



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:46 AM UTC

PDB ID : 9M7Y / pdb_00009m7y
EMDB ID : EMD-63697
Title : Cryo-EM structure of gp79-dependent RNAP promoter open complex
Authors : Xu, L.; Feng, Y.
Deposited on : 2025-03-11
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

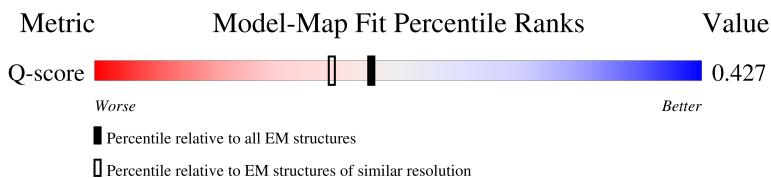
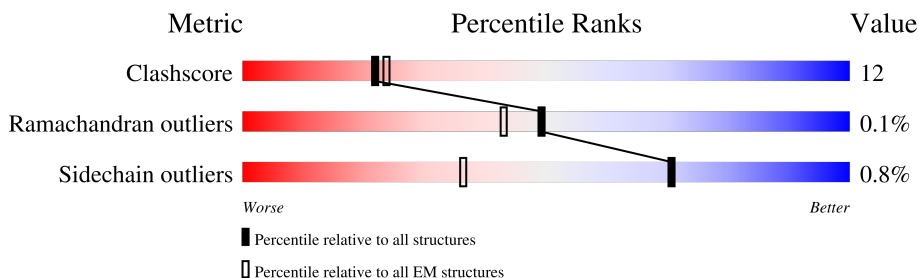
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	A	1342	
2	B	1407	
3	C	329	
3	D	329	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	91	
5	F	214	
6	G	82	
7	H	71	
8	I	71	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 28130 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 beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1341	Total	C	N	O	S	0	0
			10577	6636	1842	2056	43		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1167	Total	C	N	O	S	0	0
			9133	5747	1633	1706	47		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	228	Total	C	N	O	S	0	0
			1768	1102	312	348	6		
3	D	218	Total	C	N	O	S	0	0
			1683	1051	297	329	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	72	Total	C	N	O	S	0	0
			573	350	110	112	1		

- Molecule 5 is a protein called RNA polymerase ECF sigma factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	208	Total	C	N	O	S	0	0
			1775	1139	298	328	10		

- Molecule 6 is a protein called gp79.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	78	Total	C	N	O	S	0	0
			629	392	109	122	6		

- Molecule 7 is a DNA chain called Non-template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	55	Total	C	N	O	P	0	0
			1138	546	210	327	55		

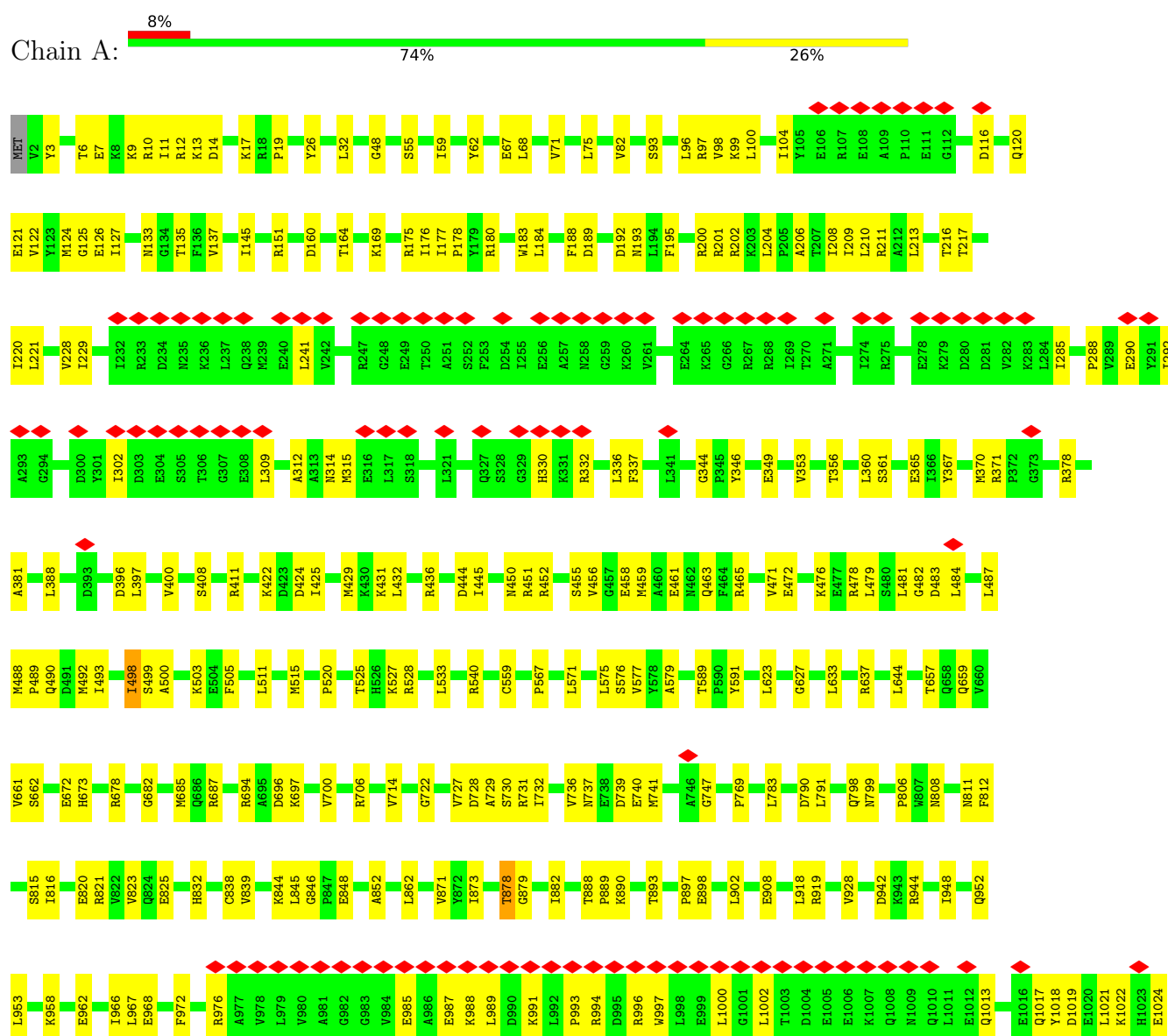
- Molecule 8 is a DNA chain called Template strand DNA.

