62
3:B:522:ARG:CB	3:B:570:GLN:NE2	2.61	0.62
1:A:1129:TRP:CB	1:A:1178:LEU:HG	2.30	0.62
2:E:136:TRP:HB3	2:E:141:MET:SD	2.39	0.62
3:B:650:THR:HB	3:B:663:TRP:HB2	1.81	0.61
5:D:180:ASP:HB2	5:D:200:ILE:HD12	1.82	0.61
1:A:425:ARG:HA	3:B:1154:VAL:HG13	1.81	0.61
1:A:342:ILE:HD12	1:A:437:GLU:HG2	1.82	0.61
4:C:96:ARG:NH2	4:C:148:GLU:O	2.33	0.61
8:F:324:GLU:HA	8:F:327:TRP:CD1	2.35	0.61
1:A:19:ASN:ND2	2:E:42:SER:O	2.33	0.61
3:B:593:ASP:OD2	3:B:634:ARG:NH2	2.26	0.61
3:B:957:TYR:CZ	3:B:959:PHE:HB2	2.35	0.61
8:F:183:ASN:O	8:F:187:MET:HG2	2.01	0.61
3:B:255:ALA:HB2	3:B:315:VAL:HG11	1.83	0.61
3:B:541:MET:SD	3:B:544:ARG:NH2	2.72	0.61
4:C:110:VAL:HB	4:C:134:ALA:HB3	1.83	0.61
8:F:142:ILE:HB	8:F:145:ARG:HD3	1.82	0.60
1:A:1262:ILE:HB	1:A:1265:ILE:HD12	1.82	0.60
3:B:580:ALA:HB2	3:B:666:VAL:HG23	1.83	0.60
5:D:101:ASN:O	5:D:105:ILE:HD12	2.01	0.60
3:B:485:SER:HG	3:B:504:VAL:N	1.99	0.60
8:F:94:LYS:HE3	8:F:96:ASP:OD2	2.02	0.60
1:A:116:ILE:HD11	1:A:119:LYS:HD3	1.83	0.60
1:A:1150:SER:O	1:A:1154:TRP:N	2.31	0.60
1:A:1172:ALA:HB2	1:A:1229:GLU:HG2	1.83	0.60
3:B:373:LEU:HB3	3:B:376:MET:HG3	1.84	0.60
4:C:305:ILE:HD11	4:C:323:ILE:HG23	1.84	0.60
3:B:330:GLU:OE2	3:B:361:ASN:ND2	2.33	0.59
5:D:17:ARG:NH2	5:D:172:VAL:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:820:ASP:HB3	3:B:823:ARG:HD3	1.84	0.59
3:B:1012:THR:HG23	3:B:1023:GLN:HE22	1.67	0.59
8:F:205:LYS:HZ1	8:F:214:SER:HA	1.66	0.59
1:A:1177:ARG:HD2	1:A:1222:ILE:HD11	1.83	0.59
8:F:273:GLN:OE1	8:F:277:SER:OG	2.20	0.59
1:A:273:ASP:O	1:A:298:SER:OG	2.18	0.59
3:B:101:HIS:N	3:B:110:ILE:O	2.34	0.59
3:B:305:MET:O	3:B:309:LEU:HD12	2.03	0.59
3:B:915:LYS:HB3	3:B:921:VAL:HG13	1.85	0.59
4:C:254:GLN:NE2	4:C:341:GLN:OE1	2.35	0.59
1:A:171:ARG:NH1	1:A:197:VAL:HG12	2.19	0.58
1:A:960:LYS:NZ	1:A:1011:THR:O	2.32	0.58
2:E:42:SER:OG	2:E:43:PRO:CD	2.48	0.58
3:B:486:ILE:HA	3:B:504:VAL:HB	1.85	0.58
3:B:917:VAL:HG12	3:B:922:PRO:HD3	1.84	0.58
3:B:74:ASP:N	3:B:74:ASP:OD1	2.36	0.58
8:F:211:SER:O	8:F:337:HIS:NE2	2.35	0.58
1:A:247:VAL:HG12	1:A:248:ARG:N	2.19	0.58
1:A:83:LEU:H	1:A:264:GLN:HE22	1.50	0.57
1:A:470:SER:O	1:A:474:ARG:HB2	2.04	0.57
8:F:101:LEU:HD21	8:F:111:THR:HG23	1.85	0.57
3:B:360:LEU:O	3:B:364:GLN:NE2	2.37	0.57
8:F:194:LYS:HD2	8:F:194:LYS:O	2.04	0.57
5:D:163:GLN:O	5:D:198:ARG:NH1	2.38	0.57
3:B:889:LEU:HD23	3:B:936:LYS:HE3	1.85	0.57
5:D:74:LEU:O	5:D:78:THR:OG1	2.14	0.57
4:C:6:GLN:HA	4:C:357:LEU:HD11	1.86	0.57
1:A:919:ASN:ND2	1:A:1337:SER:OG	2.38	0.56
3:B:369:ASP:O	3:B:386:LYS:NZ	2.39	0.56
3:B:417:ARG:NH2	3:B:744:GLU:OE1	2.37	0.56
3:B:1239:PHE:HB3	8:F:53:GLN:HG2	1.87	0.56
4:C:61:VAL:HA	4:C:65:GLU:HB2	1.88	0.56
4:C:328:SER:OG	4:C:331:ASP:OD2	2.23	0.56
6:H:61:PRO:HB2	6:H:63:ARG:HG3	1.85	0.56
4:C:252:SER:O	4:C:255:LYS:HG3	2.05	0.56
1:A:712:PRO:HB2	1:A:714:ARG:HG2	1.87	0.56
3:B:130:LEU:HD22	3:B:157:VAL:HG21	1.86	0.56
3:B:392:LEU:HD22	3:B:614:ARG:HH11	1.70	0.56
1:A:499:GLN:NE2	1:A:617:TYR:OH	2.32	0.56
1:A:656:MET:HG2	1:A:730:LEU:HD22	1.88	0.56
1:A:748:ILE:HD11	3:B:1037:MET:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:105:ILE:HD12	5:D:105:ILE:H	1.71	0.56
3:B:815:TRP:CG	3:B:816:PRO:HD3	2.40	0.56
3:B:877:PHE:O	3:B:1110:ARG:NH1	2.37	0.56
6:H:17:TYR:HB3	6:H:58:LEU:HD22	1.86	0.56
1:A:981:GLU:OE1	1:A:1027:ARG:NH2	2.39	0.55
5:D:104:ASP:O	5:D:108:GLU:HG3	2.06	0.55
3:B:235:GLN:NE2	3:B:243:SER:OG	2.40	0.55
4:C:327:ALA:HB1	4:C:331:ASP:HB2	1.89	0.55
5:D:30:LYS:O	5:D:34:MET:HG3	2.06	0.55
1:A:909:ARG:O	1:A:913:LEU:HB2	2.07	0.55
1:A:867:THR:HG22	1:A:927:VAL:HG12	1.89	0.55
3:B:256:ILE:HB	3:B:272:TRP:CD1	2.42	0.55
3:B:274:LEU:O	3:B:278:MET:HG3	2.07	0.55
5:D:76:THR:HG22	5:D:109:GLN:HE22	1.70	0.55
1:A:320:TRP:CE2	3:B:1135:PRO:HG3	2.42	0.55
5:D:22:LEU:HD11	5:D:52:ILE:HD12	1.88	0.54
3:B:82:ARG:NH1	3:B:455:GLU:OE1	2.40	0.54
5:D:102:ILE:HA	5:D:105:ILE:HD13	1.89	0.54
3:B:999:ARG:NH2	3:B:1044:GLU:OE2	2.30	0.54
1:A:1127:LEU:HB2	1:A:1181:ASN:HB2	1.88	0.54
3:B:448:LEU:HD22	3:B:465:ALA:HB2	1.89	0.54
3:B:904:THR:HA	3:B:950:TYR:HB2	1.90	0.54
3:B:994:ASP:OD2	3:B:1110:ARG:NH2	2.41	0.54
3:B:316:LEU:HD11	3:B:321:GLN:HG3	1.89	0.54
4:C:72:ASP:OD1	4:C:94:ARG:NH1	2.40	0.54
8:F:95:ASN:ND2	8:F:124:ALA:O	2.40	0.54
1:A:1185:MET:HG2	1:A:1190:ILE:HB	1.89	0.54
3:B:228:ILE:HG22	3:B:250:TYR:HB3	1.90	0.54
1:A:885:LYS:NZ	1:A:895:GLU:OE1	2.32	0.54
1:A:1419:VAL:O	8:F:61:ARG:NH2	2.41	0.54
3:B:482:MET:O	3:B:486:ILE:HG23	2.08	0.54
3:B:639:ARG:NH1	3:B:649:THR:O	2.39	0.54
7:G:73:CYS:HB3	7:G:78:LEU:H	1.73	0.54
5:D:30:LYS:O	5:D:33:GLN:HG2	2.08	0.53
3:B:881:PHE:HB3	3:B:986:TYR:HB2	1.91	0.53
5:D:102:ILE:O	5:D:106:ILE:HG12	2.09	0.53
1:A:1120:ILE:HD13	1:A:1260:ARG:HH21	1.73	0.53
1:A:26:VAL:HG12	3:B:1199:MET:SD	2.49	0.53
3:B:1059:ASP:OD2	3:B:1061:THR:OG1	2.21	0.53
1:A:874:MET:SD	1:A:1284:LEU:HD23	2.48	0.53
8:F:202:PHE:HE1	8:F:320:ILE:HD12	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:38:LEU:HD23	4:C:225:ALA:HB1	1.90	0.53
5:D:19:MET:HB3	5:D:45:ALA:HB1	1.90	0.53
5:D:76:THR:O	5:D:80:ASN:ND2	2.42	0.53
1:A:84:GLN:NE2	1:A:195:LYS:O	2.42	0.53
1:A:91:ILE:HG12	1:A:196:LEU:HD13	1.91	0.53
5:D:42:ARG:HG2	5:D:42:ARG:HH11	1.73	0.53
1:A:723:ILE:HB	1:A:728:ASN:HD22	1.74	0.52
5:D:28:TYR:O	5:D:32:VAL:HG23	2.09	0.52
8:F:195:LYS:NZ	8:F:312:ASP:OD1	2.42	0.52
1:A:877:ASP:OD1	1:A:1282:GLY:HA3	2.09	0.52
3:B:1045:THR:HG1	3:B:1106:THR:HG1	1.57	0.52
5:D:103:LEU:HD22	5:D:205:ILE:HG21	1.92	0.52
1:A:83:LEU:HD23	1:A:197:VAL:HG22	1.92	0.52
8:F:244:TYR:HA	8:F:247:LEU:HD12	1.90	0.52
3:B:304:PHE:HD2	3:B:402:MET:SD	2.32	0.52
3:B:259:GLU:HB2	3:B:269:ARG:HG2	1.92	0.52
3:B:375:HIS:HD2	3:B:620:GLU:HB3	1.75	0.52
5:D:22:LEU:HD12	5:D:44:ASN:HB3	1.92	0.52
1:A:502:ASP:HB2	3:B:861:GLN:NE2	2.25	0.52
3:B:604:ASN:HA	3:B:607:ILE:HG12	1.91	0.52
8:F:83:ALA:HB1	8:F:136:ASN:HA	1.91	0.52
1:A:681:ASN:OD1	1:A:701:TYR:OH	2.14	0.51
1:A:696:THR:HG23	1:A:699:ASP:H	1.75	0.51
3:B:526:THR:HG21	3:B:542:MET:CE	2.40	0.51
7:G:50:GLU:O	7:G:54:LYS:HB2	2.10	0.51
3:B:324:GLN:HG3	3:B:325:HIS:CD2	2.45	0.51
3:B:961:GLU:OE2	3:B:988:ARG:NH2	2.31	0.51
6:H:36:THR:HB	6:H:41:ILE:HG13	1.91	0.51
1:A:205:PRO:HG2	1:A:208:ILE:HG12	1.91	0.51
1:A:255:ASN:OD1	1:A:256:ILE:N	2.44	0.51
1:A:1132:LEU:HD22	1:A:1145:TYR:CZ	2.46	0.51
4:C:190:GLU:HB2	4:C:206:LYS:HD2	1.92	0.51
8:F:106:LEU:HD13	8:F:309:ASP:HB3	1.91	0.51
1:A:318:GLN:NE2	3:B:1144:GLY:O	2.42	0.51
3:B:816:PRO:HB3	4:C:86:LEU:HB3	1.93	0.51
8:F:304:LEU:O	8:F:308:ASN:ND2	2.42	0.51
1:A:941:ILE:HG21	1:A:1022:ILE:HD11	1.93	0.51
3:B:364:GLN:HA	3:B:367:ILE:HG22	1.91	0.51
3:B:887:VAL:HG21	3:B:955:VAL:HG21	1.93	0.51
3:B:135:ILE:HG12	3:B:149:ARG:HG2	1.93	0.51
3:B:522:ARG:NH2	3:B:572:ALA:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1410:ILE:HG12	3:B:1156:THR:HG21	1.93	0.51
8:F:125:GLU:OE1	8:F:128:GLN:NE2	2.44	0.51
1:A:1129:TRP:HZ3	1:A:1131:LEU:HB3	1.76	0.51
1:A:1371:LYS:HE3	1:A:1389:SER:OG	2.11	0.51
3:B:207:ASN:OD1	3:B:208:ILE:N	2.44	0.51
3:B:621:TRP:NE1	3:B:623:GLY:O	2.40	0.51
8:F:200:ILE:HG22	8:F:311:CYS:SG	2.50	0.51
8:F:260:PRO:HD2	8:F:263:LEU:HD22	1.92	0.51
2:E:71:LEU:HG	2:E:141:MET:HE2	1.91	0.50
1:A:592:GLN:HE22	1:A:594:ARG:HH21	1.58	0.50
4:C:178:LEU:O	4:C:224:PRO:HD3	2.12	0.50
7:G:76:CYS:SG	7:G:78:LEU:HB2	2.51	0.50
1:A:1174:TRP:HZ2	1:A:1243:ASP:HB3	1.77	0.50
3:B:142:ASN:OD1	3:B:143:GLY:N	2.45	0.50
3:B:278:MET:HE3	3:B:333:ILE:HG12	1.94	0.50
3:B:279:PHE:CD1	3:B:383:ARG:HD2	2.47	0.50
1:A:1100:ASN:HB3	1:A:1103:VAL:HG22	1.93	0.50
3:B:486:ILE:O	3:B:506:THR:OG1	2.15	0.50
3:B:573:ILE:HG23	3:B:574:THR:HG23	1.92	0.50
3:B:892:ASP:O	3:B:939:LYS:NZ	2.44	0.50
1:A:185:LEU:O	1:A:185:LEU:HD23	2.11	0.49
1:A:881:GLU:O	1:A:885:LYS:HB3	2.11	0.49
3:B:63:PHE:CE2	3:B:430:LYS:HE3	2.47	0.49
3:B:650:THR:OG1	3:B:742:THR:HG21	2.12	0.49
1:A:143:LYS:HB3	1:A:157:ASP:HB3	1.94	0.49
4:C:190:GLU:H	4:C:190:GLU:CD	2.16	0.49
8:F:94:LYS:CE	8:F:96:ASP:OD2	2.60	0.49
1:A:1349:ASN:ND2	1:A:1351:ARG:HE	2.11	0.49
1:A:480:LEU:O	1:A:485:ASN:ND2	2.45	0.49
4:C:187:LEU:HB2	4:C:216:HIS:CD2	2.48	0.49
3:B:293:PHE:HB2	3:B:608:VAL:HG11	1.94	0.49
3:B:559:ALA:HB3	3:B:565:VAL:HA	1.95	0.49
4:C:278:LYS:HE2	4:C:280:ILE:HD11	1.94	0.49
1:A:834:GLN:HE22	1:A:1411:ALA:HB2	1.78	0.49
3:B:543:ARG:HH22	3:B:563:GLU:HG2	1.78	0.49
7:G:48:GLU:HG2	7:G:52:LYS:HD2	1.93	0.48
8:F:275:GLN:N	8:F:275:GLN:OE1	2.46	0.48
1:A:109:LEU:HD23	1:A:185:LEU:HD12	1.95	0.48
2:E:122:CYS:HA	2:E:133:VAL:HG12	1.95	0.48
3:B:367:ILE:O	3:B:371:ILE:N	2.42	0.48
8:F:212:ILE:HD12	8:F:217:ILE:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LYS:O	1:A:141:HIS:N	2.39	0.48
1:A:381:LYS:HD3	1:A:397:PHE:CZ	2.49	0.48
1:A:739:LYS:HG3	3:B:1034:PRO:HG2	1.95	0.48
3:B:288:ILE:HG12	3:B:306:ILE:HG23	1.94	0.48
8:F:101:LEU:CD2	8:F:111:THR:HG23	2.43	0.48
2:E:60:ILE:HD12	2:E:134:GLU:HG3	1.95	0.48
3:B:894:GLU:OE2	3:B:953:ARG:NH2	2.40	0.48
5:D:61:ASN:HA	5:D:66:HIS:HE1	1.77	0.48
7:G:68:GLN:O	7:G:69:ILE:HD13	2.14	0.48
3:B:202:VAL:HG11	3:B:421:SER:HA	1.95	0.48
3:B:765:VAL:O	3:B:768:ARG:NH1	2.47	0.48
3:B:1122:VAL:HG11	3:B:1143:GLY:O	2.14	0.48
8:F:197:PHE:HD1	8:F:200:ILE:HD11	1.77	0.48
8:F:245:ASP:O	8:F:248:LYS:HG2	2.14	0.48
1:A:49:ARG:O	1:A:61:THR:OG1	2.31	0.48
5:D:88:LEU:HD12	5:D:118:ILE:HD12	1.96	0.48
1:A:1094:MET:HB3	1:A:1295:THR:OG1	2.12	0.47
1:A:1242:THR:OG1	1:A:1243:ASP:N	2.47	0.47
3:B:790:ASN:OD1	3:B:790:ASN:N	2.44	0.47
3:B:971:PRO:HG2	3:B:979:PHE:CZ	2.48	0.47
5:D:58:PHE:O	5:D:123:TYR:OH	2.26	0.47
1:A:147:ASP:OD1	1:A:148:SER:N	2.47	0.47
1:A:419:ARG:HD2	1:A:456:ALA:HB2	1.95	0.47
1:A:824:TYR:CZ	1:A:828:LYS:HD2	2.50	0.47
1:A:972:PRO:HB2	1:A:987:ILE:HD13	1.96	0.47
8:F:248:LYS:HG3	8:F:250:LYS:HG3	1.96	0.47
3:B:132:ALA:HB3	3:B:152:ILE:HD12	1.97	0.47
3:B:1057:VAL:HB	6:H:47:LEU:HB3	1.95	0.47
1:A:1412:ALA:HB3	1:A:1413:PRO:HD3	1.96	0.47
3:B:321:GLN:HB3	3:B:322:PRO:HD3	1.96	0.47
3:B:638:LEU:HD13	3:B:644:VAL:HG11	1.96	0.47
4:C:113:LEU:HB2	4:C:130:LEU:HD23	1.95	0.47
1:A:702:GLU:OE1	1:A:761:ARG:NE	2.45	0.47
2:E:113:ARG:HD3	2:E:139:ARG:O	2.15	0.47
3:B:822:ASN:N	3:B:882:TYR:O	2.48	0.47
8:F:328:MET:HB3	8:F:332:GLN:HE22	1.80	0.47
3:B:700:ASP:O	3:B:703:LYS:HG2	2.15	0.47
3:B:928:LYS:NZ	3:B:929:LYS:O	2.46	0.47
8:F:205:LYS:NZ	8:F:214:SER:HA	2.30	0.47
1:A:501:GLN:O	3:B:1031:HIS:CE1	2.67	0.47
1:A:534:THR:HG22	1:A:638:GLN:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:938:VAL:HG13	1:A:1014:ILE:HD11	1.96	0.47
1:A:1345:ASP:OD1	1:A:1345:ASP:N	2.41	0.47
5:D:104:ASP:O	5:D:107:VAL:HG22	2.15	0.47
1:A:499:GLN:HB3	1:A:503:SER:HB2	1.95	0.46
