



Full wwPDB EM Validation Report ⓘ

Jul 27, 2026 – 12:29 PM EDT

PDB ID : 9ZPL / pdb_00009zpl
EMDB ID : EMD-74529
Title : Cryo-EM structure of the complete *Saccharomyces cerevisiae* RNA polymerase II in open clamp conformation
Authors : Fordjour, G.N.R.; Murakami, K.; Armache, J.-P.; Murakami, K.S.
Deposited on : 2025-12-16
Resolution : 3.75 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.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

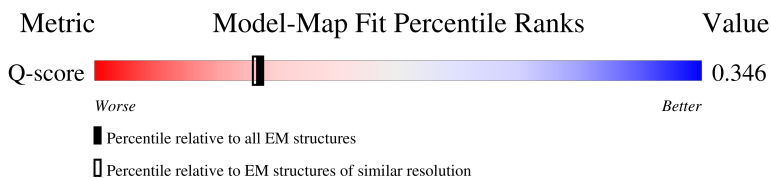
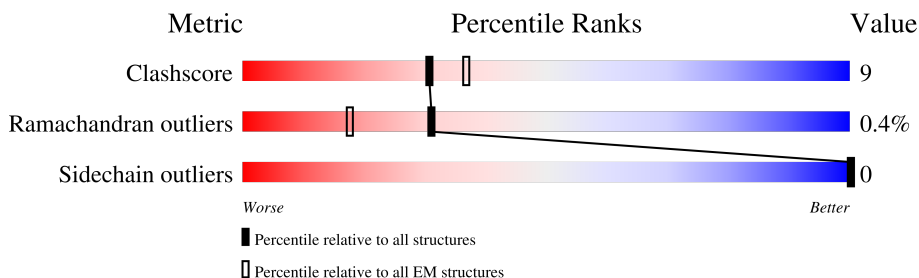
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10301 (3.25 - 4.25)

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	C	318	
2	E	215	
3	F	155	
4	G	171	

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Mol	Chain	Length	Quality of chain
5	I	122	66%27%7%
6	J	70	70%23%6%
7	K	120	12%79%17%
8	L	70	46%17%37%
9	A	1733	57%18%25%
10	B	1224	73%21%6%
11	H	146	74%19%7%
12	D	221	54%17%29%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 30372 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 II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	265	Total	C	N	O	S	0	0
			2086	1312	347	414	13		

- Molecule 2 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 3 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	87	Total	C	N	O	S	0	0
			705	451	119	132	3		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	114	Total	C	N	O	S	0	0
			927	571	168	178	10		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	66	Total	C	N	O	S	0	0
			540	345	94	95	6		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	115	Total	C	N	O	S	0	0
			924	593	157	172	2		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	1304	Total	C	N	O	S	0	0
			10253	6459	1787	1955	52		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	1153	Total	C	N	O	S	0	0
			9144	5777	1601	1711	55		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	136	Total	C	N	O	S	0	0
			1089	685	184	215	5		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	157	Total	C	N	O	S	0	0
			1253	779	220	252	2		

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
13	C	1	Total	Zn	0
			1	1	
13	I	2	Total	Zn	0
			2	2	

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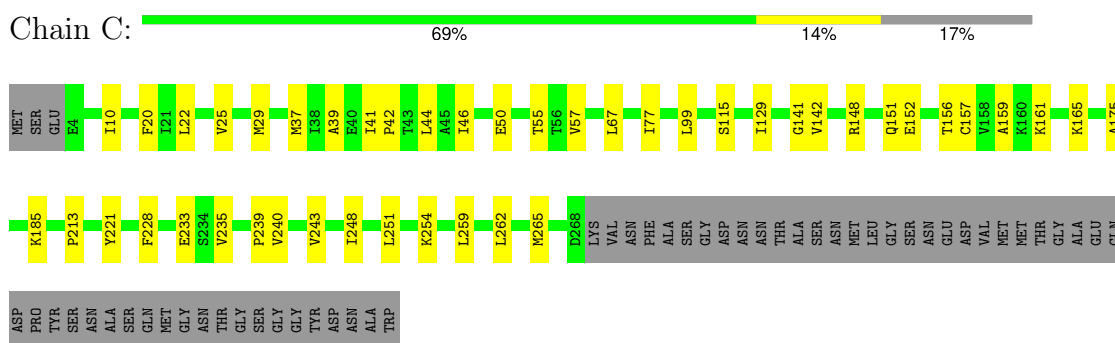
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Mol	Chain	Residues	Atoms		AltConf
13	J	1	Total 1	Zn 1	0
13	L	1	Total 1	Zn 1	0
13	A	1	Total 1	Zn 1	0
13	B	1	Total 1	Zn 1	0

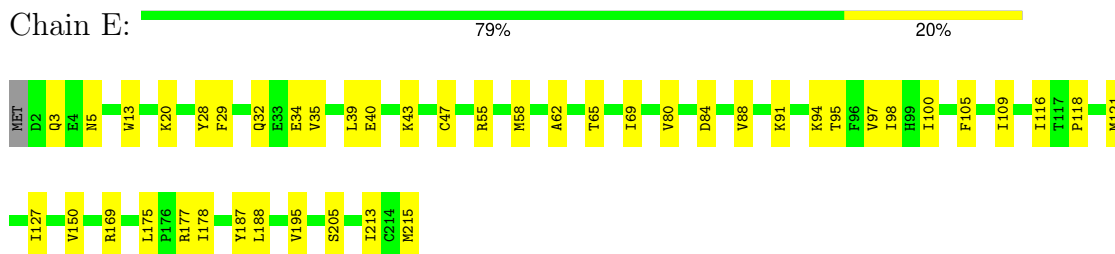
3 Residue-property plots

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.

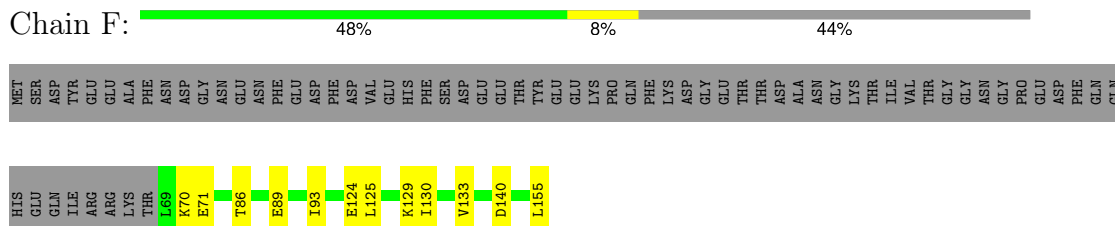
- Molecule 1: DNA-directed RNA polymerase II subunit RPB3



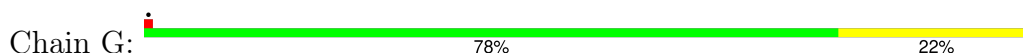
- Molecule 2: DNA-directed RNA polymerases I, II, and III subunit RPABC1



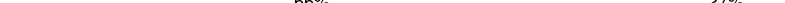
- Molecule 3: DNA-directed RNA polymerases I, II, and III subunit RPABC2

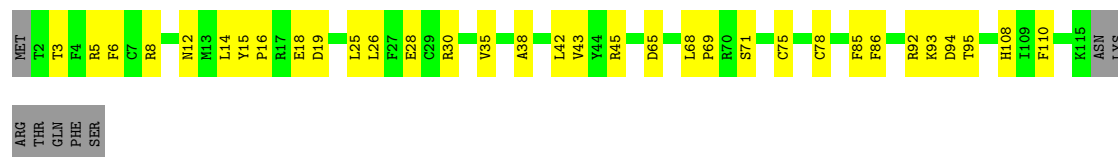


- Molecule 4: DNA-directed RNA polymerase II subunit RPB7



- Molecule 5: DNA-directed RNA polymerase II subunit RPB9

Chain I: 



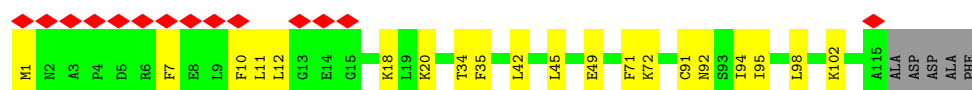
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  70% 23% • 6%

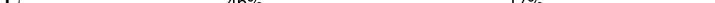


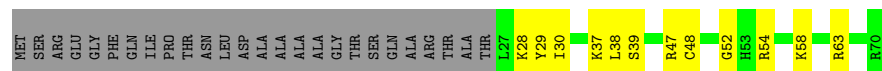
- Molecule 7: DNA-directed RNA polymerase II subunit RPB11

Chain K: 

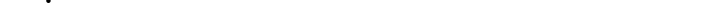


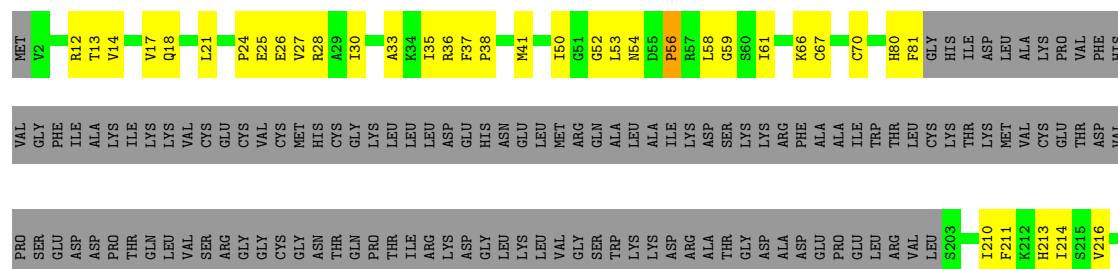
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:  46% 17% 37%