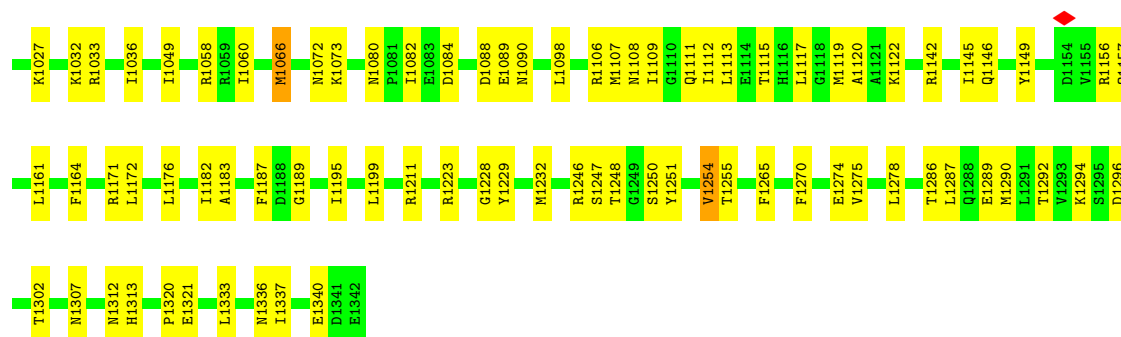
Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	42	Total	C	N	O	P	0	0
			854	413	145	254	42		

3 Residue-property plots

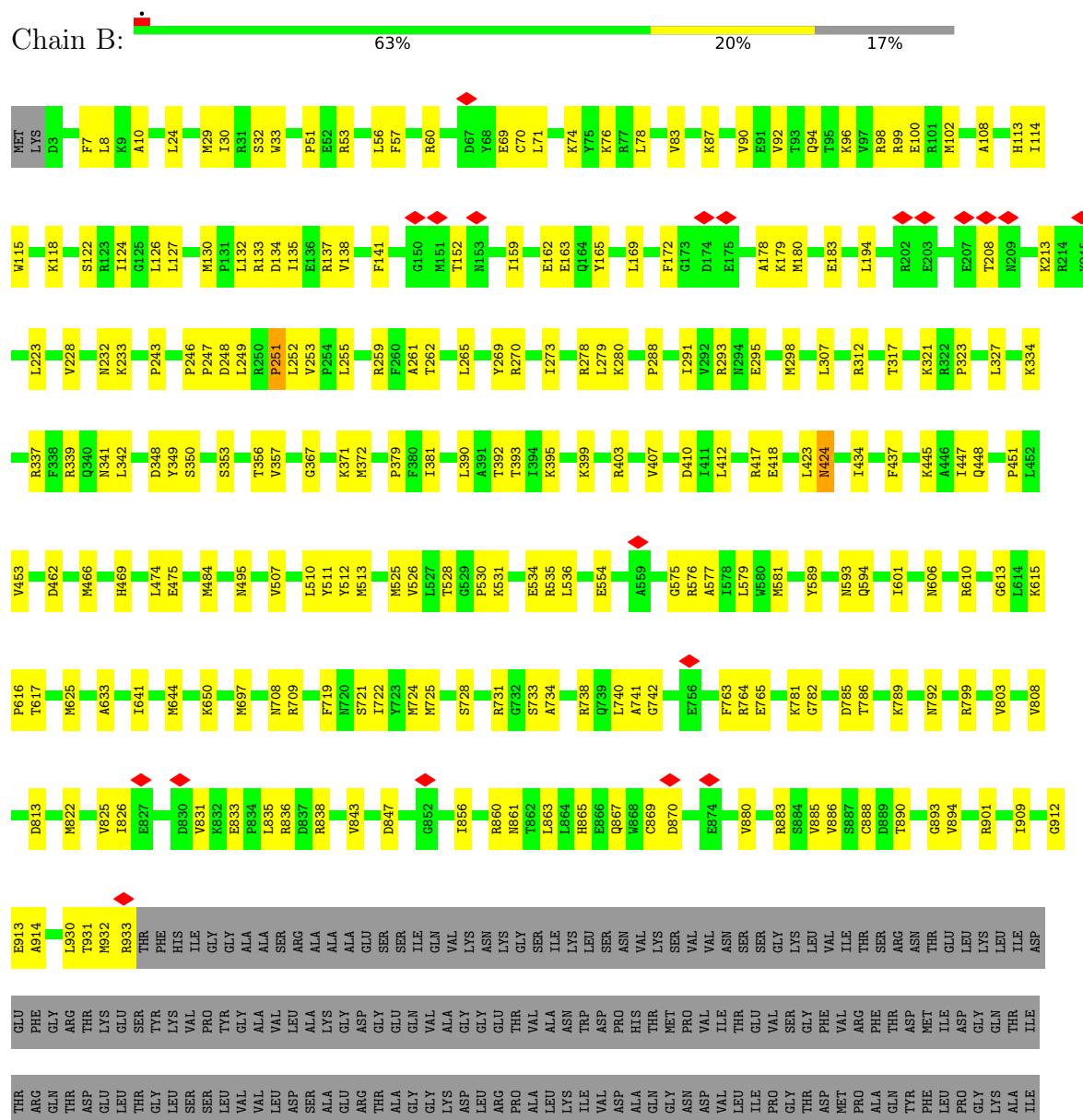
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

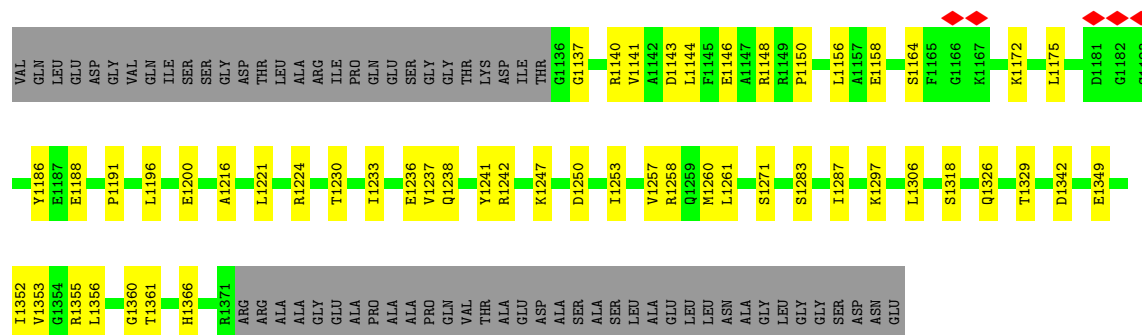
- Molecule 1: DNA-directed RNA polymerase subunit beta



