



## Full wwPDB EM Validation Report ⓘ

Feb 28, 2024 – 03:54 am GMT

PDB ID : 8Q3K  
EMDB ID : EMD-18129  
Title : The open state of the ASFV apo-RNA polymerase  
Authors : Pilotto, S.; Sykora, M.; Cackett, G.; Werner, F.  
Deposited on : 2023-08-04  
Resolution : 2.92 Å(reported)  
Based on initial model : .

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:

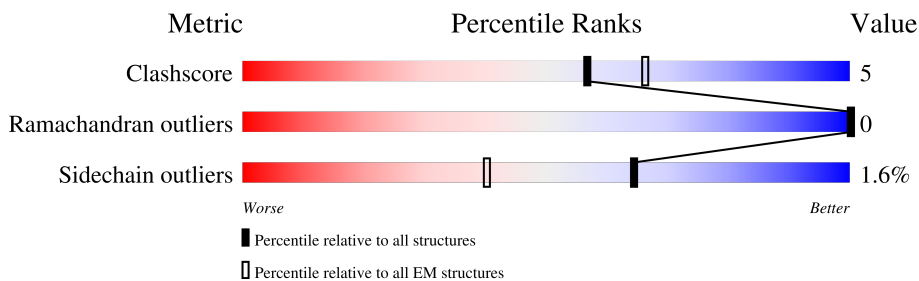
EMDB validation analysis : 0.0.1.dev70  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.92 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	
2	B	1243	
3	C	359	
4	D	339	
5	E	205	
6	F	147	
7	I	105	
8	J	80	

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 28932 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 RPB1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1420	11322	7187	1974	2099	62	1	0

- Molecule 2 is a protein called DNA-directed RNA polymerase RPB2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1020	8030	5071	1406	1505	48	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P42487

- Molecule 3 is a protein called DNA-directed RNA polymerase RPB3-11 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	359	2910	1884	484	529	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	335	2692	1730	444	503	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	204	1657	1081	277	292	7	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase RPB6 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	110	Total	C	N	O	S	0	0
			863	549	147	162	5		

- Molecule 7 is a protein called Uncharacterized protein C122R.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	105	Total	C	N	O	S	0	0
			816	507	141	153	15		

- Molecule 8 is a protein called DNA-directed RNA polymerase RPB10 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	80	Total	C	N	O	S	0	0
			635	413	102	113	7		

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	A	2	Total	Zn	0
			2	2	
9	B	1	Total	Zn	0
			1	1	
9	I	2	Total	Zn	0
			2	2	
9	J	1	Total	Zn	0
			1	1	

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

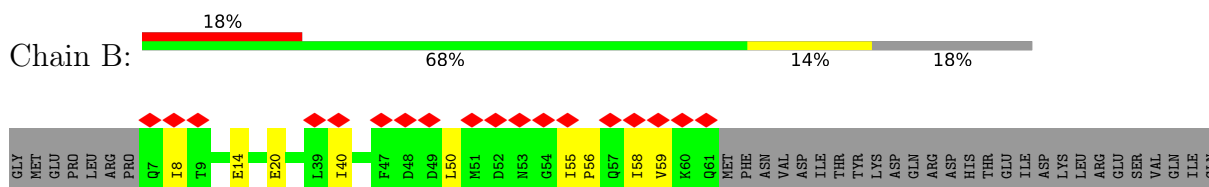
### 3 Residue-property plots

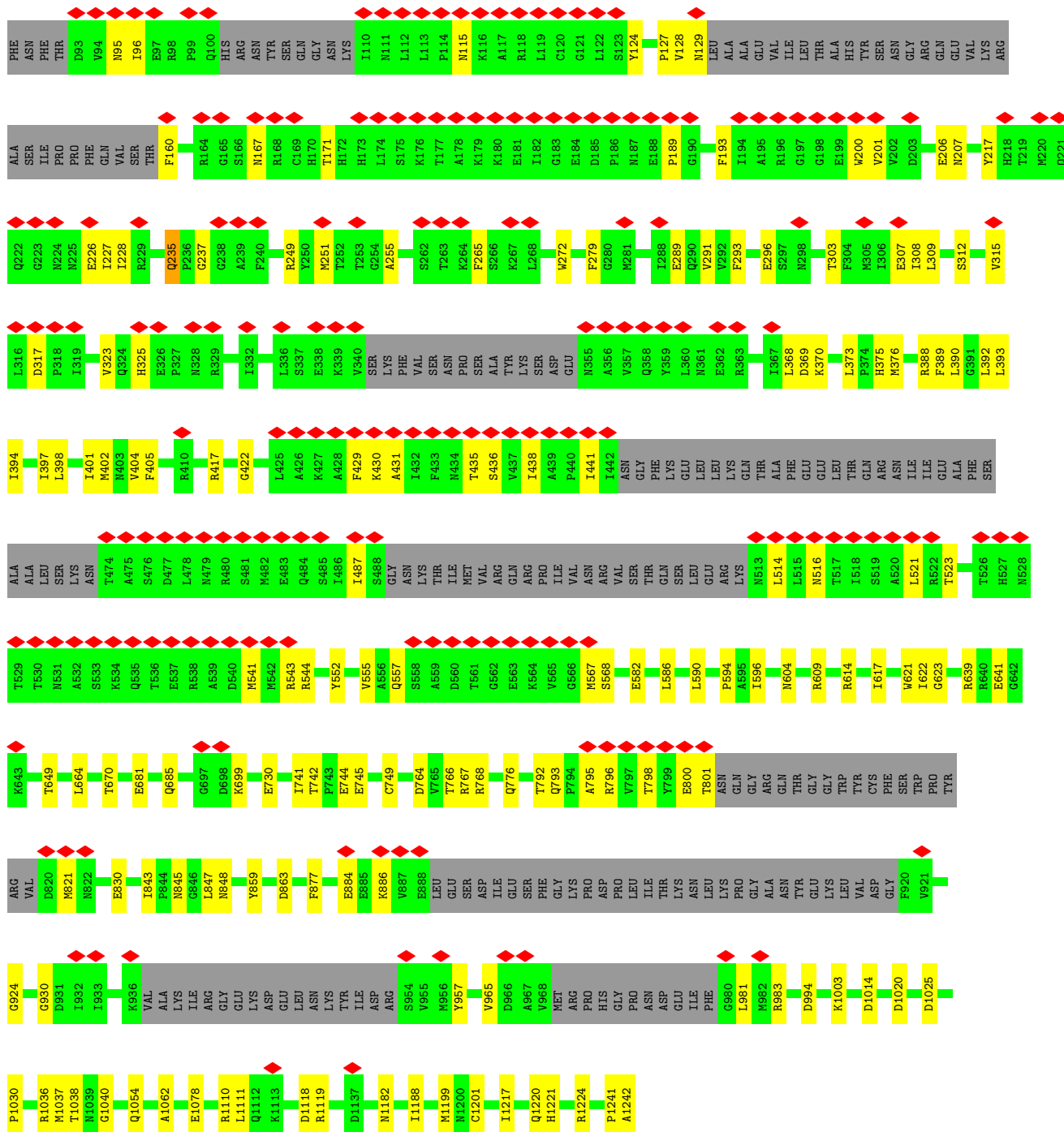
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 RPB1 homolog

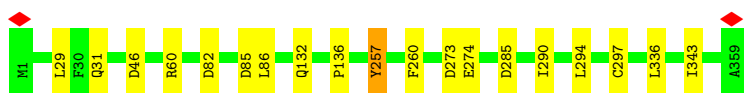


- Molecule 2: DNA-directed RNA polymerase RPB2 homolog

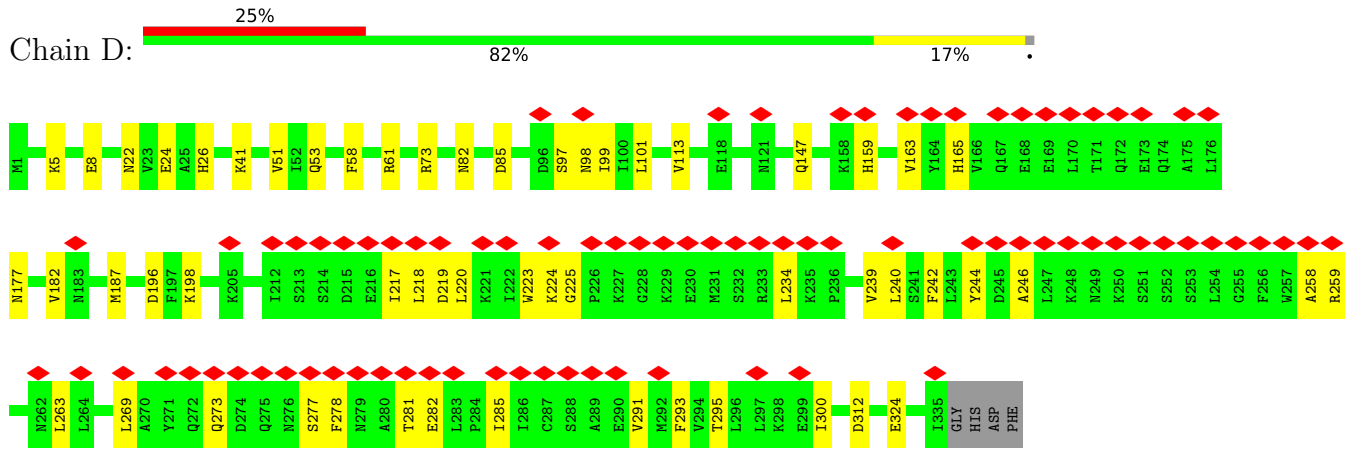




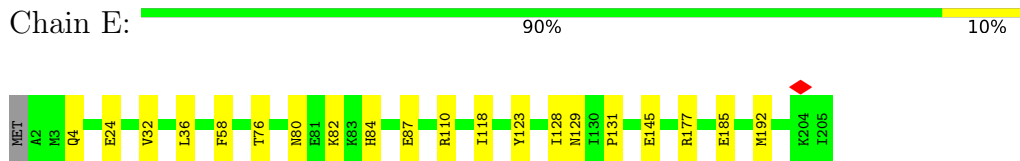
• Molecule 3: DNA-directed RNA polymerase RPB3-11 homolog