- Molecule 9: DNA-directed RNA polymerase II subunit RPB1

Chain A:  57% 18% 25%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59723	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.012	Depositor
Minimum map value	-0.363	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	377.6, 377.6, 377.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.944, 0.944, 0.944	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	C	0.15	0/2124	0.37	0/2879
2	E	0.12	0/1788	0.34	0/2406
3	F	0.18	0/717	0.46	0/967
4	G	0.14	0/1368	0.39	0/1844
5	I	0.13	0/945	0.37	0/1273
6	J	0.17	0/549	0.45	0/738
7	K	0.14	0/942	0.35	0/1272
8	L	0.17	0/354	0.59	0/468
9	A	0.16	0/10437	0.42	2/14124 (0.0%)
10	B	0.16	0/9317	0.43	3/12564 (0.0%)
11	H	0.15	0/1107	0.45	0/1498
12	D	0.10	0/1262	0.30	0/1693
All	All	0.15	0/30910	0.41	5/41726 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	334	ILE	N-CA-C	-5.79	106.14	112.80
9	A	1097	GLY	CA-C-N	5.77	123.87	120.24
9	A	1097	GLY	C-N-CA	5.77	123.87	120.24
10	B	277	LYS	N-CA-C	5.51	115.11	107.73
10	B	472	ALA	CB-CA-C	-5.07	110.34	117.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2086	0	2045	33	0
2	E	1752	0	1776	27	0
3	F	705	0	731	11	0
4	G	1340	0	1357	23	0
5	I	927	0	880	26	0
6	J	540	0	553	12	0
7	K	924	0	934	14	0
8	L	352	0	374	11	0
9	A	10253	0	10262	213	0
10	B	9144	0	9132	180	0
11	H	1089	0	1063	20	0
12	D	1253	0	1275	22	0
13	A	1	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
All	All	30372	0	30382	538	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 (538) 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)
9:A:306:ASN:H	9:A:326:ARG:HB3	1.35	0.89
3:F:155:LEU:HD11	9:A:1055:ARG:HG3	1.67	0.77
10:B:883:LEU:HA	10:B:931:TYR:HB3	1.67	0.76
9:A:513:SER:HB2	9:A:520:CYS:HB2	1.70	0.74
10:B:926:GLY:HA2	10:B:928:ARG:HH11	1.53	0.73
10:B:301:ILE:HD11	10:B:382:ILE:HB	1.69	0.73
2:E:175:LEU:HD22	2:E:213:ILE:HG13	1.71	0.73
9:A:1116:LEU:HD21	9:A:1316:VAL:HG11	1.72	0.72
10:B:72:GLU:HB3	10:B:87:LYS:HD3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:VAL:HG11	6:J:60:PHE:HB3	1.73	0.71
9:A:326:ARG:HA	9:A:329:LEU:HG	1.72	0.71
10:B:1180:PHE:HB3	10:B:1191:ILE:HG13	1.73	0.71
11:H:57:VAL:HG12	11:H:144:ILE:HG22	1.71	0.70
9:A:1107:VAL:HB	9:A:1383:SER:HB3	1.74	0.70
10:B:348:ARG:HG2	10:B:351:TYR:H	1.56	0.69
1:C:37:MET:HE1	1:C:243:VAL:HG23	1.75	0.69
9:A:38:PRO:HG3	9:A:274:ILE:HG13	1.75	0.69
4:G:27:LYS:HG2	4:G:54:ILE:HD11	1.74	0.68
9:A:14:VAL:HA	10:B:1218:THR:HA	1.76	0.68
10:B:364:ILE:HG21	10:B:585:VAL:HB	1.75	0.68
10:B:863:GLU:HB2	10:B:961:LEU:HB3	1.75	0.68
9:A:41:MET:HE1	9:A:53:LEU:HB3	1.75	0.68
10:B:512:ARG:HA	10:B:534:GLY:HA3	1.75	0.67
10:B:949:VAL:HG12	10:B:968:VAL:HG12	1.77	0.67
11:H:37:LYS:H	11:H:126:GLU:HB2	1.59	0.67
2:E:43:LYS:O	2:E:47:CYS:HB2	1.95	0.66
7:K:91:CYS:HA	7:K:94:ILE:HD12	1.77	0.66
9:A:1336:MET:HE2	9:A:1381:LEU:H	1.59	0.66
9:A:50:ILE:HB	9:A:53:LEU:HB2	1.78	0.66
9:A:1398:MET:HG3	9:A:1426:GLU:HG2	1.77	0.65
9:A:27:VAL:HA	9:A:30:ILE:HG12	1.78	0.65
10:B:67:SER:HB2	10:B:92:PHE:H	1.61	0.65
4:G:89:GLY:HA3	4:G:103:VAL:HG22	1.77	0.65
9:A:477:PRO:HG2	9:A:521:MET:HG2	1.79	0.65
9:A:917:SER:HA	9:A:920:LEU:HD13	1.79	0.64
10:B:957:ASN:HD21	10:B:961:LEU:HD12	1.63	0.64
9:A:779:PHE:HE2	9:A:785:PRO:HG3	1.63	0.64
1:C:77:ILE:HG13	1:C:161:LYS:HE3	1.78	0.63
9:A:12:ARG:HH21	10:B:1218:THR:HG23	1.63	0.63
4:G:91:VAL:HG22	4:G:101:VAL:HG22	1.81	0.62
8:L:30:ILE:HD11	8:L:37:LYS:HD3	1.81	0.62
9:A:507:VAL:HG13	9:A:521:MET:HE1	1.81	0.62
9:A:850:VAL:HG22	9:A:856:THR:HG22	1.80	0.62
4:G:131:GLN:HG3	4:G:136:VAL:HG13	1.82	0.62
6:J:44:TYR:HA	6:J:47:ARG:HB3	1.80	0.62
9:A:1115:SER:HB3	9:A:1330:ASN:HB2	1.81	0.62
9:A:18:GLN:HA	9:A:1418:LEU:HA	1.82	0.61
9:A:306:ASN:HB3	9:A:327:ALA:H	1.65	0.61
10:B:348:ARG:HD3	10:B:351:TYR:HB2	1.81	0.61
1:C:46:ILE:HA	1:C:159:ALA:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:198:LEU:HB3	12:D:207:LEU:HD22	1.81	0.61
7:K:1:MET:HB3	9:A:372:LYS:HZ3	1.66	0.61
10:B:334:ILE:HG21	10:B:336:ARG:HH21	1.65	0.61
9:A:347:PHE:H	10:B:1107:ALA:HA	1.64	0.61
1:C:115:SER:HB2	1:C:141:GLY:HA3	1.82	0.60
10:B:833:TYR:H	10:B:840:ILE:HD11	1.65	0.60
9:A:1143:LEU:HD22	9:A:1267:MET:HE3	1.84	0.60
4:G:121:PHE:HA	4:G:130:TYR:HA	1.84	0.60
9:A:247:ARG:HD3	9:A:262:LEU:HD23	1.84	0.60
9:A:446:ARG:HB2	9:A:487:MET:HE3	1.83	0.60
4:G:4:ILE:HG23	12:D:50:LEU:HD11	1.84	0.60
10:B:428:ILE:HD11	10:B:446:LEU:HB3	1.83	0.60
1:C:22:LEU:HG	1:C:25:VAL:HG21	1.84	0.59
9:A:505:CYS:HA	9:A:510:GLN:HE22	1.67	0.59
10:B:342:GLY:HA3	10:B:348:ARG:HD2	1.84	0.59
5:I:75:CYS:HB2	5:I:78:CYS:HB3	1.84	0.59
10:B:298:LEU:HA	10:B:301:ILE:HG22	1.84	0.59
10:B:1065:GLN:HG2	10:B:1069:PHE:HB2	1.84	0.59
10:B:901:PRO:HB3	10:B:950:ASP:HA	1.84	0.59
1:C:10:ILE:HD13	1:C:20:PHE:HB3	1.85	0.59
6:J:7:CYS:HB3	6:J:11:GLY:H	1.68	0.59
9:A:1143:LEU:HD23	9:A:1268:LEU:HA	1.84	0.59
9:A:1348:LEU:HD23	9:A:1372:VAL:HG23	1.85	0.59
10:B:432:MET:HA	10:B:435:THR:HG22	1.85	0.59
9:A:868:TYR:HD2	9:A:1058:VAL:HG21	1.67	0.59
9:A:1095:THR:H	9:A:1113:THR:HG21	1.66	0.59
1:C:41:ILE:HD12	1:C:42:PRO:HD2	1.85	0.58
5:I:68:LEU:HD11	5:I:86:PHE:HB3	1.86	0.58
10:B:343:ILE:HG12	10:B:348:ARG:HG3	1.85	0.58
9:A:778:GLY:HA3	10:B:516:ASN:HB2	1.86	0.58
12:D:50:LEU:HB3	12:D:55:ALA:HB2	1.86	0.57
9:A:1317:MET:HG2	9:A:1327:ILE:HD13	1.86	0.57
9:A:506:ALA:HB3	9:A:509:LEU:HD23	1.86	0.57
1:C:151:GLN:HE21	6:J:65:PRO:HB3	1.69	0.57
5:I:25:LEU:HG	5:I:38:ALA:HB3	1.85	0.57
10:B:592:ASN:HD21	10:B:595:ARG:HE	1.51	0.57
3:F:125:LEU:HA	3:F:130:ILE:HD11	1.85	0.57
5:I:12:ASN:HA	10:B:294:ASP:HB2	1.87	0.57
9:A:56:PRO:HD2	9:A:58:LEU:HG	1.87	0.57
10:B:29:ASP:HB3	10:B:658:ILE:HG12	1.85	0.57
9:A:747:VAL:HG21	9:A:758:ILE:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:350:ARG:HB3	9:A:488:ASN:HA	1.86	0.56
10:B:301:ILE:HD12	10:B:379:GLY:HA2	1.87	0.56
11:H:111:LEU:HG	11:H:127:GLY:H	1.69	0.56
5:I:65:ASP:HB2	10:B:619:ILE:HD11	1.85	0.56
2:E:80:VAL:HG12	2:E:109:ILE:HB	1.86	0.56
9:A:247:ARG:HD2	9:A:260:ASP:HB3	1.86	0.56
9:A:1194:ARG:HG2	9:A:1239:ARG:HG2	1.88	0.56
10:B:766:ARG:HH21	10:B:1020:ARG:HG2	1.71	0.56
5:I:75:CYS:CB	5:I:78:CYS:HB3	2.36	0.56
9:A:452:LYS:HD2	9:A:1067:LEU:HD21	1.87	0.56
10:B:755:ILE:HG22	10:B:983:ARG:HD2	1.88	0.56
9:A:535:THR:HG21	9:A:617:VAL:H	1.70	0.56
9:A:1373:ASP:HA	9:A:1376:THR:HG22	1.88	0.56
1:C:265:MET:HE1	7:K:20:LYS:HA	1.88	0.56
9:A:1142:THR:HG23	9:A:1145:SER:H	1.70	0.56
9:A:666:ILE:HD11	10:B:1026:LEU:HB3	1.89	0.55
12:D:164:ILE:HD13	12:D:167:LEU:HD21	1.88	0.55
1:C:254:LYS:HG2	7:K:42:LEU:HD21	1.88	0.55
6:J:9:SER:HB3	6:J:45:CYS:HB2	1.88	0.55
9:A:961:ARG:HG3	9:A:965:GLN:HE22	1.72	0.55
9:A:1136:SER:HB2	9:A:1274:ARG:HH22	1.72	0.55
11:H:63:LEU:HD12	11:H:90:ALA:H	1.72	0.55
9:A:708:MET:HB3	9:A:712:GLU:HB2	1.88	0.55
12:D:63:LEU:HG	12:D:130:LEU:HD22	1.87	0.55
9:A:1100:ARG:HH12	9:A:1111:MET:HE3	1.71	0.55
10:B:488:TYR:HE2	10:B:813:LYS:HB2	1.72	0.55
10:B:1157:ALA:H	10:B:1197:PRO:HB3	1.72	0.55
11:H:96:VAL:HG22	11:H:143:LEU:HD22	1.88	0.55
10:B:364:ILE:HG23	10:B:365:THR:H	1.71	0.54
12:D:27:LEU:HD12	12:D:29:LEU:HD11	1.88	0.54
10:B:139:ALA:HB2	10:B:150:GLU:HG2	1.90	0.54
4:G:153:GLN:HE22	4:G:158:HIS:HB2	1.73	0.54
6:J:17:LYS:HB3	6:J:39:LEU:HD21	1.90	0.54
9:A:1363:VAL:HG23	9:A:1368:MET:HE2	1.89	0.54
10:B:787:VAL:HG12	10:B:788:ARG:H	1.72	0.54
10:B:1180:PHE:H	10:B:1188:LYS:HG3	1.73	0.54
5:I:94:ASP:HA	9:A:709:THR:HG21	1.90	0.54
8:L:58:LYS:HB3	10:B:952:VAL:HB	1.89	0.54
11:H:5:LEU:HD23	11:H:134:ASN:HA	1.89	0.54
2:E:3:GLN:HG2	2:E:5:ASN:H	1.73	0.54
10:B:642:ASP:HA	10:B:649:LYS:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:865:LYS:HG3	10:B:961:LEU:HD21	1.90	0.54
1:C:175:ALA:HB3	1:C:233:GLU:HB3	1.89	0.53
2:E:40:GLU:HA	2:E:43:LYS:HG2	1.90	0.53
10:B:373:ARG:HA	10:B:566:LEU:HD23	1.90	0.53
10:B:705:MET:HE2	10:B:745:PRO:HB3	1.91	0.53
9:A:800:VAL:HG22	9:A:812:GLU:HB3	1.89	0.53
9:A:867:ILE:HD11	9:A:1010:ALA:HB1	1.89	0.53
10:B:139:ALA:HB1	10:B:148:LYS:HB3	1.91	0.53
10:B:342:GLY:H	10:B:348:ARG:HB2	1.73	0.53
10:B:580:VAL:HG23	10:B:624:LEU:HD23	1.90	0.53
9:A:709:THR:HG22	9:A:710:LEU:HD23	1.91	0.53
9:A:994:GLN:HE22	9:A:1023:ARG:HH21	1.56	0.53
10:B:824:ILE:HA	10:B:1089:PRO:HA	1.90	0.53
3:F:86:THR:HG23	3:F:89:GLU:H	1.72	0.53
3:F:133:VAL:HG21	4:G:58:ARG:HH11	1.74	0.53
9:A:346:ASP:HB2	10:B:1108:ARG:H	1.73	0.53
9:A:1143:LEU:HA	9:A:1146:VAL:HG22	1.91	0.53
9:A:1404:GLU:HG3	9:A:1408:ILE:HB	1.90	0.53
10:B:527:THR:HG21	10:B:534:GLY:H	1.73	0.53
10:B:138:GLU:HG2	10:B:159:ASP:HB3	1.91	0.53
1:C:99:LEU:HB2	1:C:157:CYS:HB2	1.90	0.53
9:A:549:MET:HG2	9:A:652:VAL:HG23	1.91	0.53
3:F:129:LYS:HZ2	9:A:1453:TYR:HD1	1.57	0.52
10:B:1065:GLN:HG3	10:B:1067:ARG:H	1.72	0.52
8:L:38:LEU:HD11	8:L:48:CYS:HA	1.92	0.52
10:B:283:VAL:HG21	10:B:318:VAL:HA	1.91	0.52
9:A:830:LYS:HE2	9:A:1080:THR:HA	1.92	0.52
10:B:336:ARG:HH22	10:B:351:TYR:HB3	1.75	0.52