1:A:1178:LEU:HB2	1:A:1223:ILE:HG23	1.98	0.46
3:B:473:ASN:OD1	3:B:474:THR:N	2.46	0.46
8:F:170:LEU:HD13	8:F:293:PHE:CD2	2.49	0.46
1:A:1265:ILE:HG23	1:A:1295:THR:HB	1.97	0.46
8:F:138:SER:O	8:F:150:ALA:HA	2.15	0.46
8:F:192:ARG:HH11	8:F:307:ILE:HG21	1.80	0.46
1:A:134:CYS:SG	1:A:135:TYR:N	2.89	0.46
1:A:1056:TYR:HE2	1:A:1074:ILE:HG22	1.80	0.46
8:F:94:LYS:NZ	8:F:96:ASP:OD2	2.44	0.46
1:A:442:SER:HB3	3:B:1119:ARG:HD3	1.96	0.46
3:B:323:VAL:HG13	3:B:326:GLU:OE1	2.15	0.46
1:A:1126:ILE:O	1:A:1126:ILE:HD12	2.16	0.46
3:B:639:ARG:NH2	3:B:745:GLU:OE2	2.41	0.46
3:B:694:ARG:HD3	3:B:701:TRP:CE2	2.51	0.46
3:B:966:ASP:OD2	3:B:983:ARG:NH2	2.48	0.46
1:A:843:ARG:HG2	1:A:853:GLN:O	2.15	0.46
3:B:37:THR:HG22	3:B:38:GLY:O	2.16	0.46
3:B:232:PHE:HB3	3:B:246:ILE:HG13	1.97	0.46
3:B:443:ASN:HA	3:B:446:LYS:HD3	1.96	0.46
1:A:247:VAL:CG1	1:A:248:ARG:N	2.78	0.46
1:A:830:ILE:HD12	3:B:1153:TRP:CE3	2.51	0.46
2:E:137:ASN:O	2:E:141:MET:HG3	2.15	0.46
3:B:809:GLY:HA2	3:B:826:GLN:HB3	1.98	0.46
1:A:334:HIS:NE2	1:A:535:GLN:OE1	2.42	0.46
1:A:536:THR:HG22	1:A:631:LYS:HE3	1.97	0.46
1:A:798:SER:OG	3:B:775:PRO:HB3	2.16	0.46
1:A:1305:LEU:HB3	5:D:1:MET:HB3	1.97	0.46
3:B:856:TYR:CE1	3:B:1016:PRO:HG3	2.51	0.46
3:B:454:PHE:HD1	3:B:457:LEU:HD12	1.81	0.46
1:A:885:LYS:HZ2	1:A:895:GLU:HA	1.81	0.46
1:A:31:ILE:HD12	1:A:33:ASN:HB3	1.97	0.45
3:B:202:VAL:HA	3:B:506:THR:HG22	1.97	0.45
3:B:838:ALA:O	3:B:842:VAL:HG22	2.14	0.45
2:E:120:MET:HG3	2:E:135:ILE:CD1	2.45	0.45
7:G:60:ALA:HB3	7:G:95:VAL:HG21	1.98	0.45
1:A:115:LEU:HD22	1:A:123:GLU:OE2	2.17	0.45
1:A:376:CYS:HA	1:A:407:ARG:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1293:ILE:HD12	1:A:1309:ILE:HD11	1.98	0.45
2:E:100:SER:O	2:E:100:SER:OG	2.34	0.45
4:C:28:LYS:HB3	4:C:28:LYS:HE2	1.68	0.45
1:A:333:LEU:O	1:A:447:ASN:ND2	2.49	0.45
2:E:120:MET:HG3	2:E:135:ILE:HD13	1.98	0.45
3:B:278:MET:HE3	3:B:278:MET:HB3	1.87	0.45
4:C:80:ILE:HG22	4:C:80:ILE:O	2.17	0.45
5:D:42:ARG:HD2	5:D:56:PHE:CE1	2.52	0.45
1:A:19:ASN:OD1	1:A:19:ASN:N	2.49	0.45
1:A:937:ILE:HG23	1:A:1025:LEU:HD23	1.98	0.45
1:A:1126:ILE:HD13	1:A:1129:TRP:CD1	2.52	0.45
3:B:887:VAL:O	3:B:980:GLY:N	2.46	0.45
1:A:115:LEU:HD13	1:A:123:GLU:OE1	2.17	0.45
1:A:1077:PRO:HG3	1:A:1342:VAL:HG11	1.99	0.45
1:A:1158:PHE:CZ	1:A:1209:MET:HA	2.52	0.45
3:B:928:LYS:HG2	3:B:929:LYS:H	1.81	0.45
7:G:58:LYS:HE3	7:G:58:LYS:HB3	1.77	0.45
8:F:194:LYS:HD2	8:F:194:LYS:C	2.38	0.45
3:B:453:ALA:O	3:B:457:LEU:HG	2.17	0.45
4:C:352:LYS:HE3	4:C:352:LYS:HB2	1.66	0.45
1:A:1074:ILE:O	1:A:1077:PRO:HD2	2.17	0.44
3:B:549:TYR:N	3:B:550:PRO:HD2	2.32	0.44
3:B:264:LYS:HE2	3:B:371:ILE:HD12	1.98	0.44
3:B:94:VAL:HG22	3:B:130:LEU:HG	2.00	0.44
3:B:800:GLU:O	3:B:804:GLY:N	2.46	0.44
8:F:101:LEU:HD21	8:F:111:THR:CG2	2.47	0.44
1:A:505:VAL:O	1:A:509:LEU:HG	2.17	0.44
1:A:1238:THR:HG23	1:A:1240:MET:SD	2.58	0.44
3:B:381:ASP:OD1	3:B:381:ASP:N	2.50	0.44
3:B:486:ILE:HG13	3:B:487:ILE:N	2.32	0.44
3:B:1047:VAL:HG22	3:B:1071:LEU:HD22	2.00	0.44
8:F:316:ASN:HD21	8:F:319:LEU:HD12	1.81	0.44
1:A:1100:ASN:O	1:A:1104:GLU:HG3	2.18	0.44
3:B:227:ILE:HD11	3:B:250:TYR:CD2	2.52	0.44
4:C:5:PHE:HB2	4:C:46:ASP:O	2.17	0.44
1:A:911:ILE:HG21	5:D:192:MET:O	2.18	0.44
1:A:1210:HIS:ND1	1:A:1211:SER:O	2.47	0.44
3:B:291:VAL:HG11	3:B:309:LEU:HD21	2.00	0.44
5:D:144:GLN:O	5:D:148:GLN:HG2	2.18	0.44
1:A:236:LYS:HE3	1:A:266:LEU:HD11	1.99	0.44
1:A:703:LYS:NZ	1:A:703:LYS:HB3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1240:GLN:HE21	8:F:56:PRO:HG3	1.82	0.44
1:A:592:GLN:NE2	1:A:594:ARG:HE	2.16	0.44
3:B:819:VAL:HG12	3:B:884:GLU:HB3	2.00	0.44
4:C:116:LEU:HD13	4:C:157:SER:HB2	2.00	0.44
5:D:109:GLN:HA	5:D:109:GLN:OE1	2.17	0.44
1:A:904:ASP:HB3	1:A:1000:MET:HG3	2.00	0.43
3:B:50:LEU:HD22	3:B:422:GLY:HA2	2.00	0.43
3:B:877:PHE:HB3	3:B:1110:ARG:HD2	2.00	0.43
3:B:1165:ILE:O	3:B:1169:HIS:HB2	2.17	0.43
6:H:52:LYS:HE2	6:H:62:MET:HE3	2.00	0.43
8:F:197:PHE:CD1	8:F:200:ILE:HD11	2.52	0.43
1:A:503:SER:O	1:A:507:SER:OG	2.25	0.43
3:B:271:PRO:HB2	3:B:273:TYR:CE1	2.52	0.43
8:F:325:ASN:O	8:F:329:LEU:HD13	2.19	0.43
2:E:97:LYS:HE2	2:E:99:TYR:CZ	2.53	0.43
3:B:417:ARG:HA	3:B:417:ARG:HD3	1.79	0.43
3:B:480:ARG:NH1	3:B:480:ARG:HA	2.34	0.43
3:B:688:TYR:O	3:B:692:GLU:HG2	2.18	0.43
3:B:1120:TYR:CE2	3:B:1122:VAL:HG13	2.54	0.43
5:D:103:LEU:O	5:D:107:VAL:HG13	2.18	0.43
3:B:309:LEU:O	3:B:312:SER:OG	2.30	0.43
3:B:432:ILE:HG21	3:B:481:SER:HB2	2.01	0.43
1:A:1233:ARG:HD2	1:A:1233:ARG:HA	1.80	0.43
3:B:39:LEU:C	3:B:40:ILE:HD13	2.39	0.43
3:B:301:VAL:HA	3:B:402:MET:HE3	2.01	0.43
3:B:558:SER:O	3:B:802:ASN:ND2	2.52	0.43
4:C:240:LYS:HG2	4:C:351:GLU:HG3	2.01	0.43
1:A:810:PHE:CZ	3:B:544:ARG:NH1	2.87	0.43
1:A:1350:HIS:HD2	5:D:190:THR:HG23	1.83	0.43
3:B:323:VAL:HG21	3:B:335:PHE:CD2	2.54	0.43
4:C:257:TYR:CZ	4:C:336:LEU:HD13	2.54	0.43
8:F:297:LEU:O	8:F:301:ILE:HG13	2.19	0.43
8:F:320:ILE:HG23	8:F:327:TRP:HE1	1.84	0.43
1:A:415:ALA:HB2	1:A:433:ILE:HD11	2.00	0.43
3:B:299:SER:OG	7:G:51:ASP:OD2	2.30	0.43
3:B:794:PRO:HA	3:B:797:VAL:HG23	2.01	0.43
3:B:825:PHE:O	3:B:879:GLY:HA3	2.19	0.43
3:B:830:GLU:HG2	6:H:73:THR:HA	2.00	0.43
5:D:87:GLU:HG3	5:D:88:LEU:N	2.34	0.43
1:A:1203:HIS:NE2	1:A:1257:SER:OG	2.49	0.43
3:B:1238:VAL:O	8:F:55:SER:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:182:VAL:O	5:D:182:VAL:HG13	2.19	0.43
8:F:101:LEU:HD23	8:F:113:VAL:HG22	2.01	0.43
1:A:725:PRO:HB3	1:A:731:PHE:CE2	2.54	0.43
3:B:585:SER:O	3:B:588:GLN:HG3	2.19	0.43
3:B:808:GLY:O	3:B:845:ASN:HB2	2.18	0.43
8:F:192:ARG:NH1	8:F:307:ILE:HG21	2.34	0.43
1:A:1395:LEU:HD11	3:B:1228:VAL:HG11	2.00	0.42
3:B:265:PHE:HE1	3:B:340:VAL:HG21	1.84	0.42
3:B:389:PHE:O	3:B:393:LEU:HG	2.18	0.42
4:C:142:ILE:HG13	4:C:143:PHE:CD2	2.54	0.42
3:B:130:LEU:O	3:B:155:PHE:N	2.52	0.42
6:H:37:LEU:HD23	6:H:40:ASN:ND2	2.34	0.42
1:A:1002:ILE:O	1:A:1006:LEU:HB2	2.19	0.42
3:B:682:LYS:O	3:B:685:GLN:HG3	2.19	0.42
5:D:42:ARG:NH1	5:D:42:ARG:HG2	2.34	0.42
1:A:88:ILE:HG21	1:A:151:TYR:O	2.19	0.42
3:B:121:GLY:HA2	3:B:197:GLY:HA3	2.01	0.42
1:A:1121:THR:OG1	1:A:1122:PHE:N	2.53	0.42
3:B:811:TYR:HE1	3:B:825:PHE:HB2	1.85	0.42
3:B:883:ARG:HD2	3:B:986:TYR:CE2	2.54	0.42
3:B:908:LYS:HA	3:B:909:PRO:HD3	1.91	0.42
1:A:226:ILE:HG23	1:A:270:PHE:HE1	1.85	0.42
1:A:438:ASN:HB2	4:C:317:GLN:HE22	1.84	0.42
5:D:9:TYR:HB2	5:D:126:PHE:O	2.20	0.42
1:A:407:ARG:NH1	1:A:408:ASP:O	2.52	0.42
1:A:1126:ILE:CG2	1:A:1178:LEU:HD23	2.49	0.42
1:A:1307:ASP:OD2	1:A:1307:ASP:N	2.53	0.42
3:B:280:GLY:HA2	3:B:329:ARG:HD3	2.01	0.42
3:B:384:VAL:O	3:B:387:LEU:HB2	2.19	0.42
3:B:442:ILE:O	3:B:446:LYS:HG3	2.19	0.42
1:A:1329:GLU:HB3	5:D:137:PRO:HG2	2.01	0.42
2:E:90:ASN:HD22	8:F:17:THR:HB	1.85	0.42
3:B:334:GLN:HE22	3:B:350:TYR:HE2	1.68	0.42
3:B:512:LYS:HE3	3:B:806:GLN:HA	2.02	0.42
3:B:731:ASP:O	3:B:735:GLN:HG2	2.20	0.42
1:A:422:SER:HB3	3:B:1154:VAL:HG21	2.01	0.42
1:A:810:PHE:HZ	3:B:544:ARG:NH1	2.18	0.42
3:B:71:ASP:CG	3:B:82:ARG:HH21	2.23	0.42
3:B:98:ARG:NH2	3:B:173:HIS:HE1	2.18	0.42
3:B:439:ALA:HB3	3:B:440:PRO:HD3	2.01	0.42
6:H:21:PHE:HB2	6:H:58:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1251:VAL:HG13	1:A:1255:LEU:HD23	2.02	0.41
3:B:116:LYS:HD2	3:B:120:CYS:SG	2.60	0.41
4:C:10:ILE:HG12	4:C:43:VAL:HG22	2.01	0.41
8:F:90:VAL:HG12	8:F:130:VAL:O	2.20	0.41
8:F:106:LEU:HD11	8:F:313:THR:OG1	2.20	0.41
1:A:150:ASP:OD1	1:A:150:ASP:N	2.53	0.41
1:A:843:ARG:NH1	5:D:154:GLU:OE1	2.46	0.41
1:A:1120:ILE:HA	1:A:1124:ARG:HD3	2.01	0.41
1:A:1125:LEU:HD13	1:A:1195:ILE:HD11	2.02	0.41
3:B:288:ILE:HD12	3:B:288:ILE:HA	1.94	0.41
3:B:890:GLU:H	3:B:894:GLU:HB2	1.85	0.41
5:D:78:THR:HA	5:D:81:GLU:OE2	2.21	0.41
1:A:438:ASN:HB3	1:A:441:ILE:HD12	2.03	0.41
1:A:533:THR:HB	1:A:642:ASN:HD21	1.84	0.41
1:A:681:ASN:ND2	1:A:780:LEU:O	2.51	0.41
1:A:938:VAL:O	1:A:941:ILE:HG22	2.20	0.41
3:B:228:ILE:HB	3:B:401:ILE:HD11	2.01	0.41
3:B:326:GLU:OE2	3:B:331:LYS:HB2	2.19	0.41
8:F:306:PHE:CZ	8:F:310:LEU:HD11	2.56	0.41
3:B:138:ALA:HB3	3:B:146:GLU:HB3	2.03	0.41
3:B:658:ASP:HB2	7:G:55:ILE:HG21	2.03	0.41
8:F:200:ILE:HG13	8:F:201:CYS:N	2.35	0.41
1:A:650:THR:OG1	3:B:853:TYR:O	2.24	0.41
3:B:227:ILE:HD11	3:B:250:TYR:CE2	2.56	0.41
3:B:855:ILE:HD11	3:B:1031:HIS:HE1	1.85	0.41
8:F:131:PRO:HG3	8:F:207:TYR:OH	2.20	0.41
1:A:67:LYS:HE2	1:A:67:LYS:HB2	1.83	0.41
1:A:993:ARG:HG3	5:D:195:VAL:HG23	2.01	0.41
3:B:14:GLU:CD	3:B:14:GLU:H	2.23	0.41
6:H:55:ILE:HG21	6:H:67:ARG:HG2	2.03	0.41
8:F:195:LYS:HE3	8:F:308:ASN:HA	2.03	0.41
2:E:99:TYR:CZ	2:E:108:GLN:HG3	2.56	0.41
3:B:251:MET:HG2	3:B:255:ALA:O	2.21	0.41
4:C:125:ILE:HD11	4:C:152:LEU:HG	2.03	0.41
1:A:46:TYR:CE1	1:A:212:ILE:HG23	2.56	0.41
1:A:656:MET:SD	3:B:1033:HIS:CE1	3.14	0.41
1:A:743:PRO:O	1:A:747:HIS:ND1	2.54	0.41
1:A:860:LEU:HD21	1:A:1030:TYR:HE1	1.86	0.41
3:B:276:PHE:HB3	3:B:287:ILE:HD12	2.01	0.41
3:B:908:LYS:HE2	3:B:954:SER:H	1.86	0.41
8:F:263:LEU:HG	8:F:269:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:TYR:HB2	1:A:843:ARG:HG3	2.03	0.40
1:A:1117:ILE:HD11	1:A:1293:ILE:HG21	2.02	0.40
1:A:419:ARG:HB2	1:A:463:MET:HG2	2.04	0.40
8:F:185:ILE:HG13	8:F:301:ILE:HG12	2.02	0.40
8:F:293:PHE:O	8:F:297:LEU:HD23	2.22	0.40
1:A:152:PHE:HD1	1:A:153:THR:HG23	1.86	0.40
1:A:680:ILE:HD13	1:A:704:LEU:HB3	2.03	0.40
3:B:382:THR:O	3:B:386:LYS:HG3	2.21	0.40
3:B:590:LEU:HD13	3:B:622:ILE:HD11	2.03	0.40
3:B:654:ASP:HB3	3:B:659:GLU:HG2	2.02	0.40
5:D:76:THR:HG22	5:D:109:GLN:NE2	2.35	0.40
6:H:44:ASP:O	6:H:48:GLN:HG2	2.21	0.40
1:A:673:LEU:HD11	1:A:712:PRO:HD3	2.03	0.40
1:A:475:VAL:HG22	2:E:103:ILE:HG23	2.04	0.40
3:B:20:GLU:HG2	3:B:716:PRO:HG2	2.04	0.40
3:B:815:TRP:CD1	3:B:816:PRO:HD3	2.56	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	A	1363/1450 (94%)	1307 (96%)	56 (4%)	0	100	100
2	E	104/147 (71%)	102 (98%)	2 (2%)	0	100	100
3	B	1186/1242 (96%)	1138 (96%)	48 (4%)	0	100	100
4	C	355/359 (99%)	346 (98%)	9 (2%)	0	100	100
5	D	203/205 (99%)	195 (96%)	8 (4%)	0	100	100
6	H	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
7	G	57/105 (54%)	51 (90%)	6 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	F	337/339 (99%)	324 (96%)	13 (4%)	0	100	100
All	All	3683/3927 (94%)	3538 (96%)	145 (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	A	1219/1279 (95%)	1186 (97%)	33 (3%)	40	67
2	E	96/136 (71%)	94 (98%)	2 (2%)	48	74
3	B	1038/1081 (96%)	1025 (99%)	13 (1%)	65	84
4	C	326/328 (99%)	322 (99%)	4 (1%)	67	85
5	D	185/185 (100%)	179 (97%)	6 (3%)	34	60
6	H	70/70 (100%)	67 (96%)	3 (4%)	25	49
7	G	54/96 (56%)	53 (98%)	1 (2%)	52	77
8	F	312/312 (100%)	305 (98%)	7 (2%)	47	73
All	All	3300/3487 (95%)	3231 (98%)	69 (2%)	49	74