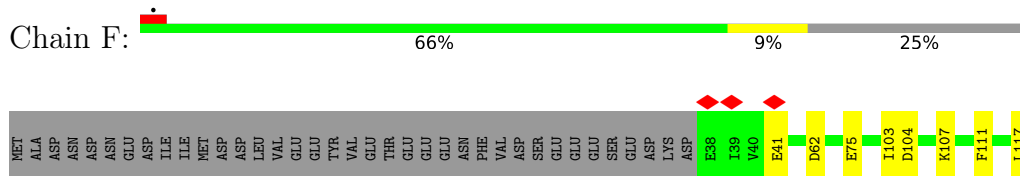
• Molecule 4: DNA-directed RNA polymerase RPB7 homolog



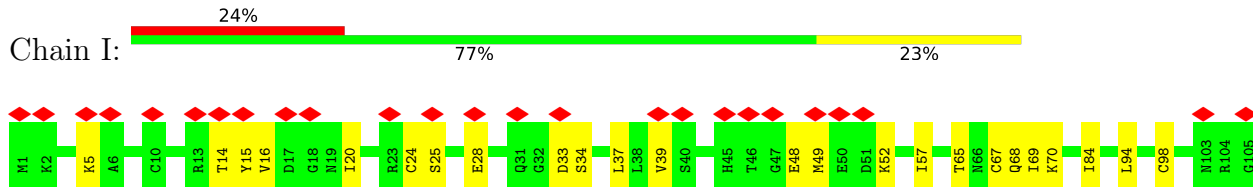
- Molecule 5: DNA-directed RNA polymerase RPB5 homolog



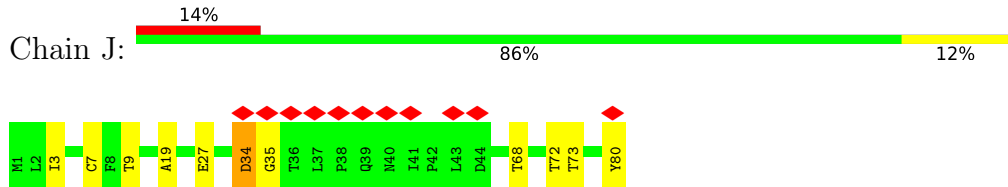
- Molecule 6: DNA-directed RNA polymerase RPB6 homolog



- Molecule 7: Uncharacterized protein C122R



- Molecule 8: DNA-directed RNA polymerase RPB10 homolog



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	352192	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 ( $e^-/\text{\AA}^2$ )	48.152	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	29.551	Depositor
Minimum map value	-15.514	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	1.019	Depositor
Recommended contour level	3.9	Depositor
Map size ( $\text{\AA}$ )	248.40001, 248.40001, 248.40001	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.828, 0.828, 0.828	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: MG, 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	A	0.25	0/11543	0.50	0/15633
2	B	0.25	0/8181	0.49	0/11064
3	C	0.25	0/2972	0.47	0/4017
4	D	0.26	0/2745	0.46	0/3716
5	E	0.26	0/1696	0.47	0/2296
6	F	0.26	0/875	0.51	0/1184
7	I	0.28	0/828	0.52	0/1109
8	J	0.28	0/648	0.51	0/878
All	All	0.26	0/29488	0.49	0/39897