9:A:239:LEU:HD12	9:A:240:PRO:HD2	1.91	0.52
9:A:587:HIS:HB3	9:A:589:GLN:HE22	1.74	0.52
9:A:928:LEU:HD12	9:A:987:VAL:HG11	1.90	0.52
10:B:803:LEU:HD21	10:B:1036:ALA:HB2	1.90	0.52
12:D:118:THR:HG23	12:D:120:GLU:H	1.73	0.52
5:I:6:PHE:HB2	5:I:8:ARG:HH21	1.74	0.52
9:A:760:GLN:HG2	9:A:765:VAL:HA	1.91	0.52
10:B:978:ASP:HA	10:B:1098:MET:HB3	1.92	0.52
3:F:124:GLU:HG2	3:F:130:ILE:HG13	1.92	0.52
9:A:765:VAL:HB	9:A:800:VAL:HB	1.92	0.52
10:B:130:VAL:HG23	10:B:167:ILE:HG13	1.92	0.52
10:B:1030:LEU:HB3	10:B:1055:ILE:HG21	1.91	0.52
11:H:143:LEU:HB3	11:H:145:ARG:HH22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:18:GLU:HA	5:I:25:LEU:HA	1.91	0.52
8:L:54:ARG:HH11	10:B:120:ARG:HH12	1.58	0.52
10:B:348:ARG:HE	10:B:350:GLN:HB3	1.74	0.52
3:F:70:LYS:O	3:F:71:GLU:HG3	2.11	0.51
4:G:37:SER:HB2	4:G:45:ILE:HD12	1.91	0.51
9:A:541:ILE:HG12	9:A:546:VAL:HG23	1.92	0.51
9:A:1405:THR:HG22	9:A:1406:VAL:H	1.76	0.51
10:B:846:ILE:HD12	10:B:974:PRO:HG2	1.92	0.51
1:C:46:ILE:HD11	1:C:67:LEU:HB3	1.90	0.51
1:C:235:VAL:HG11	6:J:6:ARG:HH22	1.76	0.51
9:A:332:LYS:H	9:A:337:ARG:HD2	1.74	0.51
9:A:1406:VAL:HG22	9:A:1409:LEU:HD12	1.91	0.51
10:B:376:PHE:HB2	10:B:566:LEU:HD21	1.92	0.51
10:B:994:TYR:HB2	10:B:999:MET:HE3	1.93	0.51
9:A:216:VAL:HA	9:A:219:PHE:HD2	1.76	0.51
10:B:401:PHE:H	10:B:517:THR:HG21	1.76	0.51
10:B:922:GLU:HB3	10:B:925:LEU:HB3	1.93	0.51
12:D:127:ASP:HA	12:D:130:LEU:HD12	1.93	0.51
4:G:27:LYS:HB3	4:G:51:TYR:HE1	1.74	0.51
9:A:33:ALA:HB3	9:A:56:PRO:HB2	1.92	0.51
9:A:436:ILE:HG22	9:A:460:VAL:HG11	1.93	0.51
1:C:50:GLU:HB2	1:C:156:THR:HB	1.92	0.51
2:E:55:ARG:HA	2:E:58:MET:HE3	1.93	0.51
9:A:532:ARG:HH21	9:A:745:GLN:HG2	1.75	0.51
5:I:15:TYR:HB2	5:I:30:ARG:HE	1.75	0.50
9:A:1214:GLU:HA	9:A:1217:LYS:HG2	1.92	0.50
10:B:22:SER:HA	10:B:654:ARG:HD3	1.92	0.50
12:D:189:ASP:HA	12:D:192:LYS:HG2	1.93	0.50
9:A:528:LEU:HD23	9:A:751:SER:H	1.75	0.50
9:A:618:GLU:HG2	9:A:620:LYS:H	1.76	0.50
10:B:270:LYS:HB3	10:B:279:ASP:HB3	1.92	0.50
10:B:828:ALA:HB2	10:B:1085:ILE:HG23	1.93	0.50
9:A:50:ILE:HG22	9:A:52:GLY:H	1.76	0.50
10:B:600:LEU:HG	10:B:615:MET:HE3	1.93	0.50
9:A:1199:ARG:HD2	9:A:1236:LEU:HD21	1.92	0.50
10:B:1198:TYR:HA	10:B:1201:LYS:HG2	1.94	0.50
9:A:35:ILE:HA	9:A:52:GLY:HA2	1.94	0.50
10:B:75:ALA:HB3	10:B:143:PRO:HG2	1.93	0.50
10:B:878:GLN:HG2	10:B:881:ASN:HB2	1.94	0.50
5:I:42:LEU:HD11	5:I:45:ARG:HD3	1.93	0.50
2:E:20:LYS:HE2	2:E:34:GLU:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:92:ASN:O	7:K:95:ILE:HG22	2.12	0.49
10:B:926:GLY:HA2	10:B:928:ARG:NH1	2.26	0.49
2:E:94:LYS:HA	2:E:97:VAL:HG12	1.94	0.49
8:L:47:ARG:HD2	8:L:54:ARG:HE	1.77	0.49
9:A:12:ARG:HG2	9:A:13:THR:H	1.77	0.49
9:A:532:ARG:HD3	9:A:749:ALA:HB2	1.94	0.49
10:B:431:TYR:CD2	10:B:445:LYS:HG2	2.47	0.49
10:B:485:ARG:HH11	10:B:782:LEU:HD21	1.77	0.49
10:B:1198:TYR:HD1	10:B:1201:LYS:HZ3	1.60	0.49
12:D:154:PHE:HZ	12:D:214:LEU:HD12	1.76	0.49
7:K:12:LEU:HD13	7:K:18:LYS:HG2	1.93	0.49
12:D:188:ALA:HB2	12:D:208:GLU:HB2	1.93	0.49
10:B:95:ILE:HD11	10:B:128:LEU:HD12	1.93	0.49
10:B:706:GLN:HG2	10:B:709:ASP:HB3	1.93	0.49
9:A:1429:ILE:HG22	9:A:1430:LEU:HD12	1.94	0.49
6:J:36:LEU:HD22	6:J:47:ARG:HG3	1.95	0.49
9:A:848:ILE:HG13	9:A:1065:GLY:HA3	1.94	0.49
10:B:36:ALA:HB2	10:B:661:LEU:HD11	1.94	0.49
10:B:165:VAL:HB	10:B:446:LEU:HD11	1.94	0.49
10:B:881:ASN:O	10:B:933:SER:HB2	2.12	0.49
9:A:804:TYR:HE2	10:B:1021:MET:HE2	1.78	0.48
10:B:757:PRO:HG3	10:B:983:ARG:HH21	1.78	0.48
9:A:868:TYR:CE1	9:A:1064:VAL:HG11	2.48	0.48
7:K:7:PHE:HB2	7:K:11:LEU:HD12	1.95	0.48
9:A:38:PRO:HA	9:A:270:LEU:HB3	1.94	0.48
9:A:1399:ARG:HA	9:A:1402:PHE:HB3	1.94	0.48
1:C:248:ILE:HG21	7:K:102:LYS:HB3	1.95	0.48
9:A:1243:VAL:HG22	9:A:1245:PRO:HD3	1.96	0.48
10:B:428:ILE:HG22	10:B:432:MET:HE3	1.96	0.48
10:B:485:ARG:HD3	10:B:782:LEU:HD23	1.95	0.48
10:B:1106:ARG:NH1	10:B:1109:GLY:H	2.10	0.48
3:F:133:VAL:HG23	9:A:1444:MET:HB2	1.95	0.48
9:A:276:LEU:HD12	9:A:289:ILE:HD11	1.94	0.48
8:L:28:LYS:HB2	8:L:39:SER:HA	1.95	0.48
10:B:117:ALA:O	10:B:121:ASN:HA	2.14	0.48
10:B:780:VAL:HG12	10:B:795:ILE:HG23	1.96	0.48
9:A:300:VAL:O	9:A:304:MET:HG2	2.14	0.48
10:B:95:ILE:HD13	10:B:130:VAL:HG22	1.95	0.48
11:H:93:TYR:HB3	11:H:145:ARG:CZ	2.44	0.48
4:G:46:LEU:HD21	4:G:105:PRO:HG3	1.95	0.48
9:A:549:MET:HE1	9:A:656:TRP:HD1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:675:THR:O	9:A:679:ILE:HG12	2.14	0.48
10:B:129:PHE:HB3	10:B:166:PHE:HA	1.95	0.48
9:A:256:GLN:CD	9:A:257:ARG:H	2.21	0.47
5:I:3:THR:HG22	10:B:308:TRP:HB3	1.97	0.47
7:K:45:LEU:O	7:K:49:GLU:HG3	2.14	0.47
9:A:70:CYS:HB2	10:B:1174:LYS:HA	1.96	0.47
9:A:929:LEU:HD21	9:A:983:ILE:HG21	1.96	0.47
9:A:1385:THR:HG23	9:A:1387:HIS:H	1.80	0.47
10:B:69:LEU:HB3	10:B:432:MET:HE1	1.95	0.47
10:B:420:LEU:HB3	10:B:453:ILE:HD12	1.96	0.47
1:C:185:LYS:HG2	1:C:213:PRO:HB3	1.95	0.47
9:A:1034:GLU:O	9:A:1036:ARG:HG2	2.15	0.47
12:D:138:ASN:HB3	12:D:141:LEU:HB3	1.97	0.47
2:E:55:ARG:HD2	2:E:84:ASP:HA	1.97	0.47
9:A:35:ILE:HG22	9:A:270:LEU:HD11	1.97	0.47
9:A:908:LEU:HD22	9:A:1032:LEU:HD13	1.97	0.47
10:B:82:ASP:H	10:B:142:VAL:HA	1.79	0.47
10:B:125:SER:HB2	10:B:169:ARG:HB3	1.96	0.47
10:B:242:SER:HB2	10:B:363:HIS:HB3	1.96	0.47
11:H:130:ARG:H	11:H:130:ARG:HD3	1.78	0.47
1:C:251:LEU:HD22	7:K:98:LEU:HD21	1.96	0.47
2:E:169:ARG:HB3	3:F:140:ASP:HB3	1.95	0.47
4:G:21:ARG:HH11	4:G:24:GLN:HE22	1.62	0.47
9:A:210:ILE:HA	9:A:213:HIS:CE1	2.49	0.47
10:B:277:LYS:HZ3	10:B:280:ILE:HD11	1.80	0.47
2:E:100:ILE:HG23	2:E:105:PHE:HB2	1.96	0.47
9:A:225:ASN:HB3	9:A:228:PHE:HB2	1.96	0.47
9:A:474:VAL:HG23	9:A:521:MET:HE2	1.96	0.47
11:H:143:LEU:HB2	11:H:145:ARG:HH12	1.80	0.47
12:D:52:LEU:HD13	12:D:151:PHE:HB3	1.97	0.47
3:F:133:VAL:HG13	9:A:1446:ASP:HB2	1.96	0.47
10:B:877:PRO:HB3	10:B:882:THR:HG21	1.97	0.47
9:A:840:ARG:NE	9:A:1385:THR:HA	2.29	0.47
10:B:916:THR:HG23	10:B:918:ILE:HG12	1.95	0.47
10:B:911:ILE:HG21	10:B:966:VAL:HG11	1.96	0.46
10:B:1171:VAL:HG23	10:B:1182:CYS:HA	1.96	0.46
11:H:94:ASP:H	11:H:145:ARG:HE	1.63	0.46
2:E:65:THR:O	2:E:69:ILE:HD12	2.16	0.46
9:A:899:VAL:HG21	9:A:908:LEU:HD23	1.97	0.46
9:A:940:ARG:HH21	9:A:944:ARG:HH21	1.63	0.46
9:A:1146:VAL:HG23	9:A:1197:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:114:PRO:HG3	10:B:181:LEU:HD11	1.97	0.46
4:G:111:THR:HG23	4:G:114:LEU:H	1.81	0.46
9:A:25:GLU:HA	9:A:28:ARG:HG2	1.96	0.46
9:A:1288:ASP:HA	9:A:1302:PRO:HA	1.96	0.46
10:B:616:ILE:HG22	10:B:697:GLU:HA	1.97	0.46
4:G:102:GLN:HA	4:G:107:LYS:HA	1.97	0.46
9:A:446:ARG:HG2	9:A:487:MET:HG2	1.96	0.46
9:A:661:GLY:HA3	10:B:1081:LEU:HD12	1.98	0.46
9:A:1029:ARG:HD2	9:A:1029:ARG:HA	1.75	0.46
9:A:741:ASN:HB3	9:A:744:LYS:HB3	1.96	0.46
10:B:174:LEU:HD23	10:B:202:TYR:O	2.16	0.46
10:B:778:MET:HE3	10:B:794:ASN:HD22	1.80	0.46
11:H:146:ARG:HD2	11:H:146:ARG:HA	1.77	0.46
9:A:37:PHE:HB2	9:A:53:LEU:HG	1.98	0.46
9:A:1079:MET:HE2	9:A:1079:MET:HB3	1.85	0.46
1:C:29:MET:HA	7:K:45:LEU:HD12	1.97	0.46
5:I:43:VAL:HB	9:A:1152:ILE:HG23	1.98	0.46
5:I:92:ARG:HB3	5:I:95:THR:HG23	1.98	0.46
9:A:1329:THR:HG22	9:A:1331:SER:H	1.80	0.45
1:C:165:LYS:NZ	10:B:995:ARG:HH12	2.14	0.45
4:G:122:ASN:HB2	4:G:131:GLN:HB2	1.99	0.45
9:A:307:ASP:H	9:A:326:ARG:HG3	1.81	0.45
9:A:869:GLY:HA3	9:A:1366:ARG:HG3	1.98	0.45
1:C:240:VAL:O	1:C:243:VAL:HG22	2.17	0.45
9:A:940:ARG:HH21	9:A:944:ARG:NH2	2.14	0.45
10:B:796:LEU:HD23	10:B:853:SER:HB3	1.97	0.45
1:C:55:THR:HG22	1:C:152:GLU:H	1.82	0.45
9:A:767:GLN:NE2	9:A:774:ARG:HD2	2.32	0.45
9:A:1209:MET:HA	9:A:1212:VAL:HG22	1.98	0.45
5:I:71:SER:HB2	5:I:85:PHE:CE2	2.51	0.45
9:A:528:LEU:O	9:A:531:ILE:HG22	2.17	0.45
9:A:1216:ILE:HG12	9:A:1267:MET:HE1	1.99	0.45
10:B:542:MET:HG2	10:B:636:PRO:HD2	1.98	0.45
10:B:1180:PHE:HB2	10:B:1188:LYS:HG3	1.98	0.45
1:C:239:PRO:O	1:C:243:VAL:HG13	2.17	0.45
11:H:100:THR:HA	11:H:138:GLU:O	2.16	0.45
5:I:92:ARG:HE	5:I:93:LYS:H	1.64	0.45
12:D:57:LEU:HD13	12:D:157:GLN:HG3	1.98	0.45
12:D:174:PRO:HA	12:D:177:VAL:HG12	1.98	0.45
9:A:325:ILE:HG23	10:B:1206:GLU:HG2	1.99	0.45
10:B:171:PRO:HG2	10:B:461:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:769:TYR:HB3	10:B:773:MET:HE1	1.99	0.45
10:B:978:ASP:HB2	10:B:990:ILE:HD12	1.98	0.45
5:I:43:VAL:HG21	9:A:1191:TRP:HZ3	1.81	0.44
9:A:24:PRO:HD3	9:A:233:TRP:HA	1.99	0.44
9:A:583:PRO:HD3	9:A:645:LEU:HD13	1.98	0.44
1:C:142:VAL:HG23	6:J:15:GLY:HA3	1.99	0.44
6:J:3:VAL:HG11	6:J:18:TRP:HB2	1.99	0.44
9:A:455:MET:HE3	9:A:455:MET:HB2	1.84	0.44
10:B:580:VAL:HA	10:B:624:LEU:HB3	1.97	0.44
11:H:35:GLN:HB2	11:H:111:LEU:HD11	1.99	0.44
12:D:67:ARG:HG3	12:D:133:THR:HG21	1.99	0.44
2:E:95:THR:HA	2:E:98:ILE:HG12	2.00	0.44
9:A:211:PHE:HA	9:A:214:ILE:HG12	2.00	0.44
10:B:448:ILE:O	10:B:452:THR:HG23	2.18	0.44
2:E:32:GLN:HA	2:E:35:VAL:HG22	1.99	0.44
9:A:343:LYS:NZ	10:B:1155:SER:HB3	2.33	0.44
9:A:590:ARG:HE	9:A:621:THR:HG22	1.82	0.44
10:B:727:LYS:HA	10:B:1051:THR:HG21	1.99	0.44
2:E:178:ILE:HG13	9:A:1341:ILE:HD11	1.98	0.44