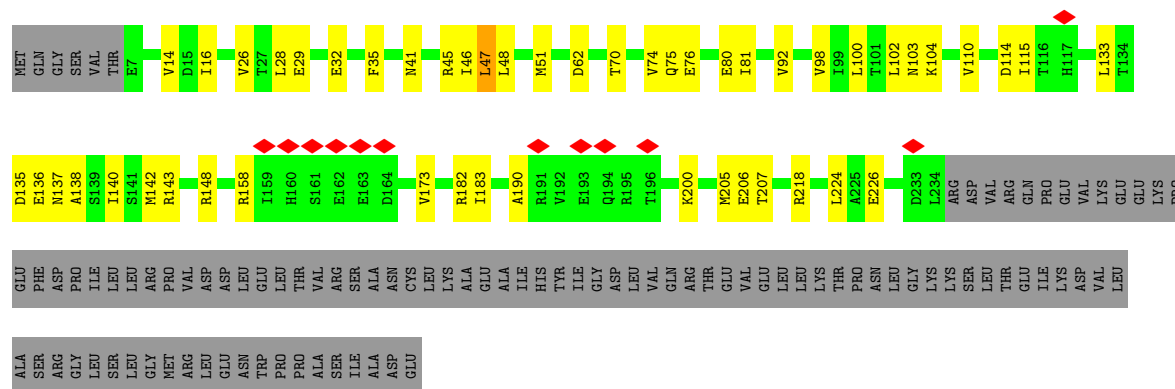


• Molecule 2: DNA-directed RNA polymerase subunit beta'

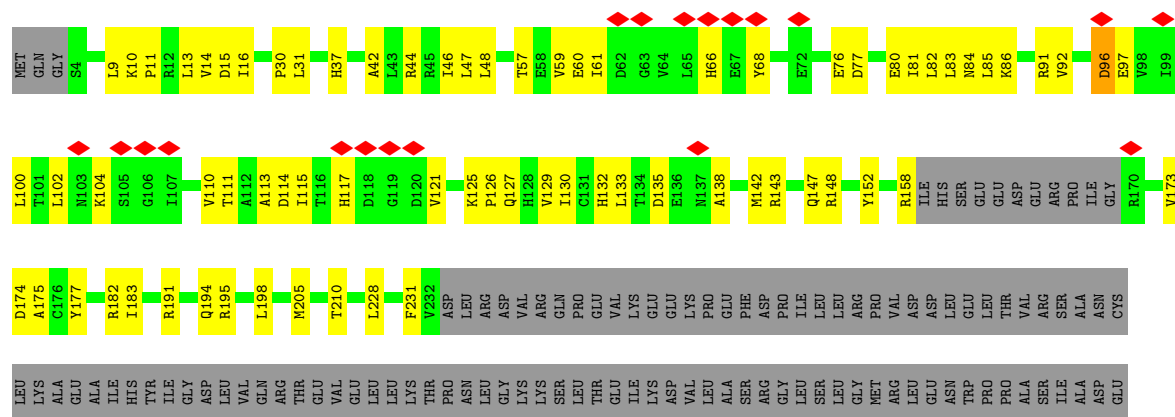
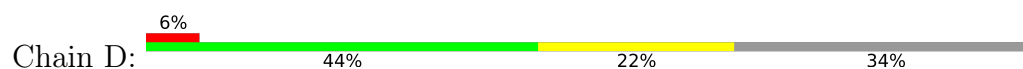




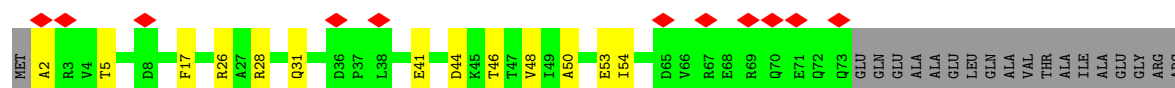
• Molecule 3: DNA-directed RNA polymerase subunit alpha



• Molecule 3: DNA-directed RNA polymerase subunit alpha



• Molecule 4: DNA-directed RNA polymerase subunit omega



Chain F:

5% 60% 36%

• •

Met Ala Lys K4 R9 Y10 I12 H13 G14 I15 Y19 I20 S21 N22 Y23 E24 E25 F26 Y27 K28 V29 V34 H35 K36 F37 F38 D41 T42 R43 D44 E47 A48 A49 E50 D50 V51 A52 A53 W60 A65 K66 Q67 D68 E69 V71 V72 L72 E73 E75 E76 E77

M81 T82 R83 R84 R85 R86 R89 W90 R93 S94 N95 V99 R102 M118 P122 L123 M127 Q130 D131 S132 G134 D135 P136 F137 M138 E139 S140 R141 I142 F145 D148 L149 S150 L158 A159 M160 M164 I169 P170 H171 I174 Q175 K176 T177

I178 G179 G180 S181 H182 G183 T184 E191 L192 K203 H203 F204 D205 K206 Q210 G211 LEU ILE THR

Chain G:

Chain H:

Segment Color	Percentage
Green	23%
Yellow	55%
Grey	23%

DT DT DA DC DT DA DC DT DT DT DA DT DT DT DT DT DT DT T12 T13 T14 T15 A16 A17 A18 T19 A20 A21 A22 A23 T27 A28 C34 A35 A36 A37 T38 T39 A43 T44 A45 A46 A47 A48 T49 A50 A51 A52 A53 A54 A55 A56 A57 A58 A59 T60 T61 T62 T63 T64 A65 A66 DT DT

Chain I:

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	230133	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.050	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	261.80002, 261.80002, 261.80002	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.19, 1.19, 1.19	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/10746	0.40	0/14499
2	B	0.34	0/9274	0.41	1/12514 (0.0%)
3	C	0.32	0/1790	0.39	0/2426
3	D	0.35	0/1702	0.55	2/2306 (0.1%)
4	E	0.27	0/575	0.34	0/774
5	F	0.34	0/1823	0.56	1/2457 (0.0%)
6	G	0.51	0/635	0.87	0/847
7	H	0.27	0/1279	0.47	0/1974
8	I	0.26	0/954	0.43	0/1466
All	All	0.33	0/28778	0.44	4/39263 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	170	PRO	CB-CA-C	-6.34	103.27	111.39
2	B	251	PRO	N-CA-C	6.22	121.28	111.38
3	D	177	TYR	CA-C-N	5.66	128.35	120.65
3	D	177	TYR	C-N-CA	5.66	128.35	120.65

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	10577	0	10591	240	0
2	B	9133	0	9346	202	0
3	C	1768	0	1793	42	0
3	D	1683	0	1719	61	0
4	E	573	0	587	8	0
5	F	1775	0	1699	74	0
6	G	629	0	637	50	0
7	H	1138	0	625	36	0
8	I	854	0	481	17	0
All	All	28130	0	27478	642	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 12.