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1224	ARG	Sidechain

## 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	11322	0	11446	110	0
2	B	8030	0	7986	128	0
3	C	2910	0	2988	11	0
4	D	2692	0	2729	38	0
5	E	1657	0	1697	13	0
6	F	863	0	909	8	0
7	I	816	0	813	17	0
8	J	635	0	660	6	0
9	A	2	0	0	0	0
9	B	1	0	0	0	0
9	I	2	0	0	0	0
9	J	1	0	0	0	0
10	A	1	0	0	0	0
All	All	28932	0	29228	299	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (299) 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:108:ASP:OD1	1:A:110:LYS:NZ	2.03	0.90
2:B:226:GLU:OE2	2:B:249:ARG:NH1	2.08	0.87
2:B:796:ARG:NH1	2:B:1037:MET:SD	2.49	0.86
6:F:128:GLU:N	6:F:128:GLU:OE1	2.10	0.85
1:A:1428:ASP:OD1	4:D:61:ARG:NH2	2.11	0.83
4:D:53:GLN:OE1	4:D:73:ARG:NH1	2.14	0.80
1:A:1425:MET:O	4:D:61:ARG:NH1	2.15	0.79
1:A:395:GLN:OE1	1:A:395:GLN:N	2.14	0.79
1:A:661:GLU:N	1:A:661:GLU:OE1	2.15	0.79
2:B:821:MET:HG3	2:B:886:LYS:HE3	1.65	0.78
2:B:1014:ASP:OD1	3:C:60:ARG:NH2	2.16	0.78
1:A:1128:GLN:N	1:A:1128:GLN:OE1	2.20	0.74
2:B:40:ILE:HD12	2:B:521:LEU:HD13	1.68	0.73
2:B:95:ASN:O	2:B:129:ASN:ND2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:431:ALA:O	2:B:435:THR:OG1	2.02	0.73
5:E:87:GLU:OE1	5:E:177:ARG:NH2	2.21	0.73
1:A:49:ARG:O	1:A:61:THR:OG1	2.07	0.72
5:E:4:GLN:N	5:E:4:GLN:OE1	2.22	0.72
2:B:58:ILE:HD11	2:B:430:LYS:CG	2.20	0.72
2:B:863:ASP:OD2	2:B:1036:ARG:NH1	2.23	0.72
4:D:273:GLN:OE1	4:D:277:SER:OG	2.04	0.71
2:B:582:GLU:N	2:B:582:GLU:OE1	2.23	0.71
2:B:541:MET:O	2:B:544:ARG:NE	2.23	0.71
2:B:830:GLU:OE2	2:B:848:ASN:N	2.23	0.71
4:D:82:ASN:N	4:D:85:ASP:OD2	2.23	0.71
7:I:24:CYS:SG	7:I:25:SER:N	2.64	0.70
4:D:324:GLU:N	4:D:324:GLU:OE1	2.24	0.70
4:D:291:VAL:O	4:D:295:THR:OG1	2.08	0.69
2:B:994:ASP:OD2	2:B:1110:ARG:NH2	2.26	0.69
2:B:58:ILE:HD11	2:B:430:LYS:HG2	1.75	0.68
4:D:147:GLN:N	4:D:147:GLN:OE1	2.26	0.68
2:B:289:GLU:O	2:B:293:PHE:N	2.27	0.68
2:B:404:VAL:O	7:I:52:LYS:NZ	2.20	0.68
6:F:75:GLU:OE2	6:F:121:ARG:NH1	2.27	0.67
2:B:402:MET:HG2	2:B:404:VAL:HG23	1.77	0.67
2:B:730:GLU:N	2:B:730:GLU:OE1	2.28	0.67
2:B:670:THR:HG22	2:B:742:THR:HG22	1.76	0.67
1:A:1393:GLN:N	1:A:1393:GLN:OE1	2.27	0.66
1:A:130:GLU:N	1:A:130:GLU:OE1	2.29	0.65
8:J:68:THR:O	8:J:72:THR:OG1	2.10	0.64
1:A:225:ASP:OD2	1:A:227:ASN:ND2	2.31	0.64
2:B:514:LEU:CD1	2:B:843:ILE:HD12	2.29	0.63
4:D:163:VAL:HG23	4:D:258:ALA:HB2	1.79	0.63
4:D:281:THR:OG1	4:D:282:GLU:OE2	2.14	0.62
5:E:24:GLU:N	5:E:24:GLU:OE1	2.32	0.62
1:A:1313:THR:O	1:A:1313:THR:HG22	1.99	0.62
5:E:32:VAL:O	5:E:36:LEU:HD22	2.00	0.61
2:B:20:GLU:OE1	2:B:20:GLU:N	2.30	0.61
5:E:145:GLU:N	5:E:145:GLU:OE1	2.35	0.60
1:A:1213:GLU:N	1:A:1213:GLU:OE1	2.34	0.59
1:A:1070:ASN:OD1	1:A:1090:GLN:NE2	2.35	0.59
1:A:781:GLU:OE2	2:B:767:ARG:NH1	2.35	0.59
2:B:227:ILE:HG22	2:B:228:ILE:HG23	1.85	0.59
3:C:31:GLN:OE1	3:C:31:GLN:N	2.36	0.58
4:D:234:LEU:HD11	4:D:273:GLN:HE21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1418:SER:OG	1:A:1419:VAL:N	2.37	0.58
1:A:367:LEU:O	1:A:371:ARG:NH2	2.36	0.57
1:A:385:GLN:N	1:A:385:GLN:OE1	2.37	0.57
2:B:681:GLU:OE1	2:B:681:GLU:N	2.36	0.57
4:D:242:PHE:O	4:D:246:ALA:N	2.37	0.57
3:C:297:CYS:SG	3:C:343:ILE:HD11	2.45	0.57
1:A:808:GLY:HA3	2:B:795:ALA:HB1	1.87	0.57
4:D:22:ASN:O	4:D:26:HIS:ND1	2.38	0.57
2:B:417:ARG:NH2	2:B:744:GLU:OE2	2.37	0.56
2:B:764:ASP:OD1	2:B:766:THR:N	2.38	0.56
2:B:1003:LYS:HG2	2:B:1111:LEU:HD11	1.87	0.56
4:D:187:MET:SD	4:D:187:MET:N	2.78	0.56
1:A:407:ARG:NH1	1:A:408:ASP:O	2.37	0.56
7:I:67:CYS:SG	7:I:68:GLN:N	2.79	0.56
1:A:100:LEU:O	1:A:176:ARG:NH1	2.38	0.56
1:A:70:MET:HE3	1:A:70:MET:HA	1.87	0.56
2:B:200:TRP:CE2	2:B:487:ILE:HG22	2.41	0.56
2:B:768:ARG:NH1	7:I:68:GLN:OE1	2.39	0.56
2:B:58:ILE:HD11	2:B:430:LYS:HG3	1.88	0.55
7:I:49:MET:SD	7:I:49:MET:N	2.78	0.55
1:A:59:CYS:O	1:A:63:SER:N	2.39	0.55
2:B:96:ILE:HG23	2:B:127:PRO:O	2.06	0.55
2:B:228:ILE:HD11	2:B:397:ILE:CG2	2.36	0.55
1:A:26:VAL:HG22	1:A:73:PRO:O	2.06	0.55
1:A:713:ASP:OD1	1:A:713:ASP:O	2.25	0.55
1:A:1205:ASN:N	1:A:1205:ASN:OD1	2.40	0.55
2:B:438:ILE:HD13	2:B:441:ILE:HD12	1.87	0.54
2:B:390:LEU:O	2:B:394:ILE:HG12	2.08	0.54
2:B:193:PHE:N	2:B:200:TRP:O	2.41	0.54
2:B:14:GLU:OE1	2:B:14:GLU:N	2.34	0.54
2:B:95:ASN:OD1	2:B:96:ILE:N	2.41	0.54
2:B:821:MET:CG	2:B:886:LYS:HE3	2.37	0.54
2:B:1182:ASN:ND2	2:B:1201:CYS:SG	2.79	0.53
1:A:400:GLU:N	1:A:400:GLU:OE1	2.41	0.53
2:B:235:GLN:NE2	2:B:237:GLY:O	2.41	0.53
3:C:132:GLN:NE2	3:C:136:PRO:O	2.39	0.53
1:A:62:CYS:HB3	2:B:1188:ILE:HG23	1.89	0.53
1:A:26:VAL:HA	2:B:1199:MET:HE1	1.91	0.53
1:A:332:ASP:OD2	2:B:859:TYR:OH	2.16	0.52
2:B:279:PHE:CE1	2:B:368:LEU:HD23	2.45	0.52
2:B:594:PRO:O	2:B:596:ILE:HD12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:GLN:NE2	1:A:407:ARG:O	2.43	0.52
1:A:97:VAL:HG12	1:A:97:VAL:O	2.10	0.52
1:A:396:ASP:OD1	1:A:396:ASP:N	2.43	0.51
7:I:34:SER:O	7:I:37:LEU:HD23	2.11	0.51
1:A:208:ILE:HD11	2:B:1221:HIS:HB2	1.93	0.51
1:A:334:HIS:NE2	1:A:535:GLN:OE1	2.40	0.51
1:A:877:ASP:OD1	1:A:905:ARG:NH2	2.38	0.51
4:D:8:GLU:OE2	4:D:73:ARG:NH2	2.42	0.51
4:D:165:HIS:N	4:D:285:ILE:O	2.40	0.51
2:B:272:TRP:CZ2	2:B:309:LEU:HD22	2.46	0.51
1:A:1430:ILE:HG22	4:D:58:PHE:HD1	1.76	0.51
2:B:685:GLN:OE1	2:B:685:GLN:HA	2.11	0.51
4:D:218:LEU:N	4:D:225:GLY:O	2.44	0.51
2:B:800:GLU:O	2:B:801:THR:OG1	2.25	0.50
1:A:777:ARG:N	7:I:65:THR:O	2.43	0.50
2:B:296:GLU:OE2	2:B:609:ARG:NH1	2.40	0.50
1:A:53:THR:HG23	1:A:206:ILE:CG2	2.41	0.50
1:A:712:PRO:O	1:A:713:ASP:HB3	2.11	0.50
6:F:136:TRP:HB3	6:F:141:MET:SD	2.52	0.50
1:A:1245:LYS:O	1:A:1248:VAL:HG22	2.11	0.49
1:A:1313:THR:O	1:A:1313:THR:CG2	2.60	0.49
2:B:981:LEU:HD23	2:B:981:LEU:N	2.28	0.49
2:B:1038:THR:HG23	2:B:1038:THR:O	2.10	0.49
2:B:58:ILE:HD13	2:B:429:PHE:CD2	2.46	0.49
2:B:206:GLU:OE1	2:B:206:GLU:N	2.41	0.49
7:I:5:LYS:HE2	7:I:5:LYS:HA	1.93	0.49
8:J:3:ILE:HA	8:J:73:THR:HG21	1.95	0.49
2:B:438:ILE:HA	2:B:441:ILE:HD12	1.94	0.49
4:D:113:VAL:O	4:D:113:VAL:HG13	2.13	0.49
5:E:76:THR:O	5:E:80:ASN:ND2	2.43	0.49
7:I:20:ILE:HD11	7:I:37:LEU:HA	1.95	0.49
2:B:312:SER:O	2:B:315:VAL:HG13	2.13	0.49
2:B:323:VAL:O	2:B:323:VAL:HG22	2.12	0.49
4:D:219:ASP:HA	4:D:224:LYS:HA	1.95	0.49
1:A:394:LYS:HE3	1:A:394:LYS:HA	1.94	0.48
5:E:58:PHE:O	5:E:123:TYR:OH	2.22	0.48
2:B:877:PHE:O	2:B:1110:ARG:NH1	2.46	0.48
3:C:257:TYR:CE1	3:C:336:LEU:HD13	2.47	0.48
3:C:274:GLU:OE1	3:C:274:GLU:HA	2.13	0.48
1:A:1345:ASP:N	1:A:1345:ASP:OD1	2.46	0.48
4:D:223:TRP:CG	4:D:224:LYS:N	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:24:GLU:OE1	4:D:24:GLU:N	2.42	0.48
5:E:129:ASN:OD1	5:E:131:PRO:HD2	2.13	0.48
2:B:1025:ASP:OD1	8:J:9:THR:HG23	2.13	0.48
4:D:239:VAL:HG21	4:D:259:ARG:HH21	1.78	0.48
1:A:123:GLU:OE1	1:A:123:GLU:HA	2.13	0.48
7:I:14:THR:HG23	7:I:14:THR:O	2.14	0.48
1:A:744:ASN:HA	2:B:1037:MET:HE1	1.96	0.47
1:A:1096:LEU:HD13	1:A:1309:ILE:HD13	1.94	0.47
2:B:699:LYS:HD2	2:B:699:LYS:N	2.29	0.47
1:A:805:GLU:OE1	2:B:555:VAL:HG23	2.14	0.47
1:A:809:ARG:NE	2:B:557:GLN:OE1	2.48	0.47
6:F:41:GLU:OE1	6:F:41:GLU:HA	2.14	0.47
2:B:55:ILE:HA	2:B:58:ILE:HG22	1.96	0.47
2:B:128:VAL:HG13	2:B:160:PHE:HE2	1.79	0.47
1:A:259:ASN:O	1:A:263:ILE:HG13	2.14	0.47
1:A:976:ILE:HG22	1:A:977:ASN:H	1.79	0.47
2:B:228:ILE:HD11	2:B:397:ILE:HG22	1.95	0.47
2:B:1054:GLN:NE2	2:B:1078:GLU:OE1	2.39	0.47
1:A:651:VAL:HG12	2:B:1030:PRO:HB3	1.97	0.47