10:B:277:LYS:HD2	10:B:337:ARG:HE	1.81	0.44
2:E:88:VAL:HB	2:E:116:ILE:HG23	2.00	0.44
5:I:5:ARG:HB2	5:I:14:LEU:HD12	2.00	0.44
9:A:662:PHE:HZ	9:A:746:MET:HG3	1.83	0.44
10:B:615:MET:HG3	10:B:626:ILE:HG23	2.00	0.44
10:B:910:VAL:HA	10:B:940:PRO:HA	1.99	0.44
12:D:153:ARG:HH21	12:D:220:LEU:HD11	1.83	0.44
9:A:1158:PRO:HB3	9:A:1187:GLN:HA	2.00	0.44
10:B:776:GLN:HG3	10:B:1096:ARG:HE	1.83	0.44
10:B:928:ARG:NH2	10:B:932:HIS:HB3	2.33	0.44
10:B:1174:LYS:HB2	10:B:1179:GLN:HB2	1.99	0.44
9:A:340:LEU:HG	9:A:1429:ILE:HG12	2.00	0.44
9:A:350:ARG:HD3	9:A:488:ASN:OD1	2.18	0.44
9:A:754:SER:O	9:A:758:ILE:HD12	2.18	0.44
10:B:259:TYR:HB2	10:B:268:THR:HG23	2.00	0.44
2:E:150:VAL:HG22	9:A:1343:ALA:HB2	1.99	0.44
9:A:210:ILE:HD13	9:A:213:HIS:NE2	2.33	0.44
9:A:800:VAL:HG13	9:A:812:GLU:HB3	1.99	0.44
10:B:1031:LEU:HD11	10:B:1042:GLY:HA3	2.00	0.44
2:E:187:TYR:HD2	2:E:188:LEU:HD12	1.83	0.43
10:B:582:VAL:HG12	10:B:583:ASN:H	1.83	0.43
1:C:22:LEU:HB3	1:C:228:PHE:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:195:VAL:HG22	2:E:213:ILE:HG12	1.99	0.43
5:I:19:ASP:HB2	5:I:26:LEU:HD23	1.99	0.43
6:J:44:TYR:O	6:J:48:ARG:HG2	2.17	0.43
9:A:59:GLY:HA2	9:A:67:CYS:SG	2.57	0.43
9:A:632:VAL:O	9:A:636:GLU:HG3	2.18	0.43
10:B:338:GLY:HA2	10:B:339:THR:HA	1.55	0.43
5:I:69:PRO:HG3	9:A:788:SER:HB2	1.99	0.43
10:B:600:LEU:HD23	10:B:615:MET:HG2	2.00	0.43
9:A:306:ASN:HD22	9:A:324:SER:H	1.66	0.43
10:B:930:ALA:O	10:B:931:TYR:HB2	2.18	0.43
2:E:177:ARG:HG2	2:E:215:MET:HB3	2.00	0.43
9:A:17:VAL:HA	10:B:1216:LEU:HA	1.99	0.43
9:A:943:LEU:HA	9:A:946:VAL:HG12	2.00	0.43
9:A:956:LEU:HG	9:A:1021:LEU:HD22	2.01	0.43
9:A:1067:LEU:HD23	9:A:1067:LEU:HA	1.87	0.43
9:A:1124:HIS:CG	9:A:1130:GLN:HG2	2.53	0.43
9:A:21:LEU:HD23	9:A:230:ARG:H	1.83	0.43
10:B:846:ILE:HD13	10:B:850:LEU:HB3	1.99	0.43
10:B:1010:LEU:HD11	10:B:1092:TYR:HE2	1.83	0.43
9:A:341:MET:O	9:A:343:LYS:HG3	2.19	0.43
9:A:774:ARG:NH2	9:A:797:LYS:HG3	2.34	0.43
9:A:1220:PHE:HB3	9:A:1223:ASP:OD1	2.19	0.43
10:B:32:ALA:HB3	10:B:658:ILE:HD11	2.00	0.43
8:L:29:TYR:HB2	8:L:38:LEU:HB2	2.01	0.43
9:A:416:ARG:HB3	9:A:417:TYR:H	1.70	0.43
9:A:308:ILE:HG12	9:A:312:PRO:HG3	2.01	0.43
9:A:534:LEU:HD13	9:A:656:TRP:CD2	2.54	0.43
4:G:110:VAL:HG22	4:G:161:GLY:HA3	2.01	0.43
9:A:266:LEU:HA	9:A:269:ILE:HG22	2.01	0.43
9:A:399:HIS:CE1	9:A:462:VAL:HG21	2.54	0.43
10:B:228:LYS:HG2	10:B:234:ILE:HG13	2.00	0.43
10:B:766:ARG:NH2	10:B:1020:ARG:HG2	2.33	0.43
10:B:778:MET:HE2	10:B:794:ASN:HB3	2.00	0.43
11:H:115:TYR:HE1	11:H:124:ARG:HG3	1.83	0.43
1:C:148:ARG:HG2	6:J:61:LEU:HD12	2.00	0.42
10:B:644:GLU:HG3	10:B:646:LEU:H	1.84	0.42
9:A:280:GLU:HG2	9:A:289:ILE:HD11	1.99	0.42
11:H:95:TYR:HB3	11:H:144:ILE:HG13	2.01	0.42
9:A:80:HIS:CE1	10:B:1173:ALA:H	2.38	0.42
10:B:952:VAL:HG22	10:B:966:VAL:HG23	2.02	0.42
11:H:56:THR:HB	11:H:145:ARG:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ALA:HB2	10:B:997:GLU:HG2	2.01	0.42
9:A:259:GLU:HG2	9:A:260:ASP:H	1.84	0.42
9:A:1100:ARG:HE	9:A:1104:ILE:HD11	1.84	0.42
10:B:521:LEU:HD22	10:B:633:VAL:HG12	2.01	0.42
2:E:28:TYR:HB3	2:E:62:ALA:HB1	2.02	0.42
5:I:42:LEU:HD21	5:I:45:ARG:HG2	2.00	0.42
9:A:613:ILE:HG23	11:H:117:SER:HB2	2.01	0.42
9:A:323:LYS:HE2	9:A:328:ARG:HA	2.02	0.42
10:B:60:GLN:HE22	10:B:94:LYS:HA	1.84	0.42
8:L:63:ARG:HH22	10:B:903:VAL:HG13	1.85	0.42
9:A:35:ILE:HD12	9:A:241:VAL:HG11	2.01	0.42
9:A:1192:LEU:HD22	9:A:1239:ARG:NH2	2.35	0.42
10:B:277:LYS:HD3	10:B:336:ARG:O	2.20	0.42
10:B:292:ILE:HD11	10:B:327:ARG:HB3	2.02	0.42
12:D:155:ARG:HH21	12:D:221:TYR:HB2	1.84	0.42
2:E:205:SER:HB3	9:A:871:ASP:HB3	2.01	0.42
4:G:116:PRO:HB2	4:G:119:LEU:HD23	2.02	0.42
9:A:599:SER:HB2	9:A:602:ASP:HA	2.01	0.42
10:B:449:ASN:O	10:B:453:ILE:HG12	2.20	0.42
10:B:577:ALA:HB1	10:B:589:VAL:HB	2.01	0.42
1:C:165:LYS:HE3	7:K:10:PHE:HB2	2.02	0.42
9:A:81:PHE:HE1	10:B:1169:MET:HB2	1.85	0.42
10:B:277:LYS:HE3	10:B:335:GLY:HA3	2.02	0.42
12:D:167:LEU:HD13	12:D:177:VAL:HG22	2.02	0.42
2:E:29:PHE:CE2	2:E:65:THR:HA	2.54	0.42
9:A:518:LYS:HE2	9:A:624:SER:HB2	2.02	0.42
9:A:1140:HIS:HB2	9:A:1276:VAL:O	2.19	0.42
2:E:118:PRO:HA	2:E:121:MET:HE2	2.01	0.41
4:G:46:LEU:HD12	4:G:77:VAL:HG22	2.01	0.41
9:A:242:PRO:HG2	9:A:266:LEU:HD21	2.02	0.41
10:B:928:ARG:HG2	10:B:929:THR:N	2.35	0.41
1:C:44:LEU:HD22	1:C:129:ILE:HG23	2.01	0.41
4:G:30:LEU:O	4:G:34:VAL:HG22	2.19	0.41
8:L:47:ARG:HA	8:L:54:ARG:HG2	2.02	0.41
9:A:210:ILE:O	9:A:214:ILE:HG12	2.20	0.41
9:A:308:ILE:HG22	9:A:326:ARG:NH1	2.34	0.41
4:G:28:THR:O	4:G:32:GLU:HG2	2.21	0.41
9:A:343:LYS:HB3	10:B:1117:GLN:HE22	1.85	0.41
9:A:542:GLU:HG2	9:A:543:LEU:H	1.86	0.41
9:A:678:GLU:O	9:A:681:GLU:HG3	2.20	0.41
9:A:961:ARG:HE	9:A:1025:ARG:CZ	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:600:LEU:HD12	10:B:600:LEU:HA	1.88	0.41
9:A:36:ARG:HA	9:A:36:ARG:HD3	1.92	0.41
9:A:239:LEU:HD22	9:A:300:VAL:HG22	2.03	0.41
9:A:1079:MET:SD	9:A:1097:GLY:HA2	2.61	0.41
10:B:48:LEU:HD13	10:B:48:LEU:HA	1.91	0.41
10:B:424:LEU:O	10:B:428:ILE:HG12	2.21	0.41
2:E:97:VAL:HG22	2:E:127:ILE:HD12	2.02	0.41
4:G:3:PHE:HB3	4:G:5:LYS:NZ	2.35	0.41
5:I:15:TYR:HA	5:I:16:PRO:HD3	1.93	0.41
5:I:45:ARG:HD2	5:I:45:ARG:HA	1.89	0.41
10:B:634:TYR:HA	10:B:694:ASP:HA	2.03	0.41
10:B:662:MET:HE2	10:B:662:MET:HB2	1.87	0.41
10:B:901:PRO:HG3	10:B:952:VAL:HG23	2.03	0.41
8:L:28:LYS:HA	8:L:28:LYS:HD2	1.82	0.41
9:A:26:GLU:O	9:A:30:ILE:HG23	2.21	0.41
9:A:54:ASN:HB3	9:A:61:ILE:HD11	2.02	0.41
9:A:1173:HIS:CD2	9:A:1227:ILE:HG23	2.56	0.41
10:B:1201:LYS:HG3	10:B:1202:LEU:N	2.35	0.41
1:C:39:ALA:HB1	1:C:165:LYS:HG3	2.03	0.41
5:I:108:HIS:CE1	5:I:110:PHE:HB3	2.55	0.41
9:A:682:THR:O	9:A:685:GLU:HG3	2.21	0.41
9:A:852:TYR:HA	9:A:1060:PRO:HB3	2.03	0.41
10:B:267:ARG:HD2	10:B:267:ARG:HA	1.82	0.41
10:B:446:LEU:HA	10:B:449:ASN:HD22	1.85	0.41
7:K:34:THR:HG22	7:K:72:LYS:HG2	2.01	0.41
9:A:340:LEU:HD21	9:A:1429:ILE:HG23	2.03	0.41
9:A:546:VAL:HG21	9:A:572:TRP:HB2	2.03	0.41
9:A:1140:HIS:CD2	9:A:1277:GLU:HA	2.56	0.41
10:B:289:LEU:HD21	10:B:374:LYS:HB2	2.02	0.41
10:B:1194:ILE:HG22	10:B:1196:ILE:HG23	2.02	0.41
12:D:34:GLN:HG3	12:D:36:LYS:H	1.85	0.41
2:E:91:LYS:HA	2:E:94:LYS:HG2	2.01	0.41
4:G:3:PHE:HD1	12:D:49:ALA:HA	1.86	0.41
5:I:69:PRO:HB2	5:I:85:PHE:CZ	2.55	0.41
9:A:853:ASP:HB3	9:A:855:THR:OG1	2.21	0.41
9:A:1191:TRP:CD1	9:A:1256:GLU:HB2	2.56	0.41
10:B:215:GLN:HA	10:B:499:ASN:O	2.21	0.41
10:B:274:PRO:HA	10:B:275:TYR:HA	1.75	0.41
10:B:1001:PHE:HB3	10:B:1007:VAL:HG12	2.02	0.41
1:C:221:TYR:HB2	9:A:569:LYS:HD2	2.03	0.41
9:A:80:HIS:CD2	10:B:1172:ILE:HD12	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:230:ARG:HB2	9:A:233:TRP:CG	2.56	0.41
9:A:424:ILE:HG22	9:A:426:LEU:H	1.86	0.41
9:A:467:THR:HG23	9:A:469:ARG:HG2	2.03	0.41
9:A:898:ARG:HD3	9:A:933:TYR:CD2	2.57	0.41
10:B:1065:GLN:HB3	10:B:1069:PHE:O	2.21	0.41
11:H:63:LEU:HG	11:H:89:LEU:HG	2.03	0.41
7:K:35:PHE:HD2	7:K:71:PHE:CZ	2.39	0.40
9:A:276:LEU:HD13	9:A:293:GLU:HB3	2.03	0.40
9:A:1153:TYR:HB2	9:A:1192:LEU:HD11	2.04	0.40
10:B:114:PRO:HB2	10:B:118:ARG:HH12	1.86	0.40
10:B:277:LYS:HG3	10:B:278:GLN:O	2.21	0.40
10:B:406:LEU:HD22	10:B:498:THR:HG21	2.02	0.40
1:C:259:LEU:O	1:C:262:LEU:HG	2.22	0.40
9:A:27:VAL:HG11	9:A:240:PRO:HD3	2.03	0.40
12:D:168:LYS:HA	12:D:168:LYS:HD2	1.77	0.40
8:L:47:ARG:HE	8:L:52:GLY:HA2	1.86	0.40
9:A:335:ARG:HA	9:A:339:ASN:HB2	2.03	0.40
9:A:894:GLU:O	9:A:898:ARG:HB3	2.21	0.40
10:B:87:LYS:HB3	10:B:139:ALA:HB3	2.03	0.40
10:B:346:GLU:CD	10:B:347:LYS:HG3	2.47	0.40
11:H:12:VAL:HG23	11:H:26:ILE:HG23	2.02	0.40
2:E:13:TRP:CE3	2:E:39:LEU:HD12	2.56	0.40
4:G:61:ILE:HD13	4:G:61:ILE:HA	1.96	0.40
9:A:211:PHE:CG	9:A:231:PRO:HB2	2.57	0.40
9:A:526:ASP:HA	10:B:1015:HIS:NE2	2.37	0.40
9:A:1356:ILE:HG21	9:A:1363:VAL:HG22	2.03	0.40
10:B:167:ILE:HD13	10:B:446:LEU:HD13	2.03	0.40
10:B:334:ILE:HD12	10:B:334:ILE:HA	1.94	0.40
3:F:93:ILE:HD13	3:F:93:ILE:HA	1.93	0.40
5:I:28:GLU:HB2	5:I:35:VAL:HG12	2.04	0.40
9:A:306:ASN:N	9:A:326:ARG:HB3	2.18	0.40
9:A:447:GLN:NE2	9:A:488:ASN:HD21	2.20	0.40
9:A:727:ASP:O	9:A:731:ARG:HG2	2.21	0.40
9:A:1106:ASN:C	9:A:1108:ALA:H	2.28	0.40
9:A:1186:ASP:HB3	9:A:1187:GLN:H	1.72	0.40
10:B:680:THR:HG23	10:B:682:SER:H	1.86	0.40
10:B:773:MET:HE3	10:B:987:LYS:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	C	263/318 (83%)	242 (92%)	21 (8%)	0	100	100
2	E	212/215 (99%)	197 (93%)	15 (7%)	0	100	100
3	F	85/155 (55%)	79 (93%)	6 (7%)	0	100	100
4	G	169/171 (99%)	149 (88%)	20 (12%)	0	100	100
5	I	112/122 (92%)	102 (91%)	10 (9%)	0	100	100
6	J	64/70 (91%)	59 (92%)	4 (6%)	1 (2%)	7	34
7	K	113/120 (94%)	111 (98%)	2 (2%)	0	100	100
8	L	42/70 (60%)	34 (81%)	8 (19%)	0	100	100
9	A	1294/1733 (75%)	1173 (91%)	113 (9%)	8 (1%)	21	52
10	B	1133/1224 (93%)	1002 (88%)	126 (11%)	5 (0%)	30	61
11	H	132/146 (90%)	114 (86%)	18 (14%)	0	100	100
12	D	153/221 (69%)	145 (95%)	8 (5%)	0	100	100
All	All	3772/4565 (83%)	3407 (90%)	351 (9%)	14 (0%)	31	61