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	23	ARG
1	A	56	HIS
1	A	66	ARG
1	A	68	GLN
1	A	168	GLN
1	A	180	ASP
1	A	184	LYS
1	A	191	SER
1	A	328	CYS

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Mol	Chain	Res	Type
1	A	363	MET
1	A	400	GLU
1	A	417	PHE
1	A	446	MET
1	A	537	ASP
1	A	646	ASN
1	A	664	GLN
1	A	682	ASN
1	A	690	MET
1	A	826	ASN
1	A	830	ILE
1	A	869	ARG
1	A	900	ARG
1	A	1099	LYS
1	A	1144	MET
1	A	1155	MET
1	A	1240	MET
1	A	1266	LYS
1	A	1269	ASN
1	A	1304	MET
1	A	1307	ASP
1	A	1358	ASP
1	A	1362	ARG
2	E	54	SER
2	E	139	ARG
3	B	25	ASP
3	B	196	ARG
3	B	293	PHE
3	B	309	LEU
3	B	311	LYS
3	B	363	ARG
3	B	480	ARG
3	B	544	ARG
3	B	886	LYS
3	B	956	MET
3	B	1140	ARG
3	B	1209	MET
3	B	1235	SER
4	C	11	LYS
4	C	210	MET
4	C	255	LYS
4	C	331	ASP