All (642) 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:898:GLU:HG2	5:F:138:MET:HE2	1.45	0.95
1:A:1302:THR:HG21	6:G:15:MET:SD	2.11	0.91
2:B:417:ARG:NH2	2:B:418:GLU:OE1	2.04	0.90
1:A:1251:TYR:H	5:F:133:VAL:HG11	1.39	0.86
5:F:138:MET:HG3	5:F:139:GLU:H	1.40	0.86
1:A:540:ARG:HD2	1:A:567:PRO:HB2	1.59	0.84
2:B:7:PHE:HD1	6:G:32:LEU:HD13	1.43	0.82
6:G:29:LEU:HD13	6:G:44:ILE:HG23	1.61	0.82
5:F:191:GLU:HG2	5:F:192:LEU:HG	1.64	0.79
1:A:1302:THR:CG2	6:G:15:MET:SD	2.70	0.79
3:C:104:LYS:HD3	3:C:110:VAL:HG22	1.66	0.78
5:F:133:VAL:HG22	5:F:134:GLY:H	1.48	0.78
1:A:1302:THR:HB	6:G:15:MET:SD	2.24	0.78
3:C:100:LEU:HD23	3:C:115:ILE:HG21	1.64	0.78
3:D:104:LYS:HD3	3:D:110:VAL:HG13	1.66	0.77
6:G:43:MET:SD	6:G:44:ILE:HG13	2.24	0.77
2:B:350:SER:HG	2:B:469:HIS:HD1	1.33	0.76
6:G:76:ASP:OD1	6:G:77:LYS:N	2.18	0.76
1:A:967:LEU:HB3	1:A:1021:LEU:HD11	1.68	0.76
2:B:94:GLN:OE1	6:G:17:GLN:HA	1.86	0.75
2:B:792:ASN:ND2	2:B:932:MET:SD	2.60	0.75
3:D:86:LYS:NZ	3:D:174:ASP:HB2	2.02	0.75
2:B:357:VAL:HG23	2:B:451:PRO:HG3	1.70	0.74
1:A:1302:THR:CB	6:G:15:MET:SD	2.76	0.74
3:D:113:ALA:HB2	3:D:126:PRO:HB3	1.71	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:91:ARG:NH1	3:D:210:THR:O	2.22	0.73
2:B:1158:GLU:N	2:B:1158:GLU:OE2	2.21	0.72
1:A:591:TYR:OH	1:A:637:ARG:NH2	2.22	0.72
5:F:20:ILE:HD13	5:F:25:GLU:HG2	1.71	0.72
2:B:141:PHE:HA	2:B:180:MET:HE2	1.68	0.72
2:B:697:MET:HE1	2:B:738:ARG:HA	1.70	0.72
1:A:478:ARG:HH21	1:A:487:LEU:HD11	1.55	0.71
2:B:1353:VAL:HG23	2:B:1355:ARG:HG3	1.71	0.71
3:C:226:GLU:HG3	3:D:10:LYS:HE3	1.70	0.71
1:A:370:MET:HE2	1:A:388:LEU:HD11	1.73	0.71
7:H:52:DA:H2''	7:H:53:DA:H2'	1.70	0.71
2:B:253:VAL:HG12	5:F:127:MET:SD	2.30	0.71
1:A:528:ARG:NH2	1:A:576:SER:O	2.23	0.70
5:F:20:ILE:HD12	5:F:26:PHE:HA	1.73	0.70
3:D:76:GLU:OE2	3:D:132:HIS:ND1	2.22	0.70
1:A:997:TRP:HA	1:A:1000:LEU:HD12	1.74	0.69
2:B:825:VAL:HG12	2:B:833:GLU:HB2	1.74	0.69
2:B:29:MET:HE1	6:G:49:SER:HB2	1.75	0.69
1:A:463:GLN:HG2	1:A:505:PHE:HB2	1.73	0.69
2:B:1156:LEU:HD21	2:B:1224:ARG:HH21	1.58	0.69
3:D:86:LYS:HZ2	3:D:174:ASP:HB2	1.57	0.69
1:A:408:SER:O	1:A:431:LYS:NZ	2.22	0.68
5:F:9:ARG:HH12	5:F:13:HIS:HB2	1.58	0.68
6:G:29:LEU:HB3	6:G:44:ILE:HG12	1.74	0.68
1:A:479:LEU:HA	1:A:492:MET:HE2	1.76	0.68
5:F:10:TYR:O	7:H:43:DA:N6	2.26	0.68
1:A:1292:THR:HG22	1:A:1320:PRO:HG3	1.76	0.68
1:A:962:GLU:O	1:A:966:ILE:HG13	1.94	0.68
2:B:7:PHE:CD1	6:G:32:LEU:HD13	2.26	0.68
2:B:789:LYS:HE2	2:B:931:THR:HA	1.76	0.67
3:C:48:LEU:HG	3:C:183:ILE:HD12	1.76	0.67
2:B:251:PRO:HD2	5:F:123:LEU:HD21	1.76	0.67
1:A:479:LEU:HD23	1:A:492:MET:HE1	1.77	0.66
2:B:909:ILE:HD11	2:B:913:GLU:HG2	1.77	0.66
5:F:139:GLU:HA	5:F:142:ILE:HD12	1.77	0.66
2:B:70:CYS:SG	2:B:71:LEU:N	2.69	0.66
1:A:1286:THR:O	1:A:1290:MET:HG2	1.96	0.66
2:B:451:PRO:HD2	2:B:625:MET:HE1	1.77	0.65
1:A:487:LEU:HD13	1:A:492:MET:HE3	1.77	0.65
1:A:727:VAL:HG11	3:C:75:GLN:NE2	2.12	0.65
1:A:360:LEU:HD13	1:A:378:ARG:HD2	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:ARG:HB3	2:B:248:ASP:HB3	1.79	0.65
5:F:9:ARG:HD3	5:F:90:TRP:CE3	2.31	0.65
1:A:9:LYS:HG2	1:A:1171:ARG:HE	1.60	0.65
1:A:985:GLU:HB3	1:A:988:LYS:HB2	1.79	0.64
1:A:1223:ARG:HD2	2:B:512:TYR:HE1	1.62	0.64
2:B:265:LEU:HD11	2:B:327:LEU:HG	1.78	0.64
1:A:189:ASP:OD1	1:A:195:PHE:HE1	1.80	0.64
3:D:30:PRO:HB2	3:D:198:LEU:HD23	1.80	0.64
1:A:209:ILE:O	1:A:213:LEU:HD12	1.98	0.64
2:B:392:THR:HG23	2:B:393:THR:HG23	1.79	0.64