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	A	256	GLN
10	B	364	ILE
9	A	1107	VAL
9	A	1221	LYS
10	B	1156	ASP
9	A	1313	LEU
10	B	84	ILE
9	A	66	LYS
10	B	82	ASP
6	J	6	ARG
9	A	1034	GLU
9	A	56	PRO

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Mol	Chain	Res	Type
9	A	612	ILE
10	B	1157	ALA

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	C	233/274 (85%)	233 (100%)	0	100	100
2	E	196/197 (100%)	196 (100%)	0	100	100
3	F	77/137 (56%)	77 (100%)	0	100	100
4	G	152/152 (100%)	152 (100%)	0	100	100
5	I	108/116 (93%)	108 (100%)	0	100	100
6	J	61/65 (94%)	61 (100%)	0	100	100
7	K	99/102 (97%)	99 (100%)	0	100	100
8	L	39/57 (68%)	39 (100%)	0	100	100
9	A	1136/1520 (75%)	1136 (100%)	0	100	100
10	B	994/1061 (94%)	994 (100%)	0	100	100
11	H	119/128 (93%)	119 (100%)	0	100	100
12	D	139/200 (70%)	139 (100%)	0	100	100
All	All	3353/4009 (84%)	3353 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	C	73	GLN
1	C	151	GLN
1	C	242	GLN
1	C	252	GLN
2	E	5	ASN
2	E	63	ASN

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Mol	Chain	Res	Type
2	E	99	HIS
2	E	106	GLN
2	E	113	GLN
2	E	174	GLN
2	E	179	GLN
4	G	24	GLN
4	G	131	GLN
4	G	153	GLN
4	G	158	HIS
5	I	89	GLN
9	A	4	GLN
9	A	273	ASN
9	A	306	ASN
9	A	313	GLN
9	A	390	GLN
9	A	394	ASN
9	A	447	GLN
9	A	589	GLN
9	A	706	HIS
9	A	935	GLN
9	A	975	HIS
9	A	994	GLN
10	B	46	GLN
10	B	350	GLN
10	B	572	HIS
10	B	573	GLN
10	B	610	ASN
10	B	686	ASN
10	B	776	GLN
10	B	881	ASN
10	B	958	GLN
10	B	1062	HIS
10	B	1117	GLN
11	H	11	GLN
11	H	33	GLN
12	D	40	HIS
12	D	138	ASN
12	D	143	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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.

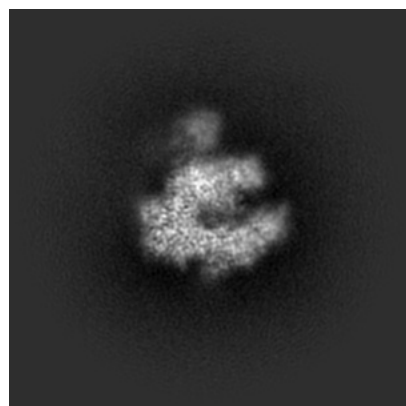
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74529. These allow visual inspection of the internal detail of the map and identification of artifacts.