7:I:15:TYR:OH	7:I:39:VAL:HG21	2.15	0.47
7:I:15:TYR:OH	7:I:39:VAL:CG2	2.63	0.47
1:A:90:GLU:OE1	1:A:93:ARG:NH1	2.48	0.47
2:B:1241:PRO:O	2:B:1242:ALA:HB2	2.14	0.47
4:D:263:LEU:HD22	4:D:269:LEU:HB2	1.97	0.47
2:B:776:GLN:NE2	2:B:1062:ALA:O	2.37	0.47
7:I:69:ILE:HG22	7:I:70:LYS:N	2.30	0.47
4:D:5:LYS:NZ	4:D:41:LYS:O	2.49	0.46
1:A:976:ILE:HG22	1:A:977:ASN:N	2.31	0.46
1:A:1432:ASP:OD2	6:F:139:ARG:NH2	2.40	0.46
2:B:404:VAL:HG12	2:B:405:PHE:CD1	2.50	0.46
1:A:171:ARG:HB2	1:A:197:VAL:HG11	1.95	0.46
1:A:1281:GLN:OE1	1:A:1281:GLN:HA	2.16	0.46
4:D:218:LEU:HD22	4:D:220:LEU:HD21	1.97	0.46
2:B:924:GLY:N	2:B:965:VAL:O	2.43	0.46
2:B:523:THR:HG23	2:B:568:SER:HB2	1.98	0.46
2:B:55:ILE:O	2:B:59:VAL:HG13	2.16	0.46
7:I:57:ILE:HD12	7:I:84:ILE:HD11	1.98	0.46
1:A:393:LEU:HD22	1:A:397:PHE:CD2	2.50	0.46
1:A:770:ARG:HG2	1:A:777:ARG:HA	1.97	0.46
1:A:1225:ILE:HD13	1:A:1225:ILE:N	2.31	0.46
2:B:617:ILE:HG23	2:B:617:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1123:GLU:HA	1:A:1126:ILE:HD12	1.98	0.45
1:A:1412:ALA:HB3	1:A:1413:PRO:HD3	1.98	0.45
1:A:1416:MET:SD	2:B:1220:GLN:NE2	2.89	0.45
2:B:50:LEU:HD22	2:B:422:GLY:HA2	1.98	0.45
1:A:1248:VAL:O	1:A:1251:VAL:HG22	2.17	0.45
2:B:8:ILE:HD12	2:B:641:GLU:OE2	2.16	0.45
2:B:639:ARG:NH2	2:B:745:GLU:OE2	2.42	0.45
3:C:85:ASP:OD1	3:C:86:LEU:N	2.49	0.45
2:B:40:ILE:HD11	2:B:189:PRO:CG	2.46	0.45
2:B:255:ALA:HA	2:B:315:VAL:HG11	1.97	0.45
1:A:1111:GLN:OE1	1:A:1115:ASN:ND2	2.46	0.45
1:A:1324:GLU:O	1:A:1324:GLU:OE2	2.35	0.45
3:C:290:ILE:HG22	3:C:294:LEU:HD12	1.97	0.45
1:A:696:THR:HG23	1:A:699:ASP:H	1.81	0.45
1:A:972:PRO:HB2	1:A:987:ILE:HG21	1.98	0.45
4:D:97:SER:O	4:D:98:ASN:OD1	2.35	0.45
2:B:228:ILE:CD1	2:B:401:ILE:HD11	2.47	0.45
2:B:388:ARG:NH2	2:B:604:ASN:OD1	2.46	0.45
2:B:402:MET:HG3	2:B:402:MET:O	2.15	0.45
1:A:70:MET:HE2	2:B:1217:ILE:HG21	1.98	0.45
1:A:918:PHE:HA	1:A:1315:VAL:HG22	1.99	0.45
1:A:259:ASN:O	1:A:262:THR:HG22	2.17	0.45
4:D:182:VAL:HG13	4:D:240:LEU:HD23	1.98	0.45
5:E:36:LEU:HD22	5:E:36:LEU:H	1.82	0.45
1:A:1401:ASP:OD1	1:A:1401:ASP:O	2.35	0.44
1:A:1187:LEU:O	1:A:1187:LEU:HD12	2.16	0.44
1:A:70:MET:HE2	2:B:1217:ILE:HG13	2.00	0.44
2:B:308:ILE:HG21	2:B:398:LEU:HD22	1.99	0.44
7:I:94:LEU:N	7:I:94:LEU:HD12	2.32	0.44
1:A:773:VAL:HG22	1:A:773:VAL:O	2.17	0.44
1:A:1312:TYR:CE1	5:E:128:ILE:HD11	2.52	0.44
2:B:369:ASP:OD2	2:B:370:LYS:NZ	2.50	0.44
4:D:113:VAL:O	4:D:113:VAL:CG1	2.65	0.44
8:J:34:ASP:OD1	8:J:35:GLY:N	2.50	0.44
1:A:934:VAL:HG13	1:A:1026:ILE:HD11	2.00	0.44
1:A:1131:LEU:HD13	1:A:1251:VAL:HG11	1.98	0.44
1:A:169:ILE:HD13	1:A:248:ARG:HA	2.00	0.44
1:A:1181:ASN:ND2	1:A:1184:THR:OG1	2.51	0.44
5:E:110:ARG:NH1	5:E:118:ILE:O	2.49	0.44
2:B:590:LEU:O	2:B:596:ILE:HD13	2.18	0.44
1:A:70:MET:HB3	2:B:1217:ILE:HG21	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:VAL:N	1:A:250:GLN:OE1	2.51	0.43
1:A:442:SER:OG	2:B:1119:ARG:NE	2.51	0.43
2:B:58:ILE:HD13	2:B:429:PHE:HD2	1.82	0.43
6:F:103:ILE:O	6:F:107:LYS:HG3	2.18	0.43
3:C:29:LEU:CD1	8:J:19:ALA:HB1	2.48	0.43
1:A:240:ILE:HG12	1:A:263:ILE:HD11	1.99	0.43
1:A:757:ILE:HG21	1:A:810:PHE:CE2	2.54	0.43
2:B:251:MET:HE3	2:B:251:MET:HA	1.99	0.43
2:B:621:TRP:NE1	2:B:623:GLY:O	2.51	0.43
1:A:1153:GLU:OE1	1:A:1154:TRP:N	2.51	0.43
4:D:99:ILE:HG22	4:D:101:LEU:HD13	1.99	0.43
5:E:32:VAL:HG22	5:E:36:LEU:HD21	2.01	0.43
6:F:107:LYS:HZ2	6:F:111:PHE:HE2	1.66	0.43
2:B:793:GLN:OE1	2:B:795:ALA:HB3	2.19	0.43
4:D:312:ASP:OD1	4:D:312:ASP:N	2.51	0.43
1:A:1051:GLU:HB3	1:A:1052:PRO:HD3	2.01	0.43
4:D:51:VAL:O	4:D:51:VAL:HG23	2.18	0.43
1:A:1429:ILE:HG21	6:F:117:LEU:HD13	2.01	0.42
1:A:142:PRO:HB2	1:A:156:VAL:HG23	2.01	0.42
2:B:397:ILE:O	2:B:401:ILE:HG12	2.18	0.42
1:A:875:LEU:O	1:A:909:ARG:NH2	2.53	0.42
2:B:373:LEU:HD13	2:B:389:PHE:HD2	1.84	0.42
2:B:649:THR:HG22	2:B:664:LEU:CD2	2.50	0.42
4:D:182:VAL:HG13	4:D:240:LEU:CD2	2.49	0.42
1:A:82:VAL:HG13	1:A:264:GLN:OE1	2.20	0.42
2:B:389:PHE:O	2:B:393:LEU:HD12	2.20	0.42
2:B:830:GLU:HG2	2:B:847:LEU:HA	2.02	0.42
1:A:226:ILE:O	1:A:229:VAL:HG22	2.20	0.42
1:A:1258:THR:O	1:A:1258:THR:HG23	2.19	0.42
2:B:649:THR:HG22	2:B:664:LEU:HD23	2.01	0.42
3:C:82:ASP:C	3:C:82:ASP:OD1	2.58	0.42
1:A:770:ARG:NH1	2:B:749:CYS:O	2.49	0.42
2:B:303:THR:O	2:B:307:GLU:OE1	2.38	0.42
2:B:373:LEU:HD11	2:B:390:LEU:CD2	2.50	0.42
4:D:196:ASP:OD1	4:D:196:ASP:O	2.38	0.42
1:A:591:THR:HA	1:A:601:GLY:HA3	2.02	0.42
1:A:678:GLU:OE1	1:A:678:GLU:HA	2.20	0.42
1:A:808:GLY:HA3	2:B:795:ALA:CB	2.49	0.42
2:B:793:GLN:NE2	2:B:796:ARG:CZ	2.83	0.42
1:A:382:GLN:O	1:A:385:GLN:NE2	2.53	0.41
1:A:770:ARG:NH2	2:B:749:CYS:O	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1438:GLU:HG2	1:A:1439:ASN:OD1	2.20	0.41
2:B:845:ASN:OD1	2:B:845:ASN:O	2.37	0.41
5:E:82:LYS:N	5:E:82:LYS:HD2	2.35	0.41
7:I:28:GLU:CG	7:I:28:GLU:O	2.68	0.41
2:B:514:LEU:HD11	2:B:843:ILE:HD12	2.01	0.41
2:B:830:GLU:HB3	8:J:73:THR:HA	2.02	0.41
3:C:273:ASP:O	3:C:274:GLU:HB3	2.21	0.41
2:B:543:ARG:HE	2:B:567:MET:CE	2.33	0.41
2:B:201:VAL:CG2	2:B:521:LEU:HD21	2.50	0.41
7:I:48:GLU:CG	7:I:48:GLU:O	2.69	0.41
2:B:228:ILE:HD13	2:B:401:ILE:CD1	2.51	0.41
2:B:291:VAL:HG11	2:B:309:LEU:HD11	2.03	0.41
1:A:240:ILE:CG1	1:A:263:ILE:HD11	2.50	0.41
4:D:217:ILE:HG13	4:D:225:GLY:O	2.21	0.41
4:D:242:PHE:CD1	4:D:242:PHE:C	2.94	0.41
1:A:147:ASP:OD1	1:A:148:SER:N	2.53	0.41
1:A:1210:HIS:ND1	1:A:1210:HIS:C	2.74	0.41
2:B:55:ILE:O	2:B:59:VAL:HG22	2.20	0.41
2:B:128:VAL:HG22	2:B:160:PHE:CD2	2.55	0.41
2:B:376:MET:HE1	2:B:389:PHE:CG	2.56	0.41
2:B:392:LEU:HD21	2:B:614:ARG:CZ	2.51	0.41
2:B:792:THR:CG2	2:B:1040:GLY:H	2.33	0.41
2:B:884:GLU:HB3	2:B:983:ARG:HA	2.03	0.41
4:D:259:ARG:HH12	4:D:300:ILE:HG13	1.86	0.41
4:D:273:GLN:CD	4:D:278:PHE:CE1	2.94	0.41
1:A:973:TYR:O	1:A:976:ILE:O	2.39	0.41
2:B:55:ILE:HB	2:B:56:PRO:HD3	2.02	0.41
1:A:156:VAL:HG13	1:A:156:VAL:O	2.21	0.40
1:A:294:ARG:HB2	1:A:295:PRO:HD3	2.03	0.40
1:A:304:PRO:O	1:A:305:ARG:HB2	2.22	0.40
2:B:930:GLY:N	2:B:957:TYR:O	2.45	0.40
1:A:961:TYR:O	1:A:964:VAL:HG22	2.21	0.40
2:B:171:THR:HG22	2:B:171:THR:O	2.21	0.40
2:B:552:TYR:OH	2:B:741:ILE:O	2.30	0.40
1:A:108:ASP:HB3	1:A:111:ARG:HB2	2.04	0.40
1:A:608:VAL:HG12	1:A:616:ILE:HD11	2.03	0.40
1:A:812:LEU:HD21	2:B:798:THR:HG22	2.03	0.40
2:B:586:LEU:HD23	2:B:664:LEU:HD11	2.03	0.40
2:B:617:ILE:HG22	2:B:622:ILE:CG2	2.50	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	1413/1450 (97%)	1392 (98%)	21 (2%)	0	100	100
2	B	998/1243 (80%)	964 (97%)	34 (3%)	0	100	100
3	C	357/359 (99%)	354 (99%)	3 (1%)	0	100	100
4	D	333/339 (98%)	330 (99%)	3 (1%)	0	100	100
5	E	202/205 (98%)	199 (98%)	3 (2%)	0	100	100
6	F	108/147 (74%)	105 (97%)	3 (3%)	0	100	100
7	I	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
8	J	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
All	All	3592/3928 (91%)	3521 (98%)	71 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1261/1279 (99%)	1243 (99%)	18 (1%)	67	88
2	B	882/1081 (82%)	868 (98%)	14 (2%)	62	85
3	C	328/328 (100%)	324 (99%)	4 (1%)	71	90
4	D	309/312 (99%)	304 (98%)	5 (2%)	62	85
5	E	183/185 (99%)	180 (98%)	3 (2%)	62	85
6	F	100/136 (74%)	98 (98%)	2 (2%)	55	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	I	96/96 (100%)	93 (97%)	3 (3%)	40	72
8	J	71/71 (100%)	67 (94%)	4 (6%)	21	50
All	All	3230/3488 (93%)	3177 (98%)	53 (2%)	64	85