2:B:644:MET:HE2	2:B:722:ILE:HD11	1.78	0.64
3:C:16:ILE:HG12	3:C:26:VAL:HG13	1.78	0.64
1:A:741:MET:HE2	1:A:747:GLY:HA3	1.79	0.64
2:B:252:LEU:HD13	2:B:262:THR:HG22	1.80	0.64
1:A:1117:LEU:HD13	1:A:1195:ILE:HG12	1.80	0.63
2:B:162:GLU:OE2	2:B:163:GLU:HG3	1.98	0.63
2:B:321:LYS:NZ	7:H:49:DT:OP1	2.25	0.63
3:C:158:ARG:NH2	3:C:173:VAL:O	2.31	0.63
1:A:124:MET:HE2	1:A:493:ILE:HG21	1.80	0.63
3:D:92:VAL:O	3:D:148:ARG:NH2	2.32	0.62
3:D:125:LYS:HD2	3:D:127:GLN:HG3	1.80	0.62
1:A:229:ILE:HD13	1:A:332:ARG:HH21	1.63	0.62
1:A:48:GLY:N	1:A:461:GLU:OE2	2.32	0.62
1:A:1254:VAL:O	2:B:99:ARG:NH2	2.27	0.62
5:F:65:ALA:H	5:F:70:ARG:HD3	1.65	0.62
1:A:589:THR:OG1	1:A:659:GLN:NE2	2.32	0.62
1:A:400:VAL:HG11	1:A:452:ARG:HD2	1.82	0.62
2:B:278:ARG:NH2	5:F:50:ASP:OD1	2.28	0.62
3:C:76:GLU:HB3	3:C:80:GLU:HB3	1.82	0.62
2:B:528:THR:HG23	3:D:86:LYS:HD3	1.82	0.62
7:H:36:DA:H2'	7:H:37:DA:H8	1.64	0.62
1:A:425:ILE:O	1:A:429:MET:HG3	1.99	0.61
2:B:133:ARG:O	2:B:133:ARG:HD3	2.00	0.61
2:B:1175:LEU:HD13	2:B:1196:LEU:HD11	1.81	0.61
1:A:839:VAL:HG12	1:A:1049:ILE:HG12	1.81	0.61
3:D:158:ARG:NH2	3:D:173:VAL:O	2.34	0.61
3:C:98:VAL:HG12	3:C:100:LEU:HD12	1.83	0.61
2:B:813:ASP:OD1	2:B:883:ARG:NH2	2.33	0.61
5:F:164:MET:SD	5:F:178:ILE:HD11	2.41	0.61
2:B:644:MET:O	2:B:764:ARG:NH1	2.29	0.60
4:E:50:ALA:O	4:E:54:ILE:HG12	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ILE:HD11	1:A:472:GLU:HG3	1.82	0.60
2:B:890:THR:OG1	2:B:893:GLY:O	2.20	0.60
1:A:478:ARG:NH2	1:A:487:LEU:HD11	2.16	0.60
2:B:24:LEU:HD12	2:B:232:ASN:HB3	1.84	0.60
7:H:34:DC:H2"	7:H:35:DA:H5"	1.83	0.60
1:A:478:ARG:HH22	1:A:482:GLY:HA3	1.67	0.60
3:D:92:VAL:HG22	3:D:121:VAL:HG12	1.83	0.60
3:C:190:ALA:HB2	3:C:200:LYS:HB2	1.84	0.60
2:B:255:LEU:HD22	2:B:259:ARG:HB2	1.84	0.59
2:B:1261:LEU:HD21	2:B:1306:LEU:HD12	1.84	0.59
3:C:92:VAL:O	3:C:148:ARG:NH2	2.32	0.59
1:A:1119:MET:HB2	1:A:1228:GLY:HA2	1.83	0.59
1:A:682:GLY:HA2	1:A:685:MET:HE2	1.84	0.59
1:A:1251:TYR:HE2	5:F:136:PRO:HD3	1.67	0.59
8:I:4:DC:H2"	8:I:5:DA:C8	2.37	0.59
1:A:211:ARG:NH1	1:A:356:THR:O	2.35	0.59
1:A:1088:ASP:OD2	1:A:1088:ASP:N	2.34	0.59
3:D:60:GLU:HB2	3:D:143:ARG:HG2	1.84	0.59
1:A:55:SER:OG	1:A:465:ARG:NE	2.33	0.59
1:A:1024:GLU:OE1	1:A:1027:LYS:NZ	2.35	0.58
1:A:533:LEU:HD21	1:A:571:LEU:HD13	1.85	0.58
1:A:3:TYR:HB3	1:A:7:GLU:HB2	1.85	0.58
1:A:731:ARG:NH2	1:A:962:GLU:OE1	2.34	0.58
2:B:799:ARG:NH1	2:B:1146:GLU:OE2	2.37	0.58
1:A:93:SER:OG	1:A:126:GLU:OE1	2.20	0.58
1:A:972:PHE:HB3	1:A:994:ARG:HH11	1.68	0.58
2:B:133:ARG:HH11	2:B:137:ARG:HG3	1.67	0.58
6:G:30:ARG:HH22	6:G:82:LEU:HD12	1.68	0.58
1:A:806:PRO:HA	1:A:811:ASN:HD21	1.68	0.58
1:A:515:MET:HE1	1:A:527:LYS:HE3	1.85	0.58
1:A:59:ILE:HG22	1:A:68:LEU:HB3	1.85	0.57
1:A:309:LEU:HD21	1:A:312:ALA:HB2	1.85	0.57
1:A:204:LEU:HB3	1:A:208:ILE:HD12	1.86	0.57
6:G:40:ASN:ND2	6:G:76:ASP:O	2.34	0.57
2:B:826:ILE:HG13	2:B:831:VAL:HA	1.86	0.57
2:B:1172:LYS:HG2	2:B:1191:PRO:HA	1.85	0.57
1:A:844:LYS:HG3	1:A:845:LEU:HD12	1.85	0.57
7:H:22:DT:H2"	7:H:23:DA:C8	2.39	0.57
2:B:424:ASN:HB2	2:B:434:ILE:HG12	1.86	0.57
4:E:31:GLN:HB2	4:E:46:THR:HG21	1.86	0.57
3:D:113:ALA:HB2	3:D:126:PRO:CB	2.34	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:15:ILE:HG21	5:F:37:PHE:HB2	1.87	0.56
1:A:188:PHE:CE2	1:A:436:ARG:HG2	2.41	0.56
1:A:1250:SER:HB3	5:F:131:ASP:OD2	2.04	0.56
2:B:708:ASN:OD1	2:B:709:ARG:N	2.34	0.56
2:B:33:TRP:HB3	2:B:102:MET:HE3	1.87	0.56
3:D:47:LEU:HD22	3:D:205:MET:HE1	1.88	0.56