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Mol	Chain	Res	Type
5	D	4	GLN
5	D	17	ARG
5	D	63	LYS
5	D	101	ASN
5	D	125	LEU
5	D	202	LYS
6	H	32	LYS
6	H	46	SER
6	H	62	MET
7	G	83	GLN
8	F	62	THR
8	F	70	MET
8	F	91	LYS
8	F	140	TYR
8	F	194	LYS
8	F	197	PHE
8	F	269	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	224	HIS
1	A	264	GLN
1	A	265	GLN
1	A	355	GLN
1	A	420	GLN
1	A	485	ASN
1	A	592	GLN
1	A	646	ASN
1	A	721	ASN
1	A	826	ASN
1	A	834	GLN
1	A	910	GLN
1	A	919	ASN
1	A	1161	ASN
1	A	1349	ASN
1	A	1350	HIS
1	A	1439	ASN
2	E	63	ASN
2	E	90	ASN
3	B	173	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	B	216	HIS
3	B	235	GLN
3	B	314	HIS
3	B	325	HIS
3	B	364	GLN
3	B	419	HIS
3	B	557	GLN
3	B	570	GLN
3	B	845	ASN
3	B	861	GLN
3	B	1112	GLN
3	B	1142	HIS
3	B	1162	GLN
3	B	1227	ASN
3	B	1229	ASN
4	C	254	GLN
4	C	345	GLN
5	D	66	HIS
6	H	48	GLN
8	F	4	GLN
8	F	121	ASN
8	F	272	GLN
8	F	332	GLN

### 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 ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

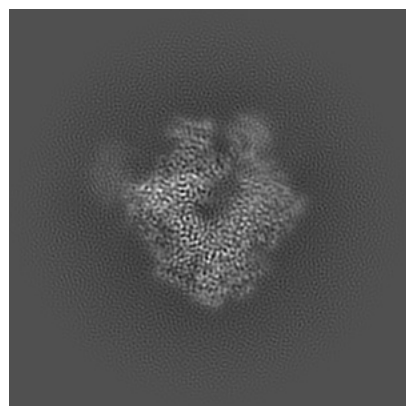
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39507. These allow visual inspection of the internal detail of the map and identification of artifacts.