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	66	ARG
1	A	157	ASP
1	A	397	PHE
1	A	417	PHE
1	A	767	SER
1	A	833	LEU
1	A	877	ASP
1	A	1030	TYR
1	A	1124	ARG
1	A	1161	ASN
1	A	1178	LEU
1	A	1213	GLU
1	A	1214	ASN
1	A	1252	ASP
1	A	1351	ARG
1	A	1370	GLU
1	A	1397	ASP
2	B	115	ASN
2	B	124	TYR
2	B	167	ASN
2	B	207	ASN
2	B	217	TYR
2	B	235	GLN
2	B	265	PHE
2	B	317	ASP
2	B	325	HIS
2	B	375	HIS
2	B	436	SER
2	B	516	ASN
2	B	1020	ASP
2	B	1118	ASP
3	C	46	ASP
3	C	257	TYR

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Mol	Chain	Res	Type
3	C	260	PHE
3	C	285	ASP
4	D	159	HIS
4	D	177	ASN
4	D	198	LYS
4	D	244	TYR
4	D	293	PHE
5	E	84	HIS
5	E	185	GLU
5	E	192	MET
6	F	62	ASP
6	F	104	ASP
7	I	16	VAL
7	I	33	ASP
7	I	98	CYS
8	J	7	CYS
8	J	27	GLU
8	J	34	ASP
8	J	80	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	375	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

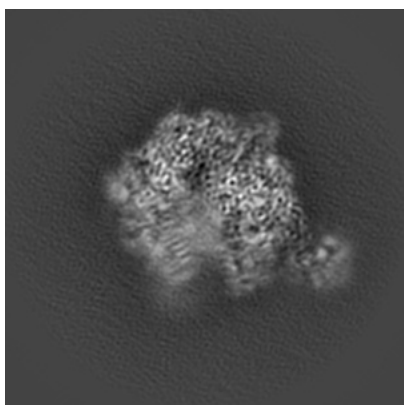
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18129. These allow visual inspection of the internal detail of the map and identification of artifacts.

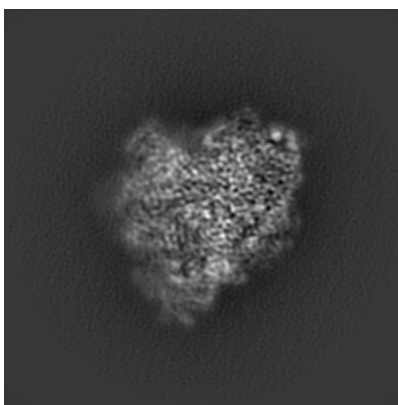
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

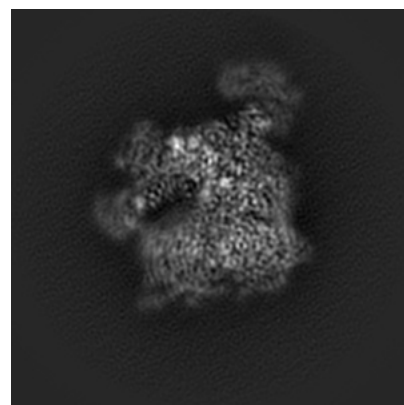
#### 6.1.1 Primary map



X



Y

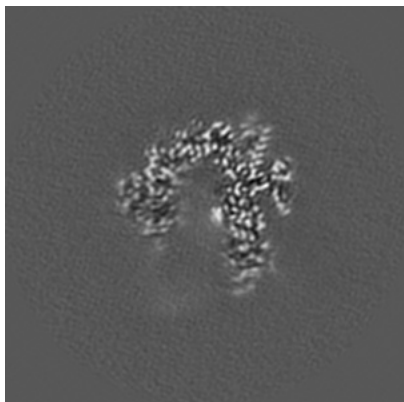


Z

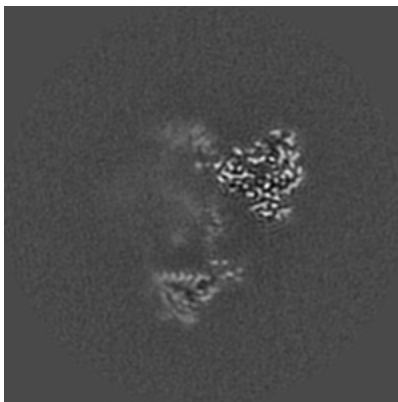
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

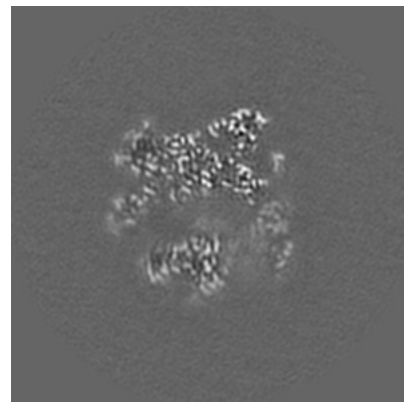
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

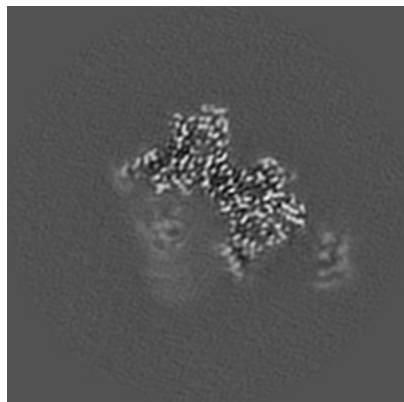


Z Index: 150

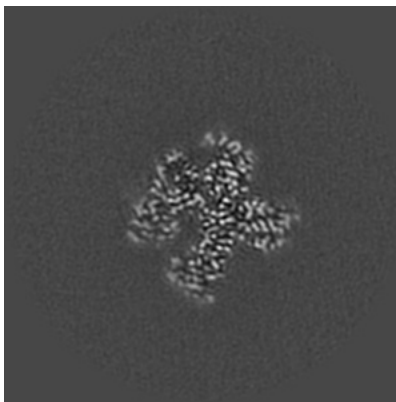
The images above show central slices of the map in three orthogonal directions.