6:G:29:LEU:HD22	6:G:44:ILE:HG12	1.88	0.56
1:A:455:SER:OG	1:A:456:VAL:N	2.37	0.56
1:A:478:ARG:NE	1:A:478:ARG:O	2.37	0.56
1:A:878:THR:OG1	1:A:879:GLY:N	2.38	0.56
5:F:19:TYR:CD2	5:F:78:GLN:HG2	2.40	0.56
5:F:171:HIS:O	5:F:175:GLN:HG3	2.06	0.56
2:B:782:GLY:O	2:B:786:THR:HG23	2.05	0.56
8:I:10:DC:H2"	8:I:11:DT:H71	1.86	0.56
1:A:483:ASP:OD2	1:A:483:ASP:N	2.37	0.56
1:A:993:PRO:HG2	1:A:996:ARG:HG2	1.88	0.56
5:F:21:SER:OG	5:F:72:LEU:O	2.22	0.56
1:A:201:ARG:NH1	1:A:370:MET:SD	2.79	0.55
2:B:410:ASP:OD1	3:D:191:ARG:NH2	2.38	0.55
2:B:1238:GLN:NE2	2:B:1250:ASP:OD1	2.39	0.55
1:A:145:ILE:HD12	1:A:456:VAL:HG23	1.87	0.55
5:F:41:ASP:OD1	5:F:93:ARG:NH1	2.39	0.55
2:B:113:HIS:CE1	2:B:307:LEU:HD13	2.42	0.55
1:A:202:ARG:NH2	1:A:365:GLU:OE2	2.39	0.55
2:B:835:LEU:HD21	2:B:880:VAL:HG23	1.89	0.55
3:D:66:HIS:CE1	3:D:68:TYR:HD2	2.25	0.55
4:E:2:ALA:N	4:E:5:THR:O	2.39	0.55
6:G:42:ARG:NH1	6:G:73:ALA:HA	2.21	0.55
2:B:885:VAL:HG22	2:B:894:VAL:HG11	1.88	0.55
3:D:44:ARG:HG3	3:D:183:ILE:HG23	1.89	0.55
1:A:189:ASP:OD2	1:A:192:ASP:N	2.40	0.55
1:A:210:LEU:HD13	1:A:220:ILE:HG12	1.88	0.55
2:B:179:LYS:HE3	2:B:183:GLU:HG3	1.88	0.55
3:C:74:VAL:HG11	3:C:81:ILE:HD11	1.88	0.55
1:A:1294:LYS:HE2	2:B:349:TYR:HB2	1.89	0.54
3:C:62:ASP:OD2	3:C:143:ARG:NH2	2.40	0.54
3:D:57:THR:HB	3:D:158:ARG:HH12	1.73	0.54
7:H:55:DA:H2"	7:H:56:DA:C8	2.43	0.54
2:B:606:ASN:O	2:B:610:ARG:HG2	2.07	0.54
2:B:733:SER:OG	2:B:734:ALA:N	2.39	0.54
2:B:1356:LEU:O	2:B:1366:HIS:NE2	2.29	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:LYS:HD2	6:G:17:GLN:HG2	1.89	0.54
2:B:30:ILE:HD13	2:B:243:PRO:HD3	1.90	0.54
5:F:74:ASP:HB2	5:F:78:GLN:HG3	1.90	0.54
1:A:169:LYS:NZ	1:A:192:ASP:OD2	2.39	0.54
1:A:1106:ARG:CZ	2:B:731:ARG:HH22	2.20	0.54
2:B:108:ALA:HB2	2:B:280:LYS:HG3	1.90	0.54
1:A:96:LEU:HD22	1:A:127:ILE:HD11	1.90	0.54
2:B:69:GLU:HG3	2:B:76:LYS:HG2	1.90	0.54
2:B:721:SER:O	2:B:725:MET:HG3	2.08	0.54
3:C:102:LEU:HB3	3:C:142:MET:HG2	1.89	0.54
5:F:138:MET:HG3	5:F:139:GLU:N	2.16	0.54
1:A:206:ALA:O	1:A:209:ILE:HG22	2.07	0.53
1:A:10:ARG:NH2	1:A:790:ASP:OD2	2.41	0.53
5:F:23:TYR:CZ	5:F:60:TRP:HB2	2.43	0.53
5:F:160:ASN:HD21	6:G:7:GLU:HB3	1.73	0.53
5:F:174:ILE:O	5:F:178:ILE:HD12	2.09	0.53
1:A:349:GLU:O	1:A:353:VAL:HG23	2.09	0.53
2:B:507:VAL:HG22	2:B:601:ILE:HD12	1.89	0.53
2:B:836:ARG:NH1	2:B:870:ASP:OD2	2.42	0.53
8:I:49:DC:H2'	8:I:50:DT:C6	2.44	0.53
5:F:118:MET:HE1	5:F:122:PRO:HG3	1.90	0.53
1:A:133:ASN:O	1:A:527:LYS:NZ	2.38	0.53
1:A:479:LEU:HA	1:A:492:MET:CE	2.38	0.53
5:F:133:VAL:HG22	5:F:134:GLY:N	2.20	0.53
2:B:118:LYS:HG3	2:B:312:ARG:HG2	1.91	0.53
5:F:170:PRO:O	5:F:174:ILE:HG13	2.09	0.53
7:H:36:DA:H2'	7:H:37:DA:C8	2.44	0.53
2:B:418:GLU:OE2	4:E:48:VAL:HG21	2.09	0.53
2:B:576:ARG:HD3	2:B:593:ASN:HA	1.91	0.53
1:A:14:ASP:HA	1:A:1183:ALA:HB3	1.90	0.52
1:A:520:PRO:HG3	1:A:714:VAL:HG21	1.91	0.52
1:A:1032:LYS:O	1:A:1036:ILE:HG13	2.10	0.52
1:A:944:ARG:O	1:A:948:ILE:HG13	2.09	0.52
1:A:1145:ILE:HG22	1:A:1161:LEU:HD11	1.90	0.52
2:B:124:ILE:HG22	2:B:135:ILE:HD13	1.90	0.52
1:A:820:GLU:N	1:A:1080:ASN:O	2.39	0.52
2:B:127:LEU:HD22	2:B:223:LEU:HD21	1.91	0.52
2:B:252:LEU:CD1	2:B:262:THR:HG22	2.39	0.52
1:A:176:ILE:HD12	1:A:184:LEU:HD23	1.92	0.52
3:D:194:GLN:OE1	3:D:194:GLN:N	2.32	0.52
5:F:44:ASP:HB3	5:F:47:GLU:HB3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:42:ARG:HH12	6:G:73:ALA:HA	1.75	0.52
2:B:29:MET:HE3	2:B:33:TRP:HE1	1.75	0.52