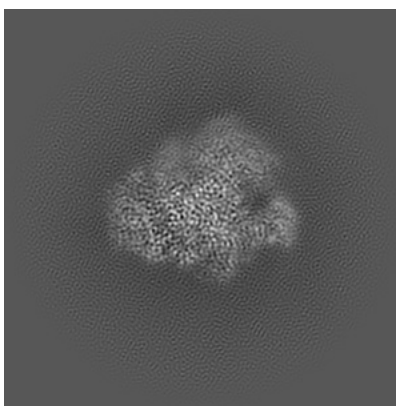
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

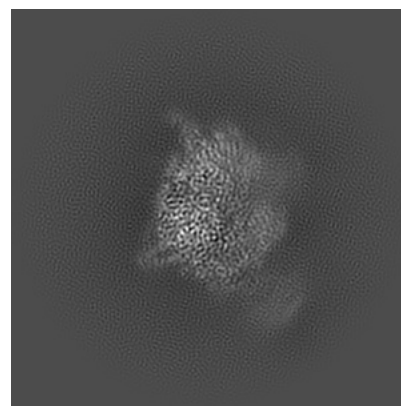
#### 6.1.1 Primary map



X

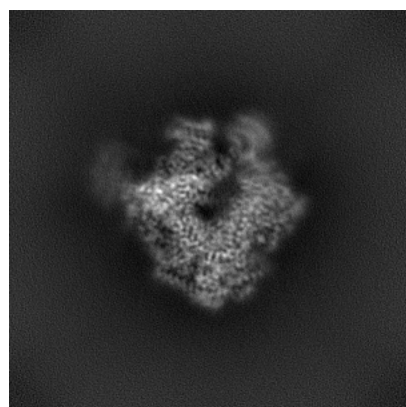


Y

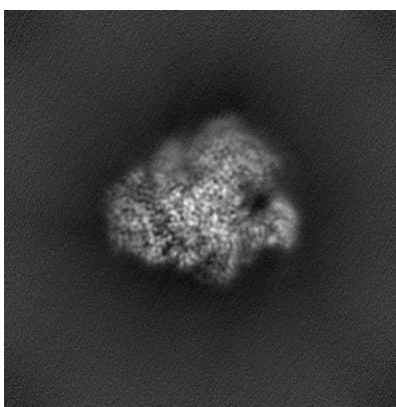


Z

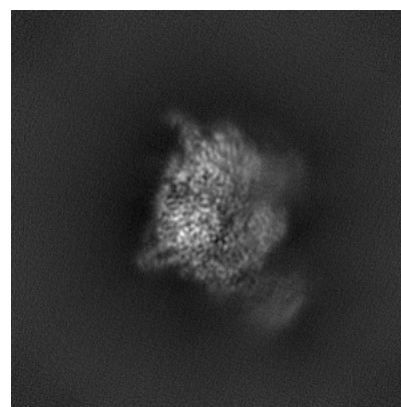
#### 6.1.2 Raw map



X



Y

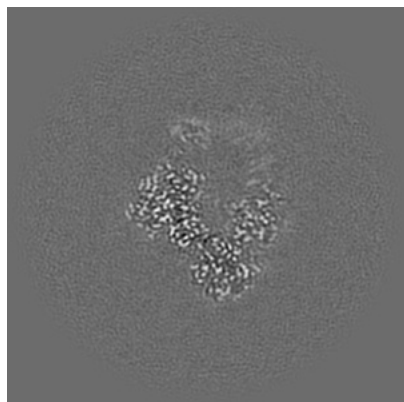


Z

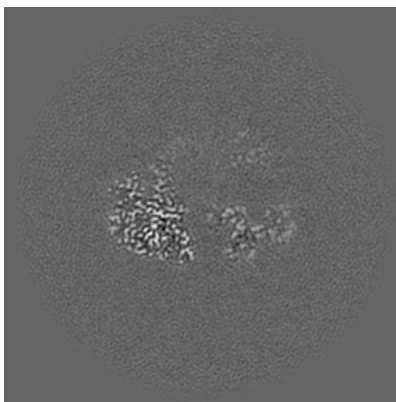
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

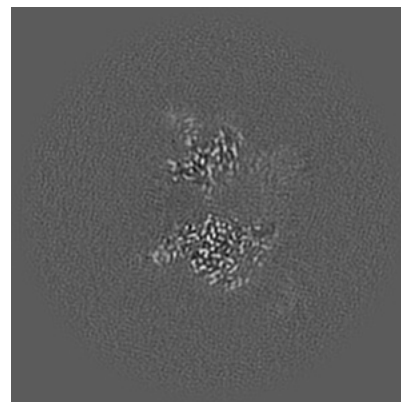
### 6.2.1 Primary map



X Index: 180

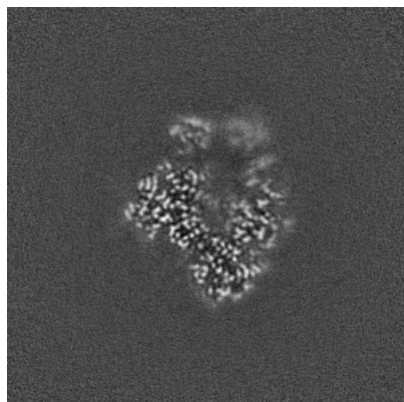


Y Index: 180

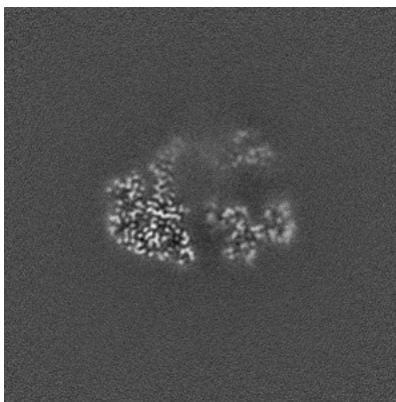


Z Index: 180

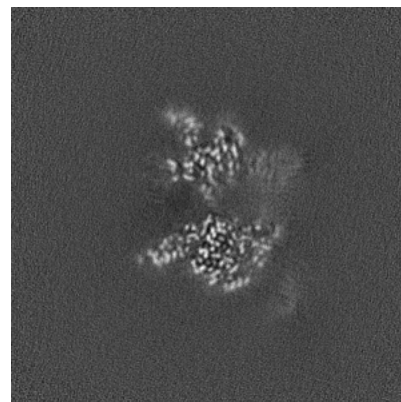
### 6.2.2 Raw map



X Index: 180



Y Index: 180

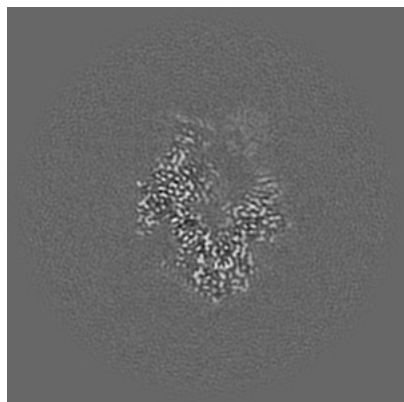


Z Index: 180

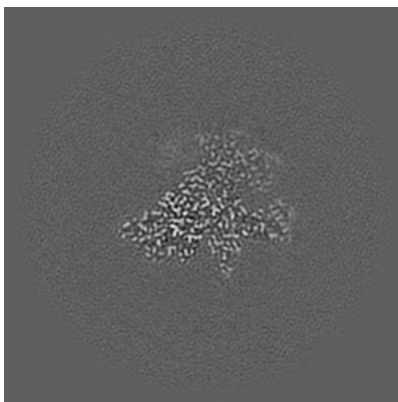
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

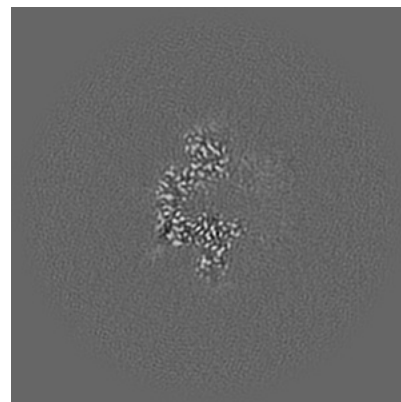
### 6.3.1 Primary map



X Index: 172

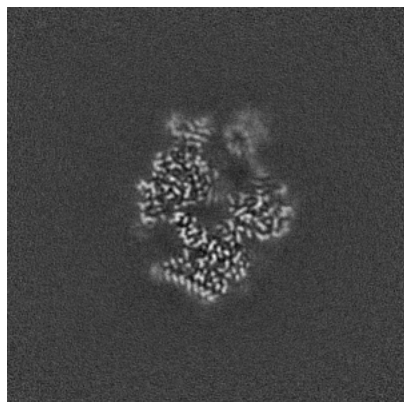


Y Index: 159

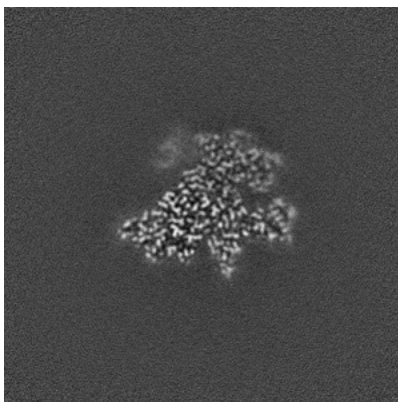


Z Index: 166

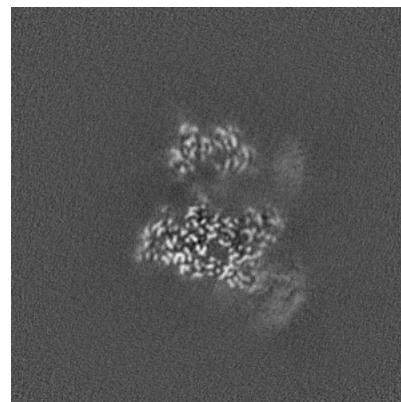
### 6.3.2 Raw map



X Index: 167



Y Index: 159

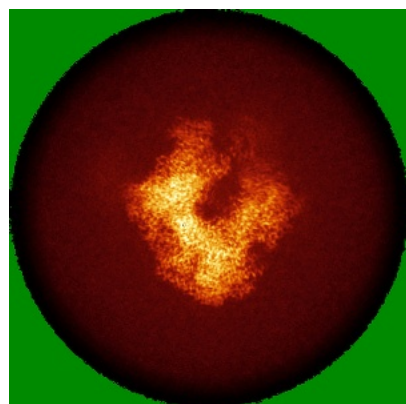


Z Index: 197

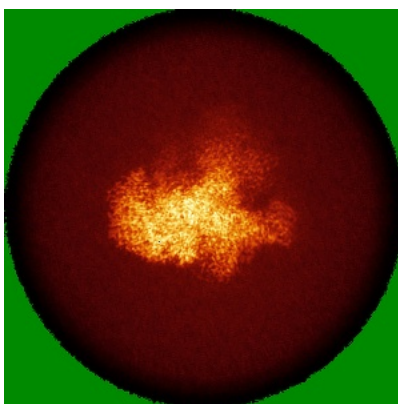
The images above show the largest variance slices of the map in three orthogonal directions.