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

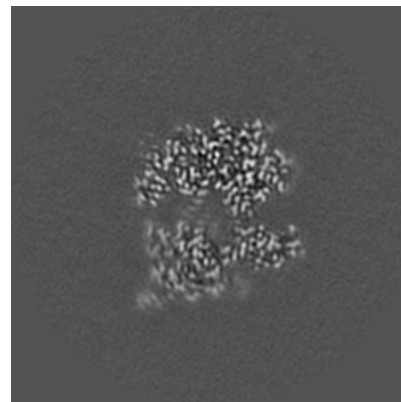
### 6.3.1 Primary map



X Index: 173



Y Index: 189

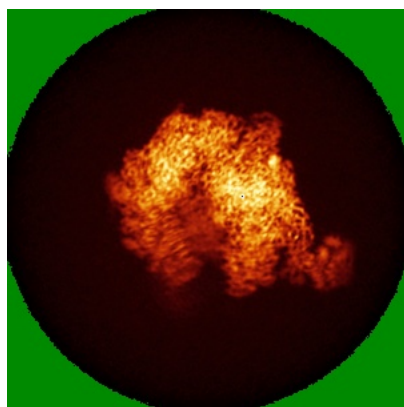


Z Index: 165

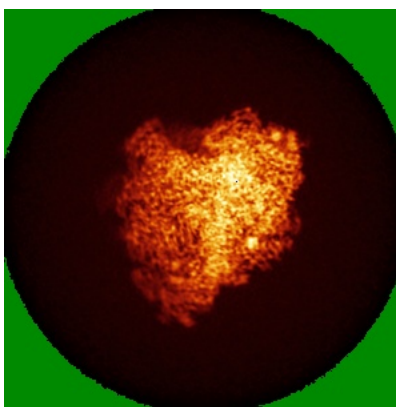
The images above show the largest variance slices of the map in three orthogonal directions.

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

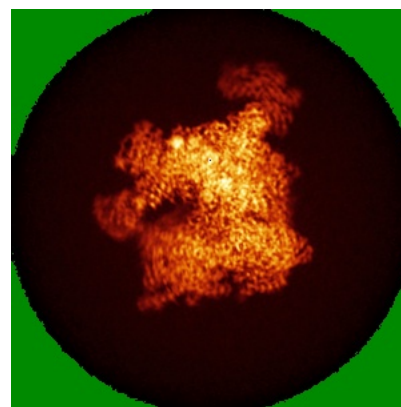
### 6.4.1 Primary map



X



Y

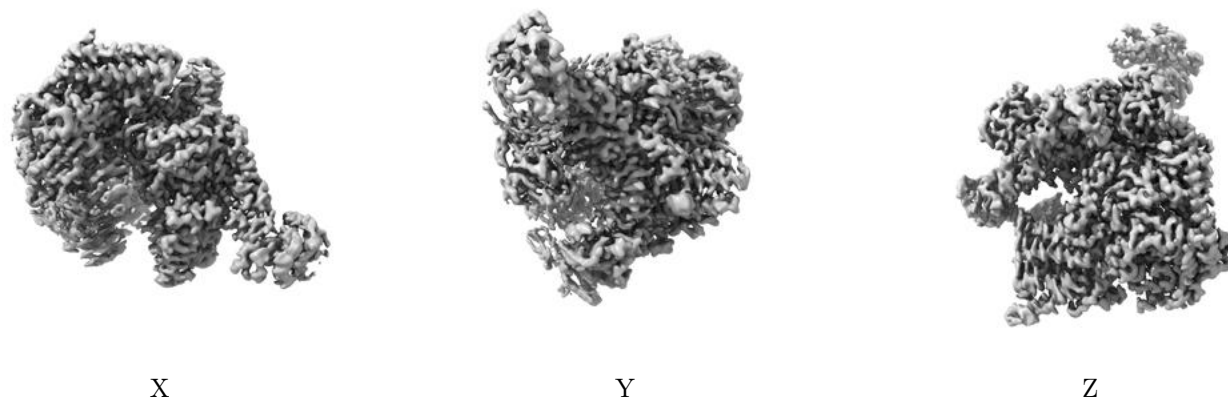


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

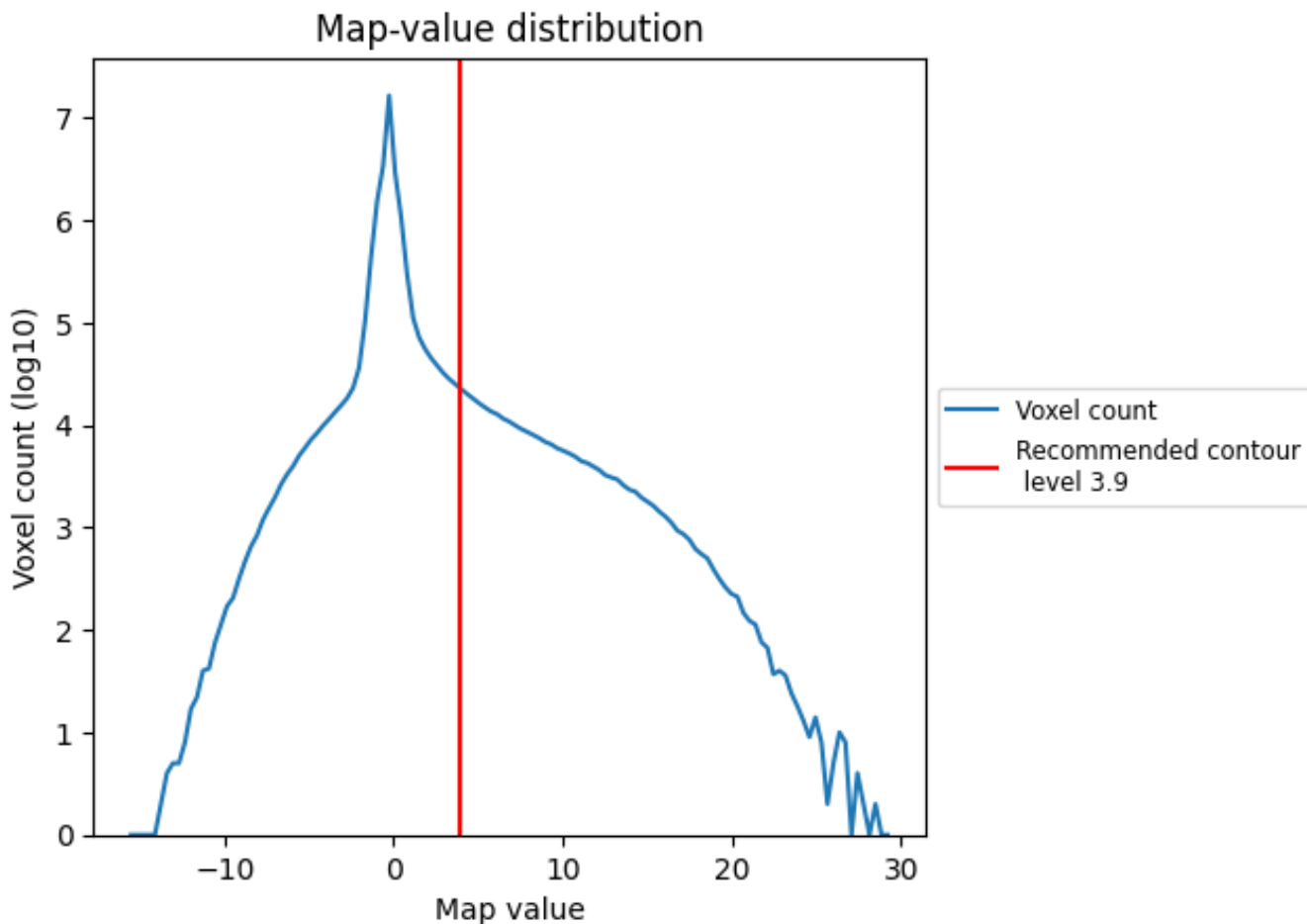
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

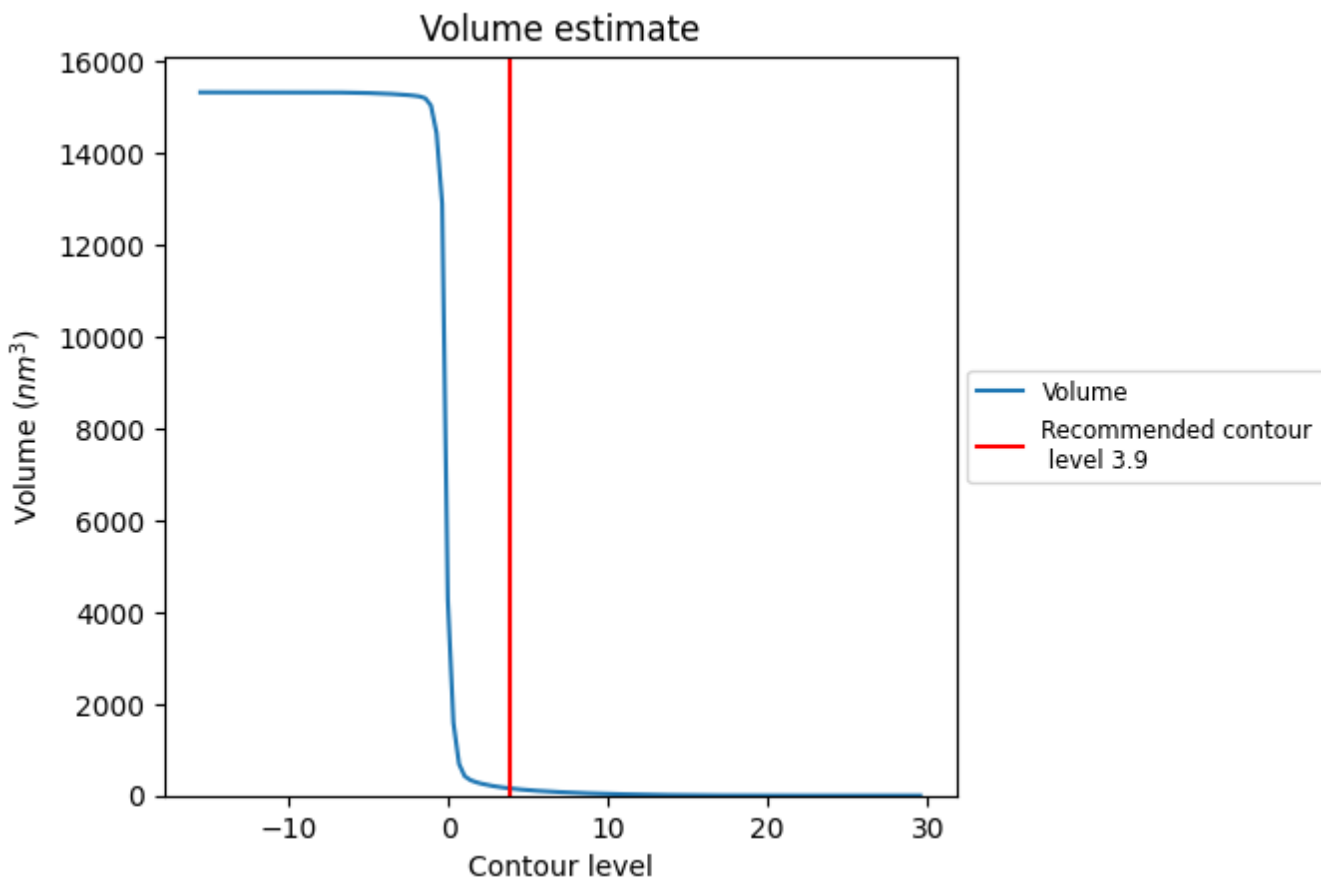
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