2:B:342:LEU:HD21	2:B:1352:ILE:HG23	1.91	0.52
2:B:863:LEU:HD11	2:B:901:ARG:HB2	1.92	0.52
1:A:694:ARG:NH2	1:A:825:GLU:O	2.31	0.52
6:G:40:ASN:HB3	6:G:42:ARG:HG2	1.91	0.52
1:A:193:ASN:OD1	1:A:349:GLU:HB3	2.10	0.52
1:A:897:PRO:HB2	5:F:135:ASP:HB2	1.91	0.52
2:B:437:PHE:HZ	2:B:453:VAL:HG11	1.75	0.52
1:A:728:ASP:OD1	1:A:729:ALA:N	2.42	0.51
2:B:334:LYS:HA	2:B:339:ARG:HD2	1.92	0.51
6:G:39:THR:HG23	6:G:77:LYS:O	2.10	0.51
1:A:192:ASP:HB3	1:A:346:TYR:HD1	1.76	0.51
5:F:25:GLU:O	5:F:29:VAL:HG23	2.10	0.51
7:H:20:DG:H2''	7:H:21:DA:C8	2.44	0.51
2:B:56:LEU:HD21	2:B:269:TYR:HB3	1.93	0.51
2:B:1140:ARG:NH2	2:B:1236:GLU:OE1	2.44	0.51
1:A:623:LEU:HD23	1:A:627:GLY:HA2	1.92	0.51
1:A:1336:ASN:OD1	1:A:1337:ILE:N	2.43	0.51
3:C:47:LEU:HA	3:C:51:MET:HG2	1.92	0.51
8:I:32:DG:H2''	8:I:33:DA:C8	2.45	0.51
1:A:488:MET:HE3	1:A:489:PRO:HD2	1.92	0.51
2:B:799:ARG:O	2:B:803:VAL:HG12	2.11	0.51
1:A:371:ARG:HH22	7:H:46:DG:H5'	1.76	0.51
1:A:1336:ASN:HD22	6:G:46:ASN:CG	2.19	0.51
1:A:722:GLY:HA3	1:A:736:VAL:HA	1.92	0.51
1:A:1066:MET:HE3	1:A:1232:MET:HE3	1.92	0.51
2:B:697:MET:SD	2:B:742:GLY:N	2.84	0.51
2:B:1271:SER:HB2	2:B:1297:LYS:HB3	1.92	0.51
1:A:678:ARG:CZ	1:A:1106:ARG:HD3	2.41	0.50
1:A:902:LEU:HG	5:F:138:MET:HE3	1.92	0.50
2:B:208:THR:HG21	2:B:213:LYS:HD3	1.93	0.50
3:D:135:ASP:HB3	3:D:138:ALA:HB2	1.93	0.50
5:F:65:ALA:H	5:F:70:ARG:CD	2.23	0.50
5:F:78:GLN:O	5:F:82:THR:HG23	2.11	0.50
3:D:102:LEU:HD12	3:D:115:ILE:HD13	1.92	0.50
1:A:948:ILE:O	1:A:952:GLN:HG3	2.11	0.50
1:A:62:TYR:CZ	1:A:476:LYS:HB3	2.47	0.50
2:B:130:MET:HG2	2:B:135:ILE:HG13	1.92	0.50
5:F:9:ARG:HD3	5:F:90:TRP:HE3	1.77	0.50
1:A:189:ASP:OD1	1:A:193:ASN:HB2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:13:HIS:HA	5:F:86:LYS:HD3	1.94	0.50
6:G:43:MET:HA	6:G:47:GLN:HB2	1.94	0.50
2:B:526:VAL:HG12	3:D:83:LEU:HD13	1.94	0.50
1:A:1246:ARG:NH1	1:A:1265:PHE:O	2.37	0.49
7:H:58:DA:H2''	7:H:59:DA:C8	2.47	0.49
1:A:6:THR:HB	1:A:706:ARG:HH21	1.77	0.49
1:A:673:HIS:ND1	2:B:763:PHE:O	2.45	0.49
2:B:180:MET:SD	2:B:293:ARG:HD3	2.52	0.49
2:B:613:GLY:O	2:B:617:THR:OG1	2.23	0.49
5:F:138:MET:C	5:F:140:SER:H	2.20	0.49
1:A:314:ASN:O	1:A:314:ASN:ND2	2.45	0.49
1:A:808:ASN:H	2:B:633:ALA:HB2	1.77	0.49
1:A:1084:ASP:OD1	3:C:45:ARG:NH2	2.46	0.49
2:B:534:GLU:OE1	2:B:581:MET:HE1	2.13	0.49
3:D:11:PRO:HB3	3:D:31:LEU:HG	1.95	0.49
1:A:1113:LEU:HD21	2:B:641:ILE:HG12	1.95	0.49
1:A:685:MET:SD	1:A:1073:LYS:HB3	2.53	0.49
2:B:295:GLU:HB2	5:F:53:GLN:HE21	1.77	0.49
1:A:82:VAL:HG13	1:A:137:VAL:HG21	1.95	0.49
2:B:554:GLU:OE1	2:B:589:TYR:N	2.31	0.49
8:I:50:DT:H2''	8:I:51:DA:H5'	1.95	0.49
1:A:452:ARG:HH12	1:A:458:GLU:CD	2.21	0.49
2:B:312:ARG:HB3	2:B:312:ARG:NH1	2.28	0.49
7:H:55:DA:H2''	7:H:56:DA:H8	1.77	0.49
3:C:32:GLU:HB3	3:C:35:PHE:HD1	1.78	0.49
1:A:135:THR:HG23	1:A:527:LYS:HE2	1.94	0.48
1:A:151:ARG:NH2	1:A:451:ARG:HH21	2.11	0.48
1:A:188:PHE:HE1	1:A:432:LEU:HG	1.78	0.48
2:B:1156:LEU:HD21	2:B:1224:ARG:NH2	2.27	0.48
5:F:148:ASP:OD2	5:F:202:LYS:NZ	2.35	0.48
1:A:821:ARG:HH11	1:A:1082:ILE:HD13	1.78	0.48
1:A:1142:ARG:NH2	1:A:1164:PHE:O	2.46	0.48
5:F:150:SER:HA	5:F:159:ALA:HB1	1.94	0.48
6:G:30:ARG:NH2	6:G:81:TYR:O	2.46	0.48
2:B:1283:SER:O	2:B:1287:ILE:HG13	2.13	0.48
5:F:66:LYS:O	5:F:70:ARG:NH2	2.34	0.48
1:A:1019:ASP:O	1:A:1022:LYS:HG2	2.13	0.48
1:A:1122:LYS:HG2	1:A:1229:TYR:CZ	2.49	0.48
1:A:1223:ARG:NH2	2:B:719:PHE:O	2.46	0.48
2:B:390:LEU:HD21	2:B:407:VAL:HG21	1.94	0.48