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

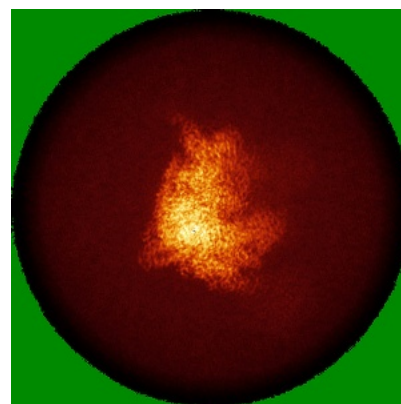
### 6.4.1 Primary map



X

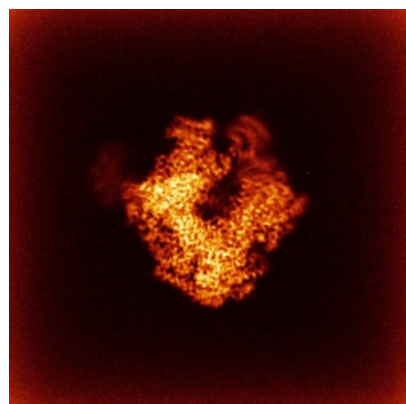


Y

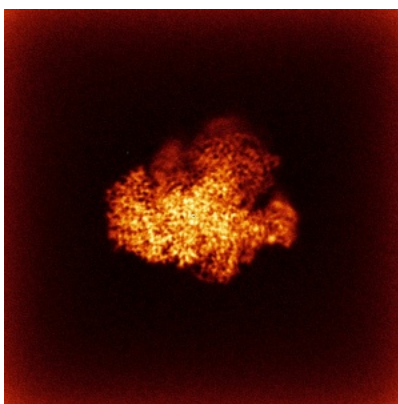


Z

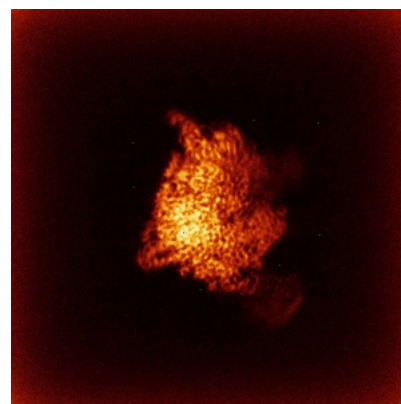
### 6.4.2 Raw map



X



Y

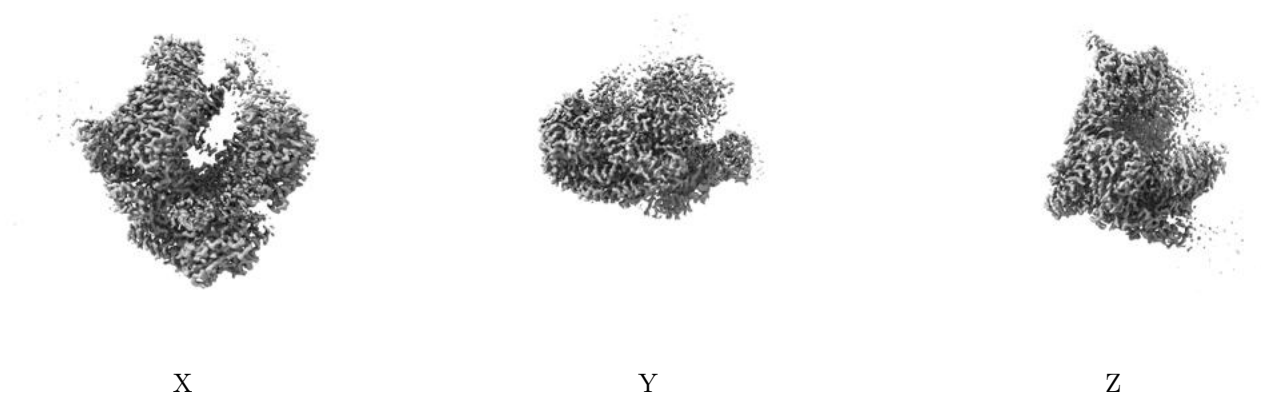


Z

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.

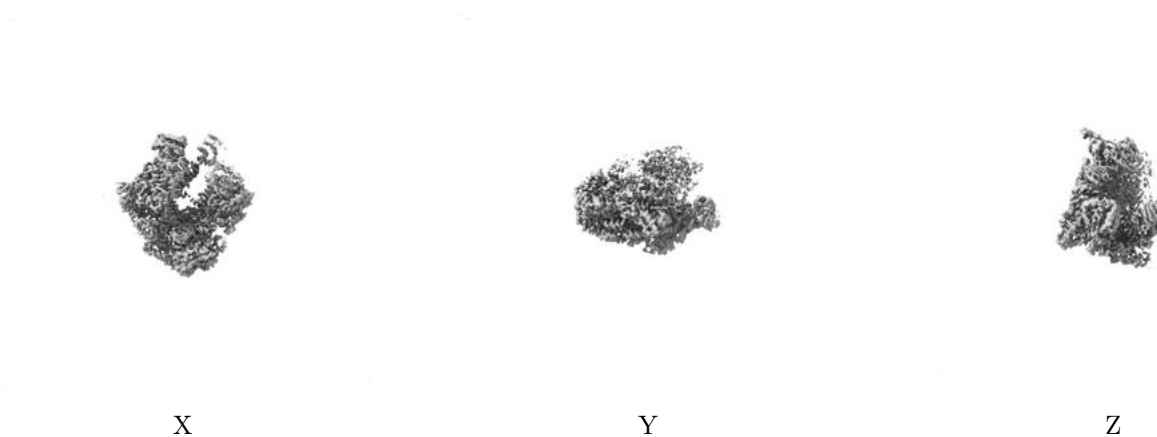
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.488. 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.

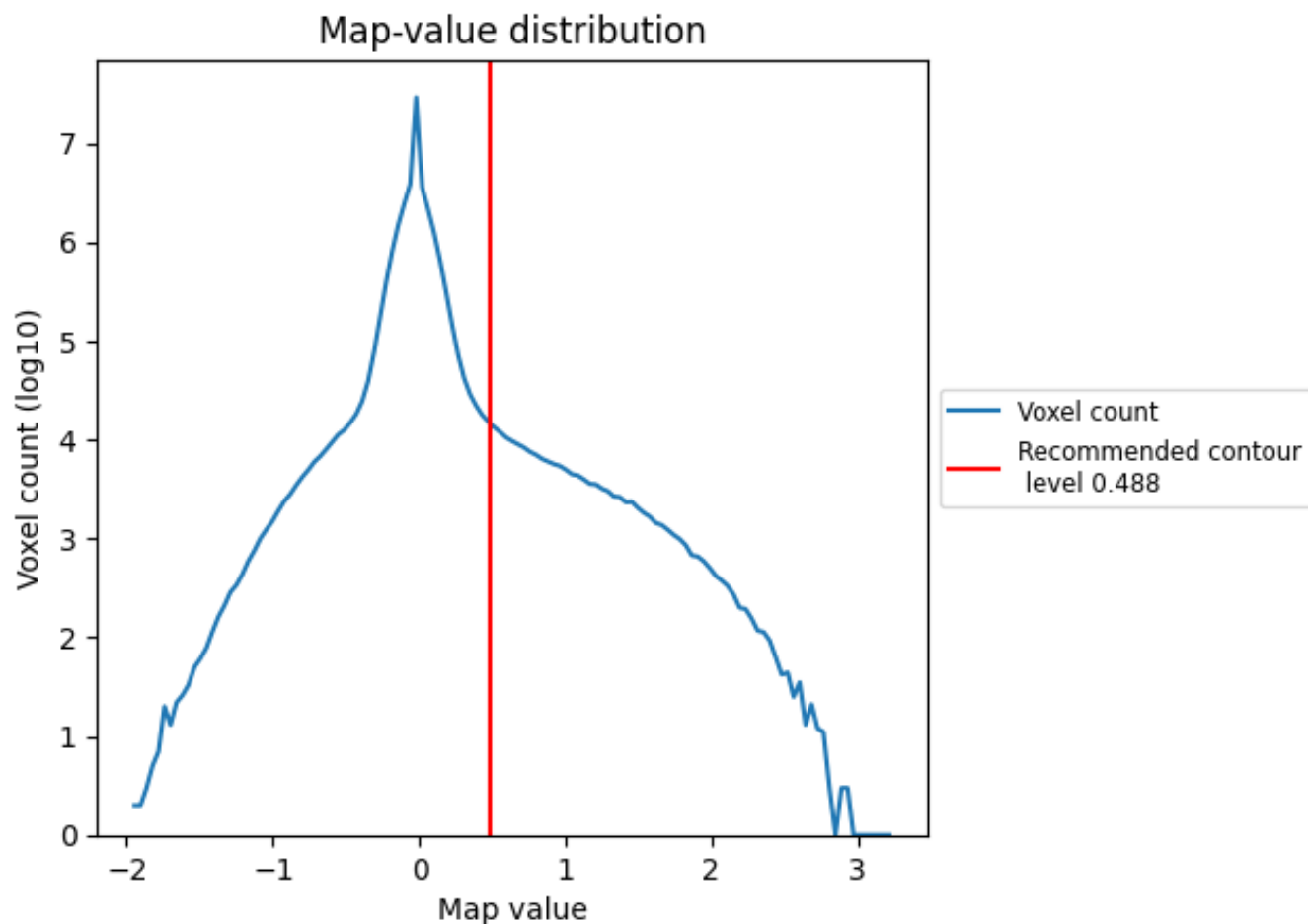
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