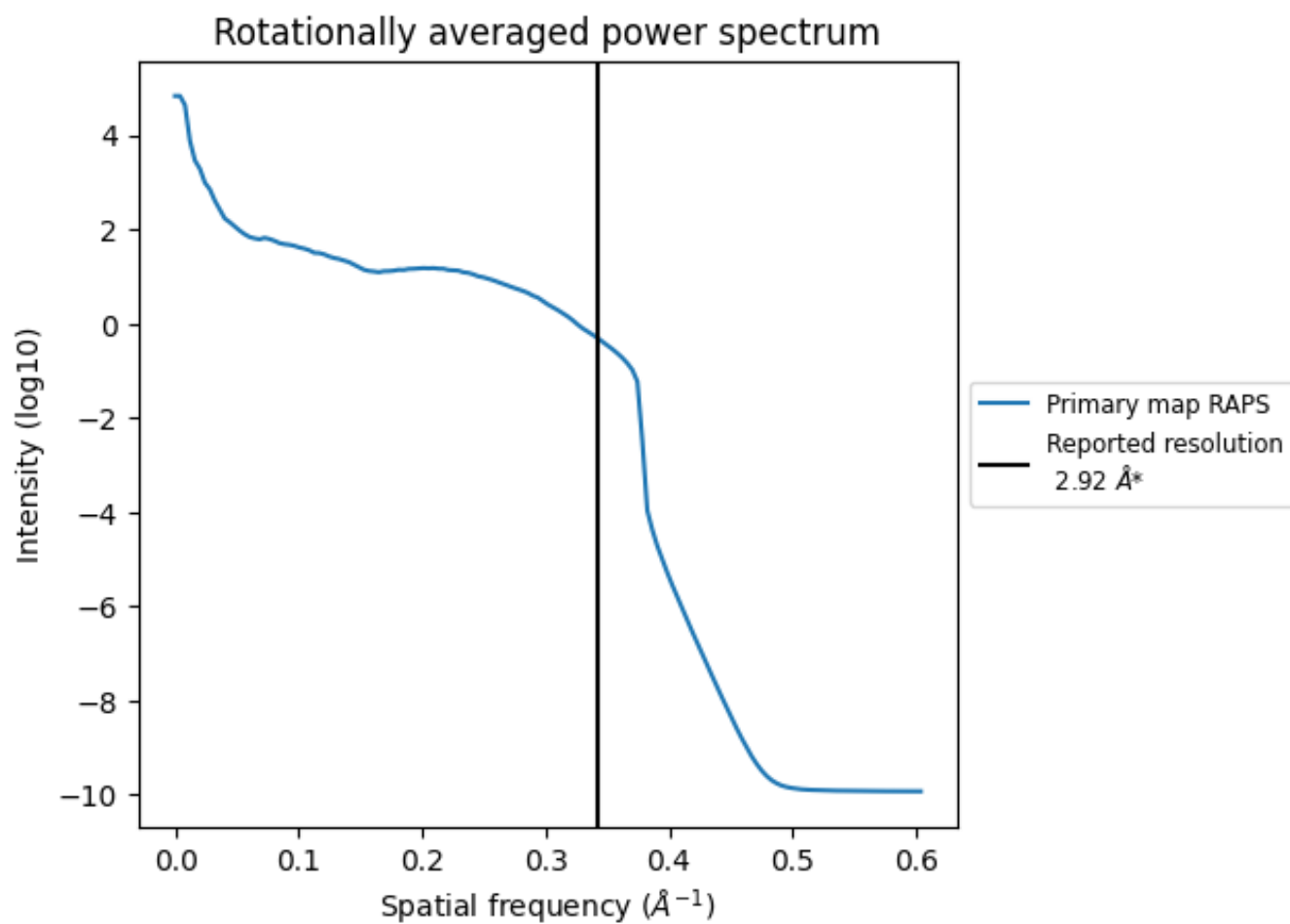
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 155 nm<sup>3</sup>; this corresponds to an approximate mass of 140 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 [\(i\)](#)

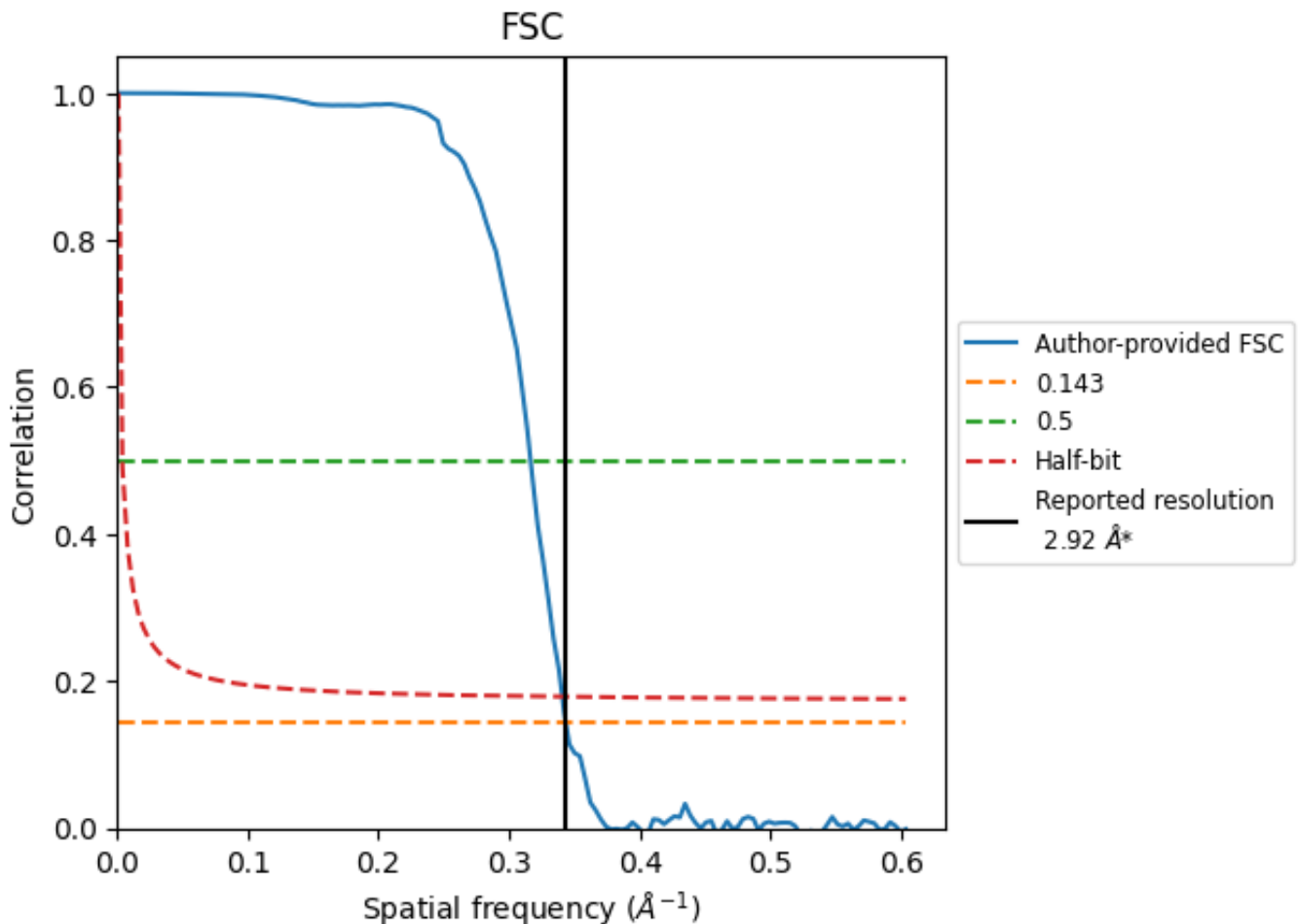


\*Reported resolution corresponds to spatial frequency of 0.342 Å<sup>-1</sup>

## 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 0.342 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

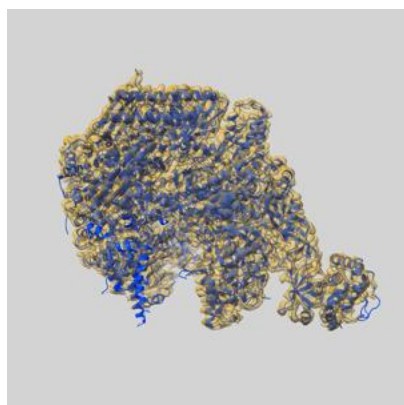
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	2.91	3.16	2.94
Unmasked-calculated*	-	-	-

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

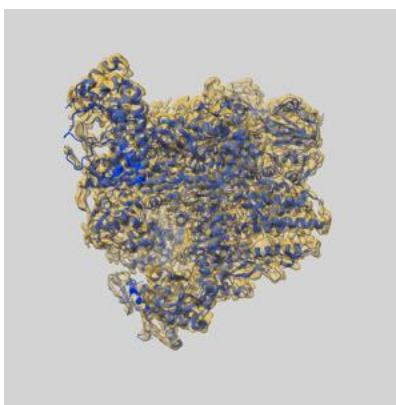
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18129 and PDB model 8Q3K. Per-residue inclusion information can be found in section 3 on page 5.