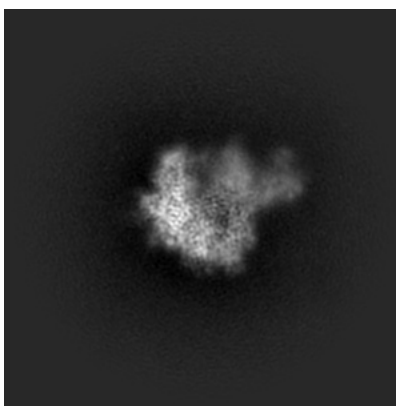
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

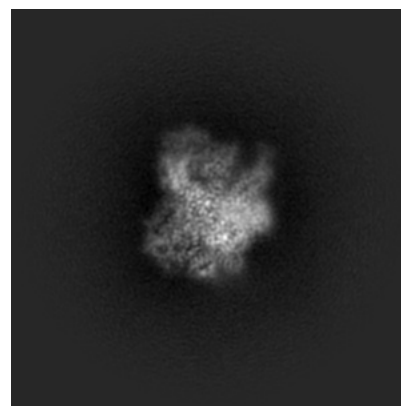
6.1.1 Primary map



X

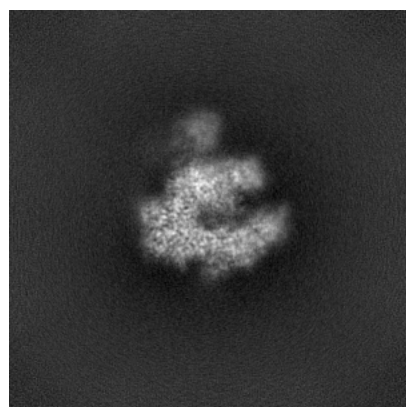


Y

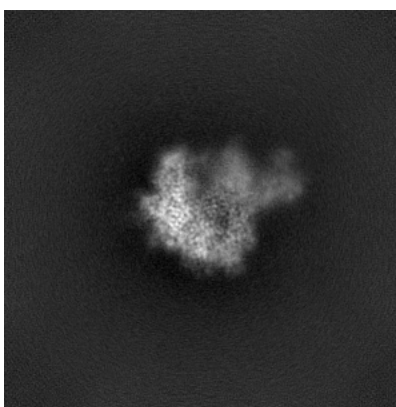


Z

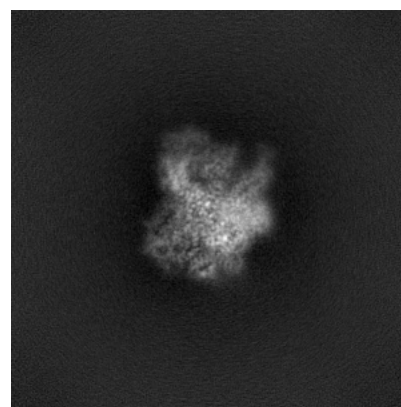
6.1.2 Raw map



X



Y

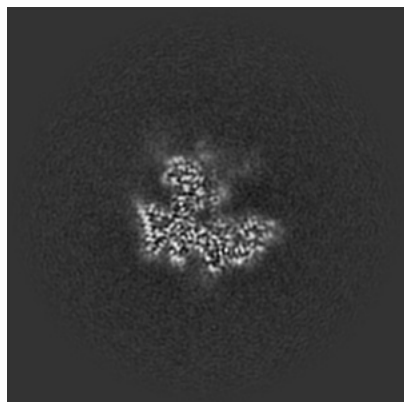


Z

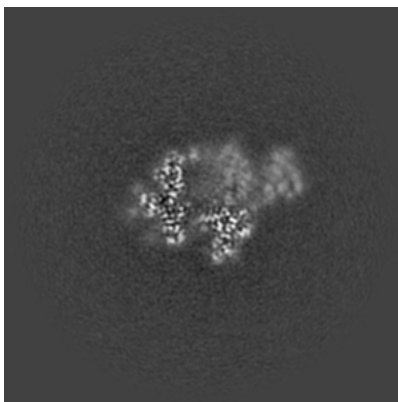
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

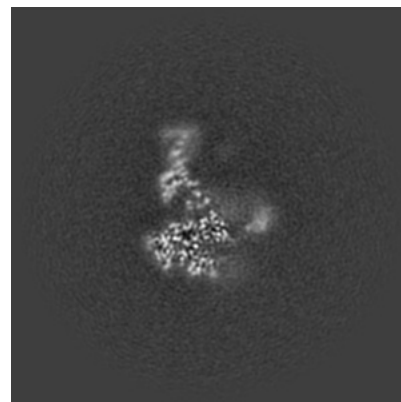
6.2.1 Primary map



X Index: 200

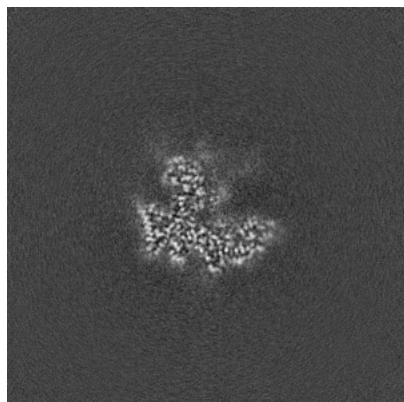


Y Index: 200

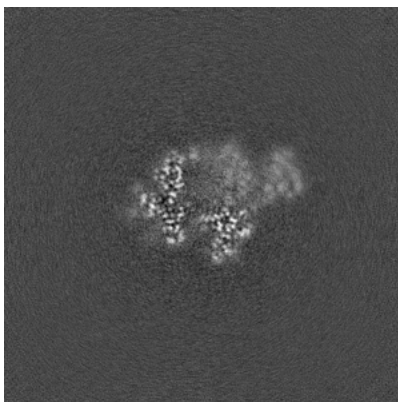


Z Index: 200

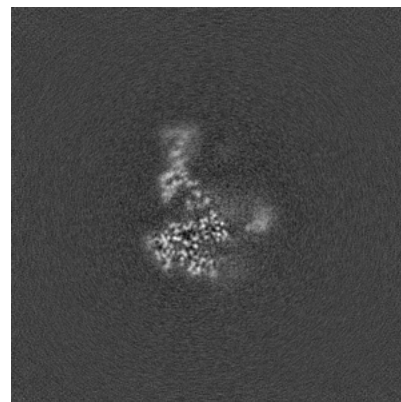
6.2.2 Raw map



X Index: 200



Y Index: 200

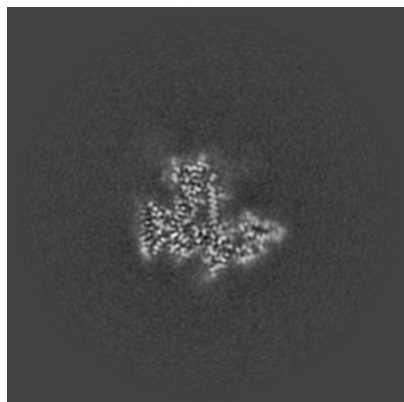


Z Index: 200

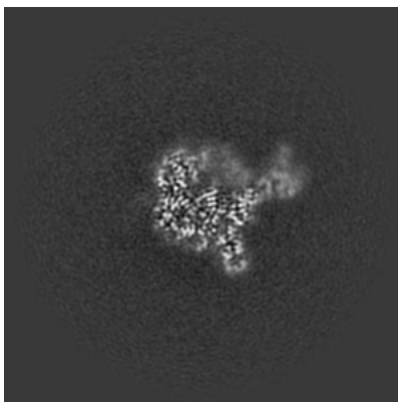
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

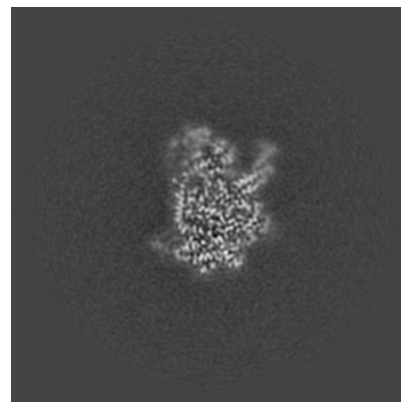
6.3.1 Primary map



X Index: 196

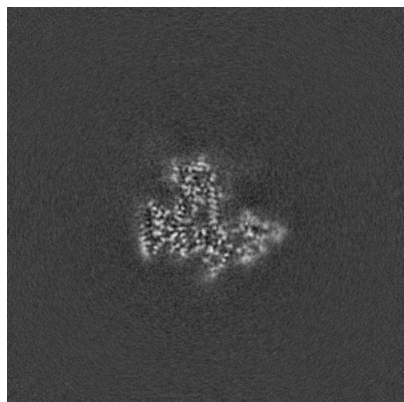


Y Index: 182

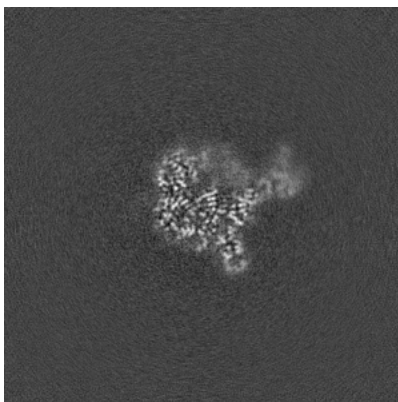


Z Index: 175

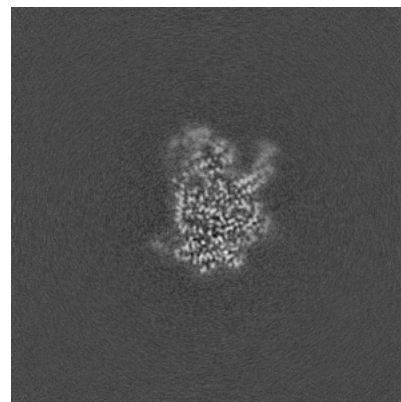
6.3.2 Raw map



X Index: 195



Y Index: 182

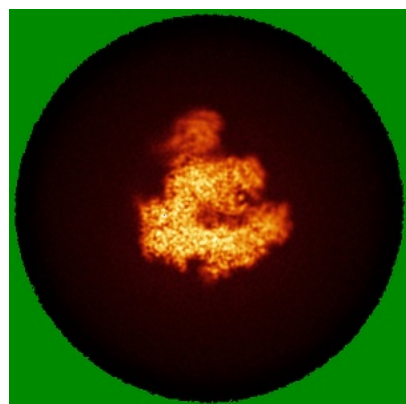


Z Index: 175

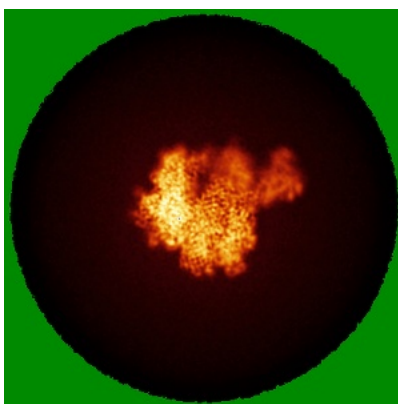
The images above show the largest variance slices of the map in three orthogonal directions.

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

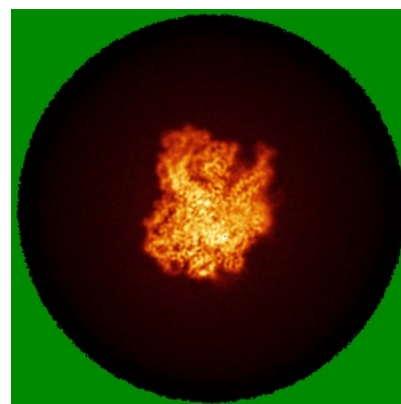
6.4.1 Primary map



X

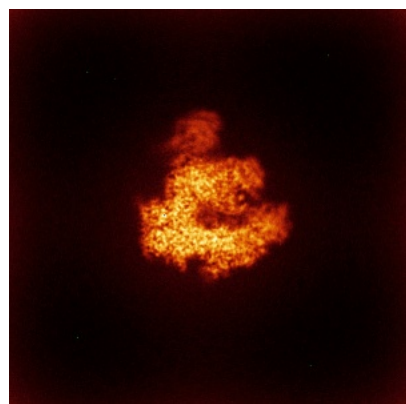


Y

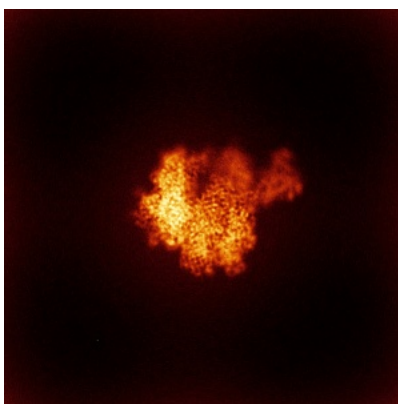


Z

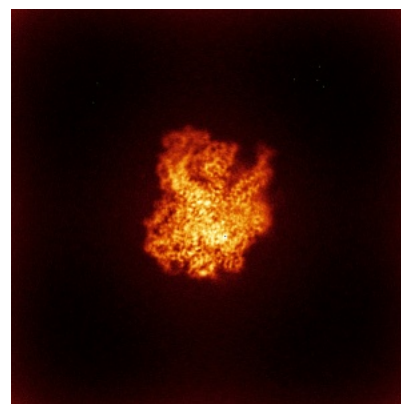
6.4.2 Raw map



X



Y



Z

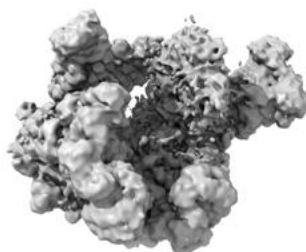
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. 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



X



Y



Z

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.