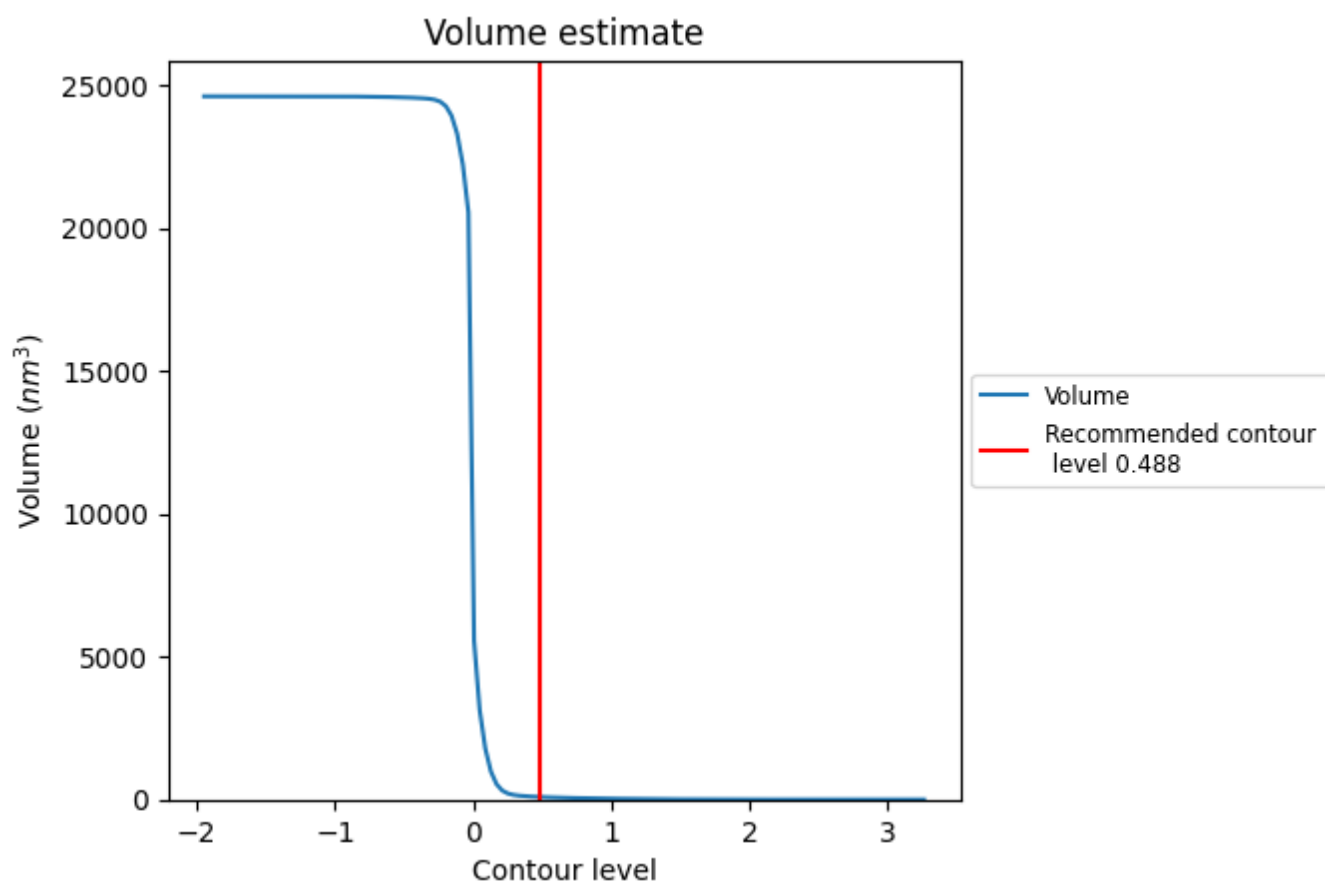
This section contains the results of statistical analysis of the map.

### 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.

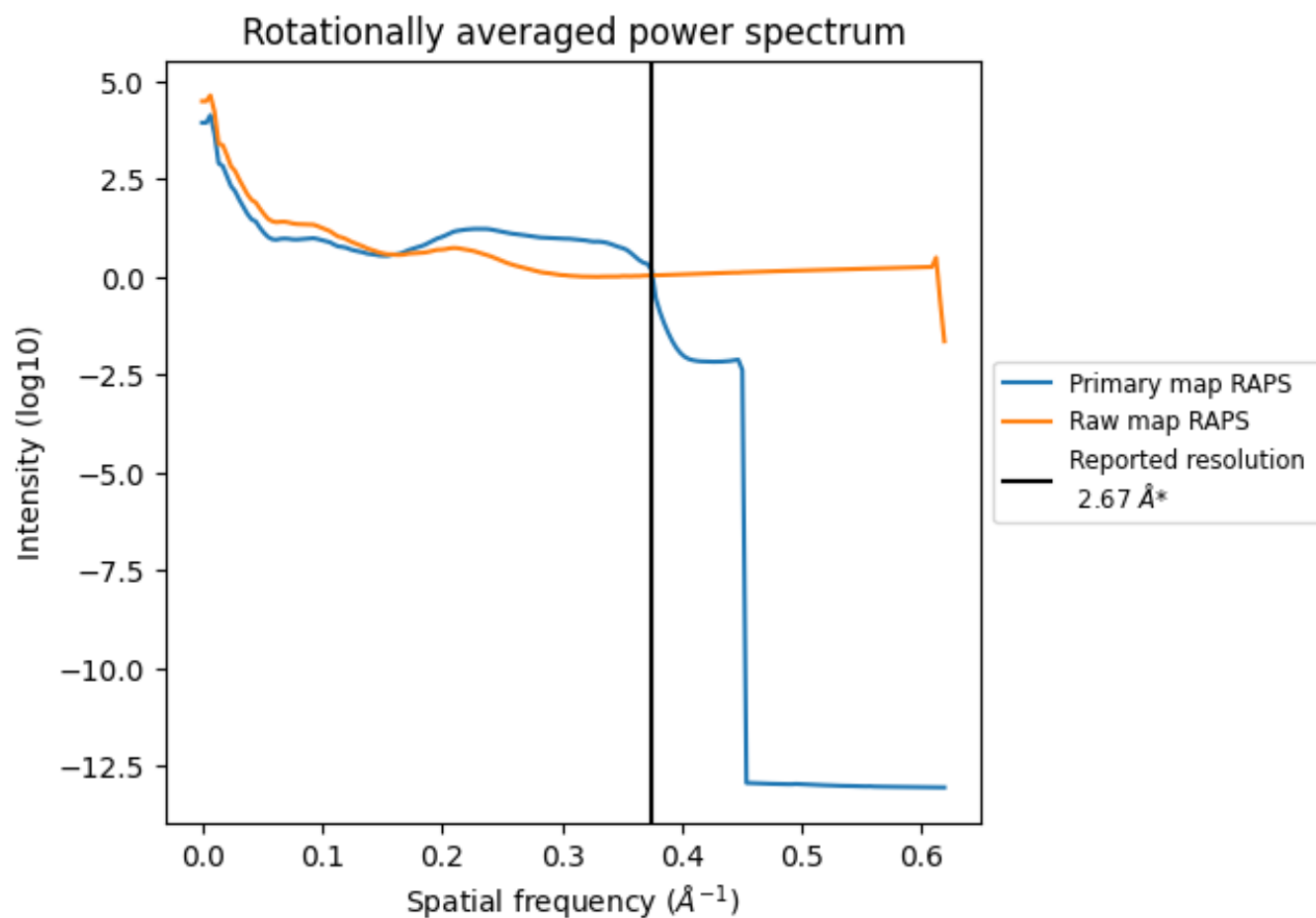
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 89  $\text{nm}^3$ ; this corresponds to an approximate mass of 80 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 ⓘ

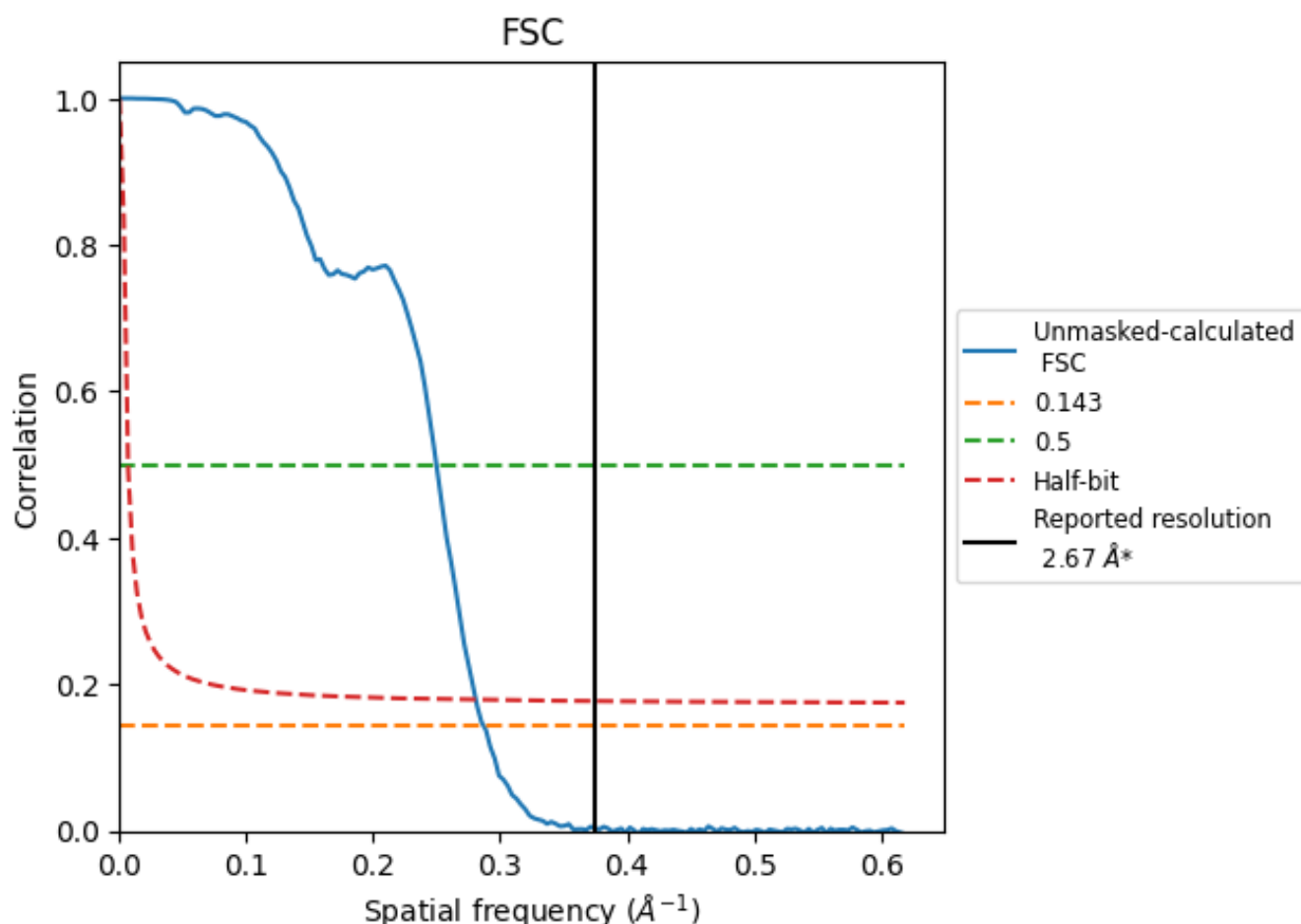


\*Reported resolution corresponds to spatial frequency of 0.375 Å<sup>-1</sup>

## 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 0.375  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

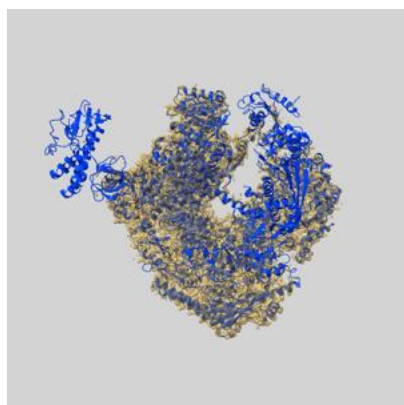
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.67	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.48	4.00	3.56