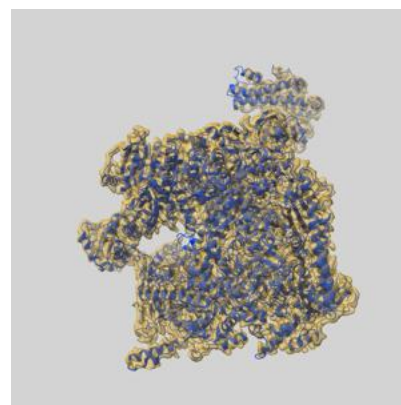
### 9.1 Map-model overlay [i](#)



X



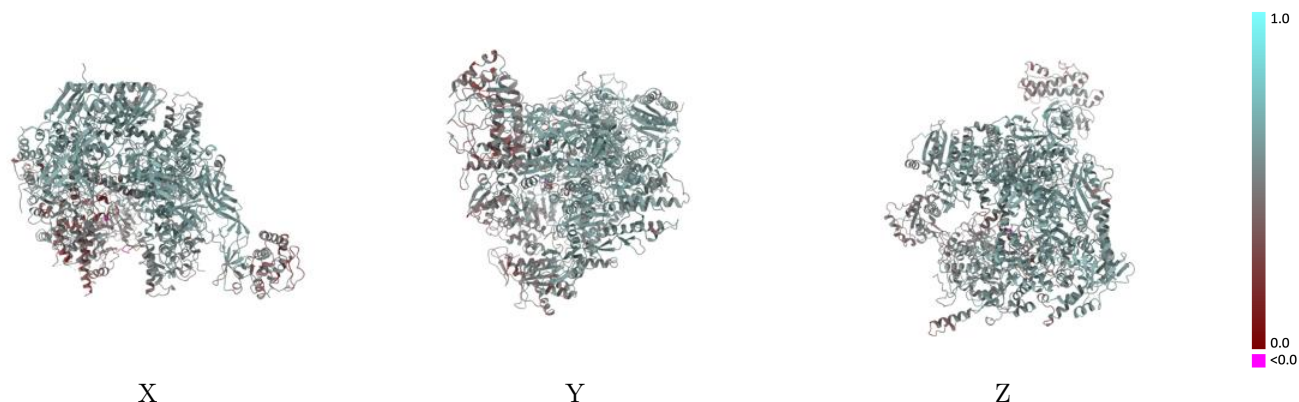
Y



Z

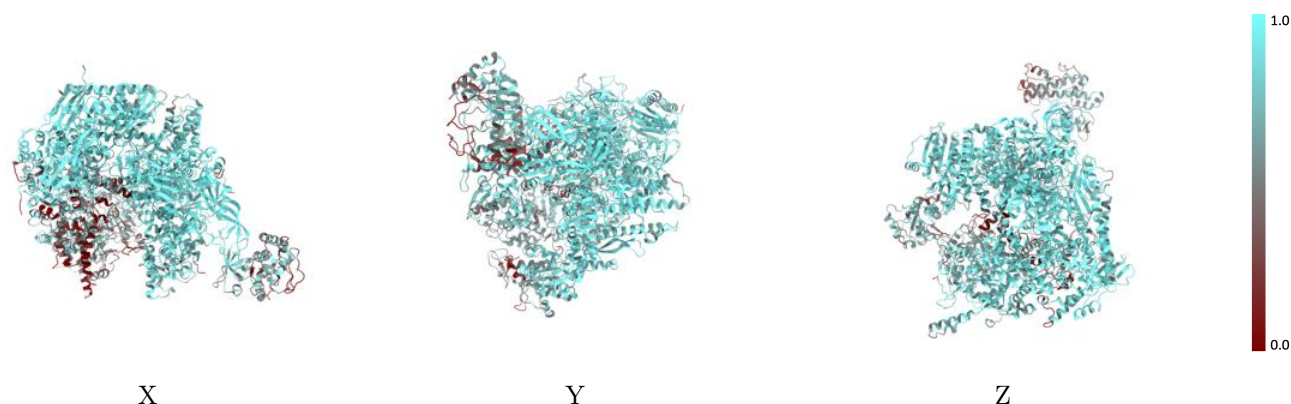
The images above show the 3D surface view of the map at the recommended contour level 3.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



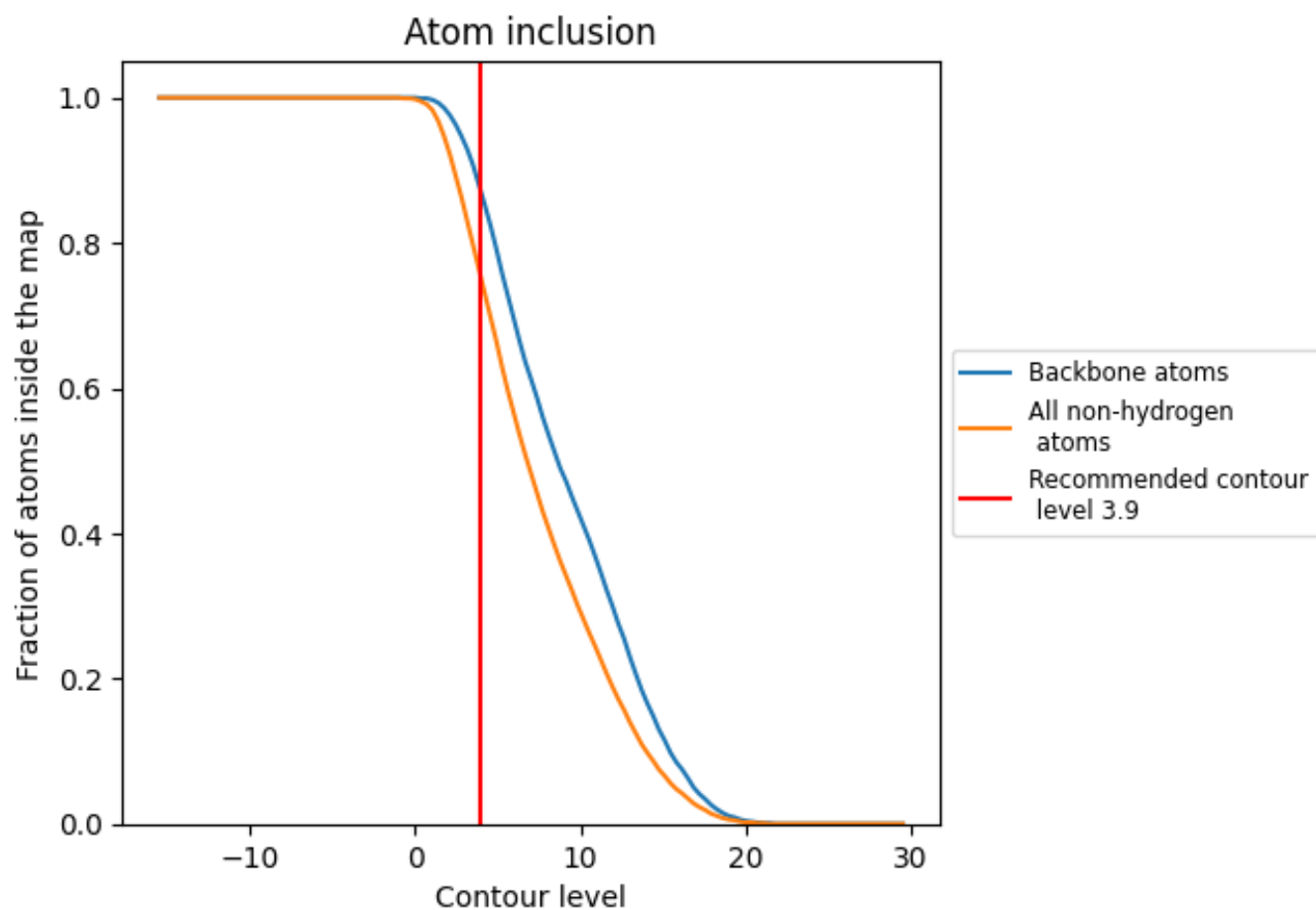
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.9).

## 9.4 Atom inclusion [i](#)





















At the recommended contour level, 88% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (3.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7600	 0.5310
A	 0.8190	 0.5490
B	 0.6650	 0.5000
C	 0.8730	 0.5760
D	 0.6100	 0.4810
E	 0.8660	 0.5580
F	 0.8690	 0.5820
I	 0.6310	 0.4650
J	 0.7700	 0.5480