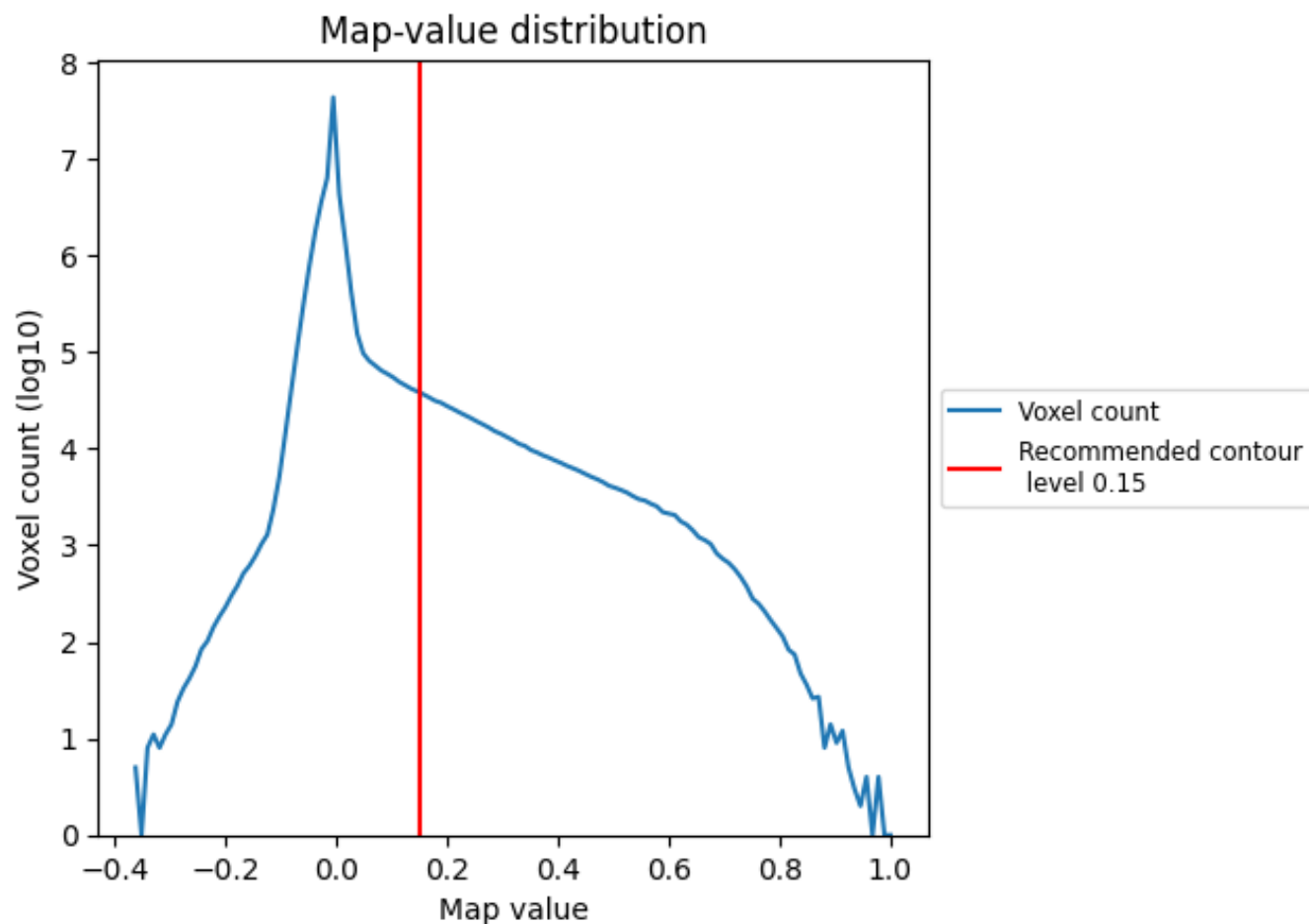
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

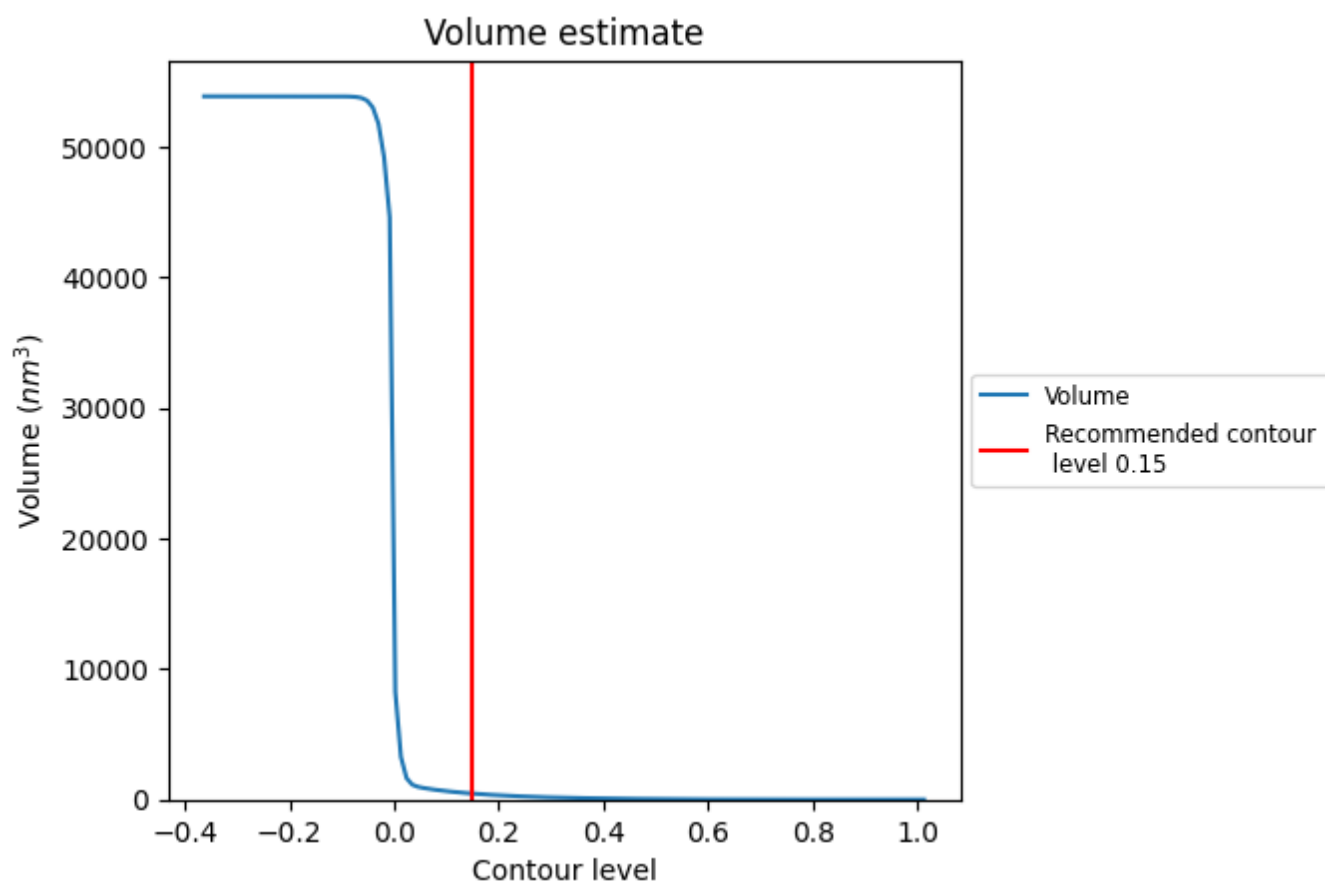
This section contains the results of statistical analysis of the map.

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.

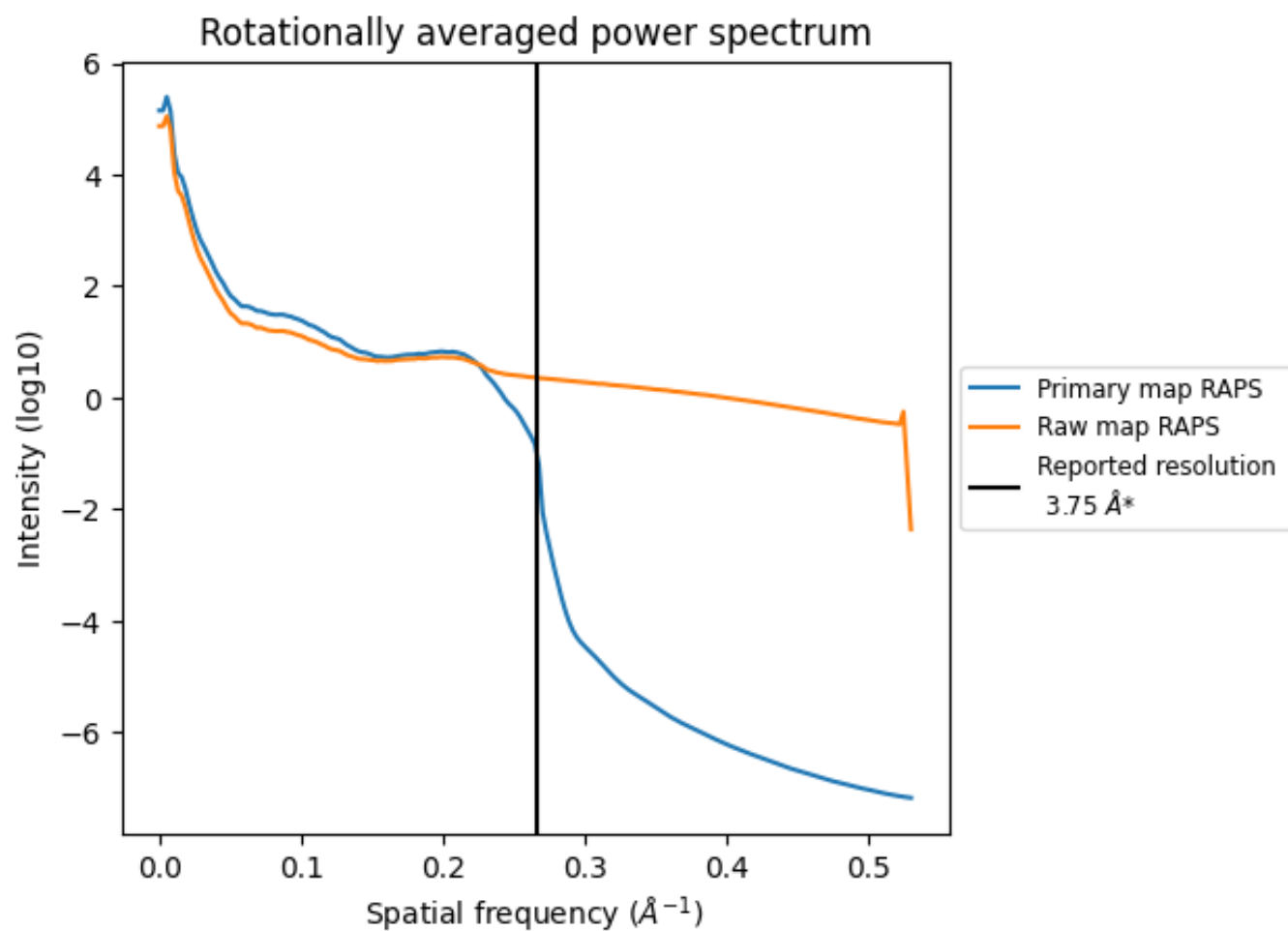
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 458 nm^3 ; this corresponds to an approximate mass of 414 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 ⓘ