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.48 differs from the reported value 2.67 by more than 10 %

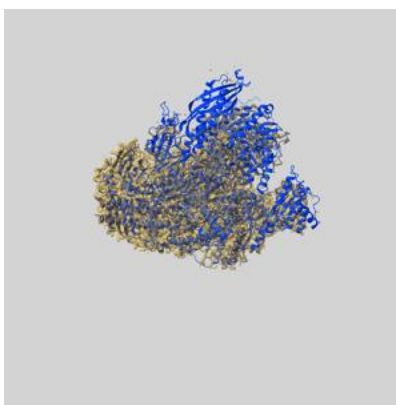
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39507 and PDB model 8YQV. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

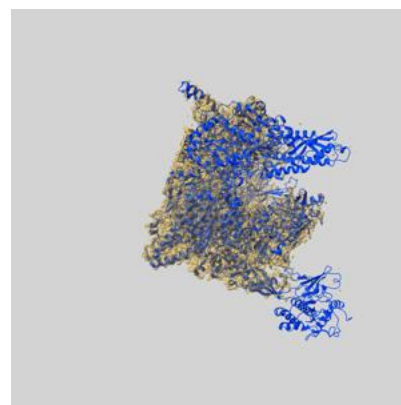
### 9.1 Map-model overlay [i](#)



X



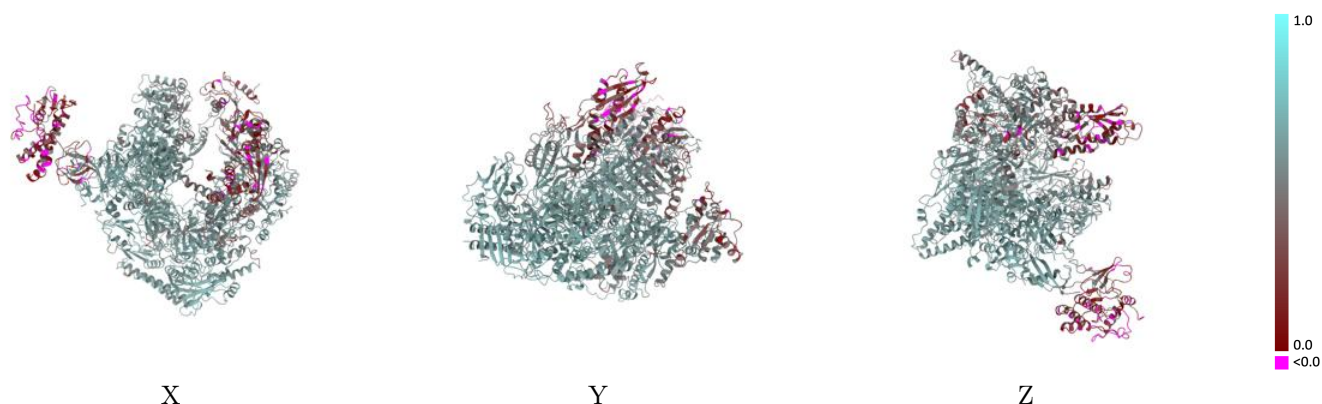
Y



Z

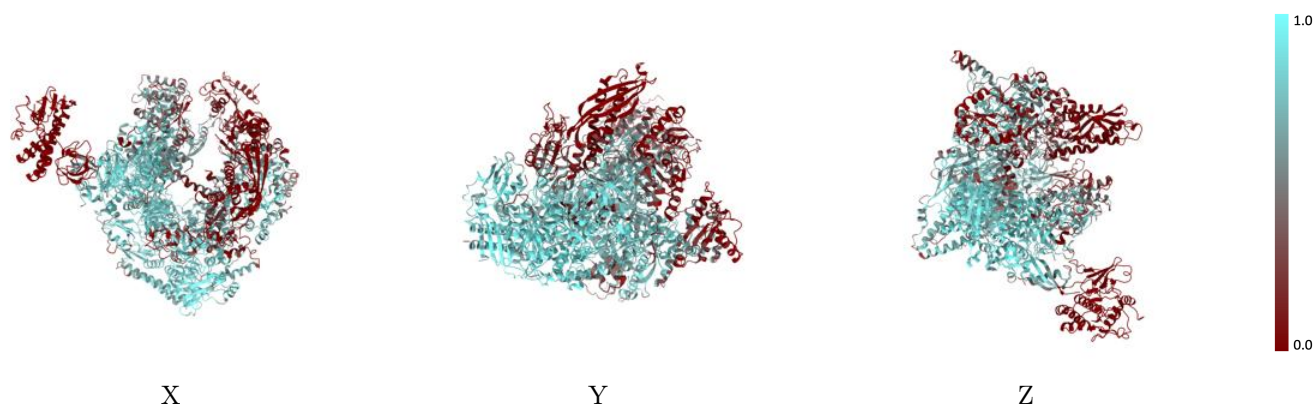
The images above show the 3D surface view of the map at the recommended contour level 0.488 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



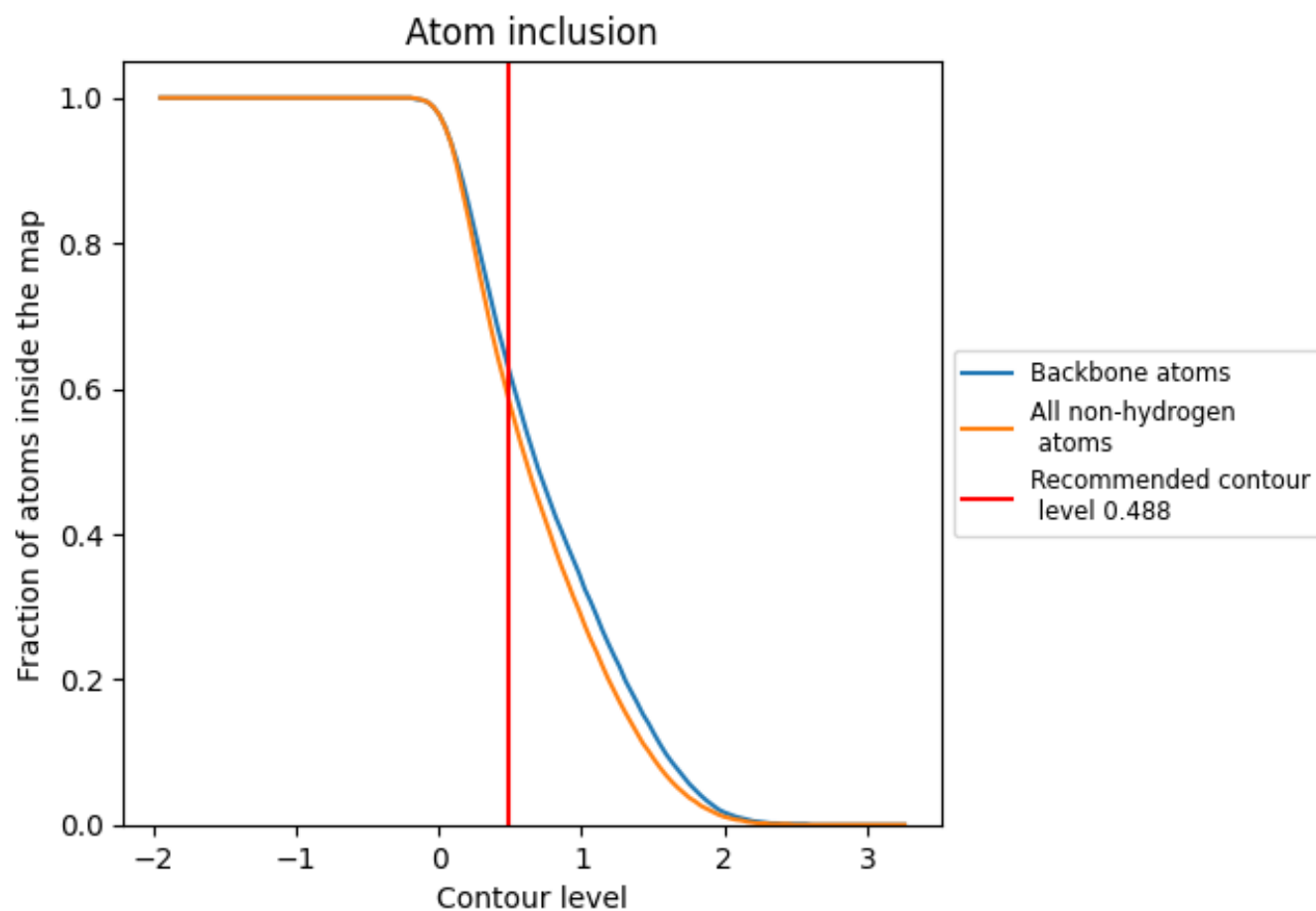
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.488).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 59% 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 (0.488) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5870	<div></div> 0.5370
A	<div></div> 0.6880	<div></div> 0.5840
B	<div></div> 0.4690	<div></div> 0.5080
C	<div></div> 0.8290	<div></div> 0.6230
D	<div></div> 0.6960	<div></div> 0.5940
E	<div></div> 0.7910	<div></div> 0.6170
F	<div></div> 0.1610	<div></div> 0.2850
G	<div></div> 0.5950	<div></div> 0.5490
H	<div></div> 0.7640	<div></div> 0.6010

1.0

0.0

<0.0