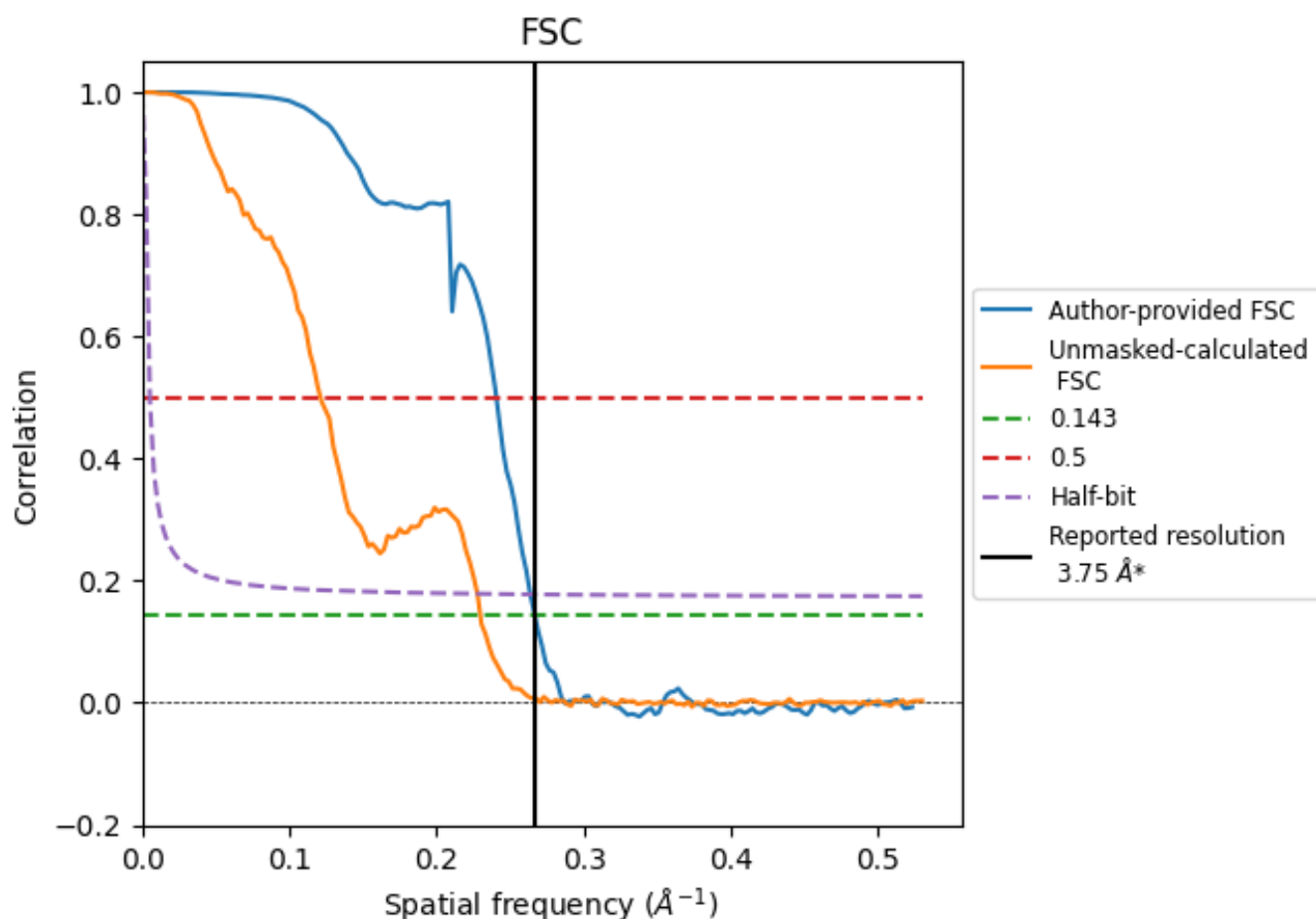


*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

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 $0.267 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

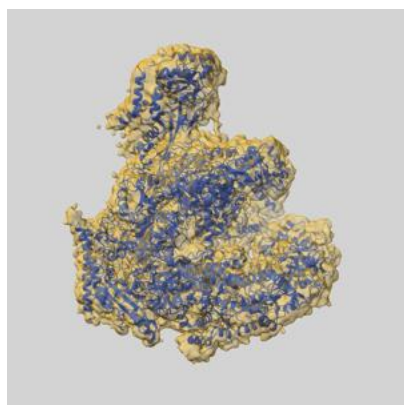
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.75	-	-
Author-provided FSC curve	3.75	4.16	3.79
Unmasked-calculated*	4.36	8.26	4.39

*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 4.36 differs from the reported value 3.75 by more than 10 %

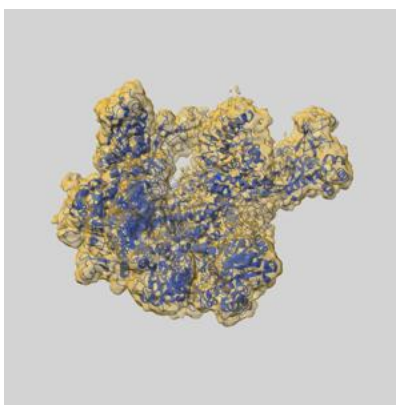
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-74529 and PDB model 9ZPL. Per-residue inclusion information can be found in section [3](#) on page [7](#).

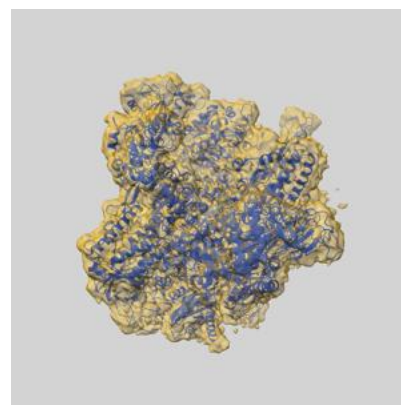
9.1 Map-model overlay [i](#)



X



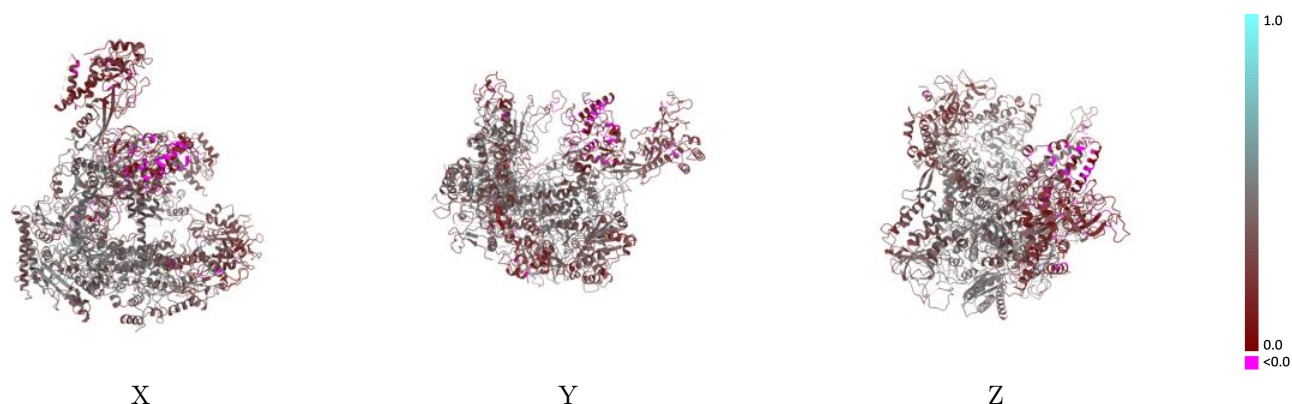
Y



Z

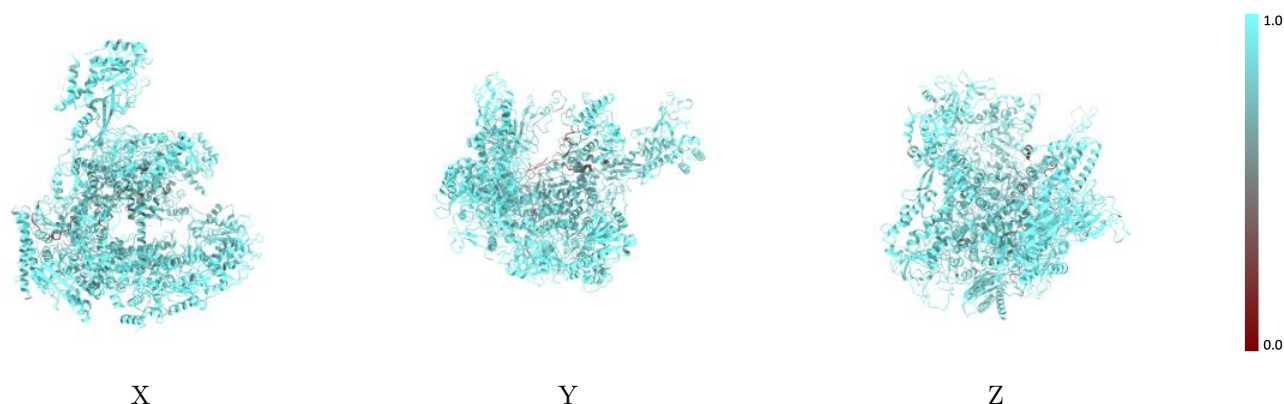
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



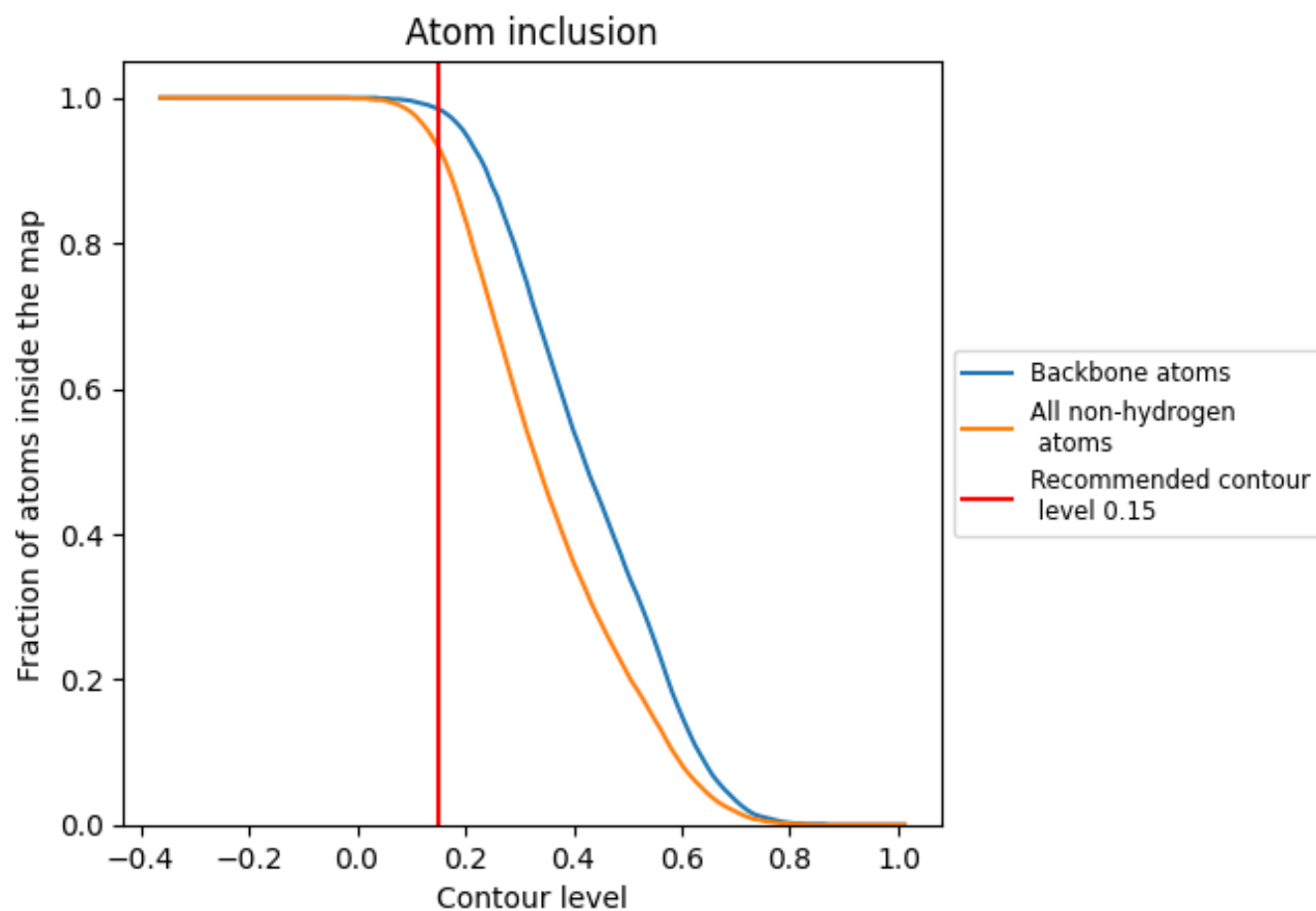
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 93% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9330	 0.3460
A	 0.9270	 0.3360
B	 0.9380	 0.3710
C	 0.9490	 0.4140
D	 0.9470	 0.1920
E	 0.9490	 0.3360
F	 0.9460	 0.4020
G	 0.9360	 0.2420
H	 0.9430	 0.3740
I	 0.9490	 0.2890
J	 0.9330	 0.4080
K	 0.8440	 0.3640
L	 0.9380	 0.3810