2:B:246:PRO:HD2	2:B:249:LEU:HD12	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:808:VAL:HG22	2:B:914:ALA:HA	1.94	0.48
5:F:184:THR:OG1	7:H:13:DG:OP2	2.23	0.48
1:A:59:ILE:O	1:A:67:GLU:HG3	2.13	0.48
2:B:78:LEU:HD11	6:G:9:LEU:HD21	1.96	0.48
2:B:353:SER:OG	2:B:445:LYS:O	2.31	0.48
2:B:530:PRO:HB3	2:B:577:ALA:O	2.14	0.48
1:A:968:GLU:OE1	1:A:1018:TYR:HE1	1.97	0.48
2:B:615:LYS:HB2	2:B:616:PRO:HD3	1.96	0.48
2:B:1233:ILE:HD13	2:B:1260:MET:HE1	1.96	0.48
5:F:47:GLU:O	5:F:51:VAL:HG23	2.13	0.48
1:A:200:ARG:HE	7:H:50:DA:H1'	1.79	0.48
2:B:510:LEU:HA	2:B:513:MET:HG2	1.96	0.48
8:I:35:DA:H2''	8:I:36:DG:C8	2.49	0.48
1:A:838:CYS:HB2	1:A:918:LEU:HD22	1.95	0.47
5:F:169:ILE:HD11	6:G:6:LEU:HD21	1.95	0.47
3:D:97:GLU:HG3	3:D:147:GLN:HG2	1.96	0.47
2:B:291:ILE:HG13	5:F:27:TYR:CE2	2.49	0.47
1:A:177:ILE:HG23	1:A:183:TRP:CE2	2.49	0.47
1:A:696:ASP:HB2	1:A:798:GLN:HE22	1.78	0.47
1:A:1321:GLU:CD	2:B:99:ARG:HH12	2.22	0.47
5:F:95:ASN:O	5:F:99:VAL:HG23	2.13	0.47
1:A:1313:HIS:HB2	2:B:474:LEU:HG	1.96	0.47
2:B:1326:GLN:HG2	8:I:14:DT:H5''	1.95	0.47
1:A:481:LEU:HD11	5:F:10:TYR:CD1	2.50	0.47
1:A:559:CYS:HB2	1:A:662:SER:HB3	1.96	0.47
1:A:987:GLU:O	1:A:991:LYS:HG3	2.14	0.47
1:A:1120:ALA:HB2	1:A:1199:LEU:HG	1.96	0.47
1:A:1340:GLU:HG3	6:G:25:SER:OG	2.15	0.47
2:B:7:PHE:HE1	6:G:32:LEU:HB3	1.79	0.47
3:D:110:VAL:O	3:D:130:ILE:HG22	2.14	0.47
5:F:9:ARG:NH1	5:F:13:HIS:HB2	2.25	0.47
7:H:62:DT:H2''	7:H:63:DG:C8	2.50	0.47
8:I:45:DT:H2''	8:I:46:DC:C6	2.49	0.47
1:A:1112:ILE:O	1:A:1115:THR:HB	2.15	0.47
7:H:46:DG:H1'	7:H:47:DA:H5'	1.96	0.47
3:D:9:LEU:HD13	3:D:198:LEU:HD21	1.96	0.47
2:B:650:LYS:NZ	2:B:765:GLU:OE2	2.43	0.47
3:D:42:ALA:O	3:D:46:ILE:HG12	2.14	0.47
3:D:104:LYS:HE3	3:D:110:VAL:HG22	1.95	0.47
1:A:848:GLU:HG2	1:A:888:THR:HG22	1.97	0.46
1:A:871:VAL:HG11	1:A:928:VAL:HG21	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1013:GLN:O	1:A:1017:GLN:HG2	2.15	0.46
2:B:350:SER:OG	2:B:469:HIS:ND1	2.36	0.46
2:B:785:ASP:HB3	2:B:789:LYS:HE3	1.97	0.46
3:C:51:MET:HA	3:C:51:MET:HE2	1.97	0.46
8:I:12:DT:H2''	8:I:13:DA:C8	2.50	0.46
1:A:730:SER:OG	3:C:70:THR:HG21	2.15	0.46
1:A:1072:ASN:ND2	1:A:1111:GLN:OE1	2.48	0.46
5:F:160:ASN:O	5:F:164:MET:HG3	2.14	0.46
6:G:23:VAL:HG21	6:G:49:SER:OG	2.15	0.46
3:D:96:ASP:OD2	3:D:96:ASP:N	2.48	0.46
3:C:14:VAL:HG21	3:C:29:GLU:HG3	1.98	0.46
5:F:145:PHE:CD2	5:F:204:PHE:HE1	2.33	0.46
7:H:35:DA:H2''	7:H:36:DA:H8	1.81	0.46
3:C:28:LEU:HD22	3:D:231:PHE:CE2	2.50	0.46
3:D:102:LEU:HD12	3:D:115:ILE:CD1	2.46	0.46
5:F:38:PHE:O	5:F:42:ILE:HB	2.16	0.46
5:F:99:VAL:HG22	5:F:102:ARG:NH2	2.30	0.46
6:G:17:GLN:O	6:G:18:LYS:C	2.58	0.46
1:A:873:ILE:HG13	1:A:944:ARG:NH2	2.31	0.46
2:B:8:LEU:HD21	6:G:55:LEU:HB3	1.97	0.46
2:B:888:CYS:HB3	2:B:1258:ARG:HH12	1.80	0.46
1:A:10:ARG:NH2	1:A:791:LEU:HB2	2.29	0.46
1:A:180:ARG:O	1:A:396:ASP:N	2.41	0.46
1:A:890:LYS:HE3	1:A:908:GLU:OE2	2.15	0.46
2:B:114:ILE:HD11	2:B:312:ARG:HG3	1.97	0.46
5:F:84:ARG:NH2	7:H:37:DA:H5'	2.30	0.46
6:G:36:TRP:N	6:G:36:TRP:CD1	2.84	0.46
1:A:976:ARG:HD2	1:A:989:LEU:HD21	1.98	0.46
2:B:822:MET:SD	2:B:838:ARG:HD3	2.55	0.46
6:G:28:GLU:O	6:G:32:LEU:HG	2.15	0.46
1:A:812:PHE:HB3	2:B:357:VAL:HG21	1.98	0.46
7:H:56:DA:H2''	7:H:57:DG:C8	2.50	0.46
1:A:120:GLN:OE1	1:A:490:GLN:N	2.48	0.46
2:B:535:ARG:HG3	3:D:48:LEU:HD22	1.98	0.46
5:F:12:ILE:HG22	5:F:13:HIS:H	1.81	0.46
1:A:1073:LYS:HD2	2:B:462:ASP:HB3	1.97	0.45
2:B:74:LYS:HD2	2:B:87:LYS:HD3	1.98	0.45
3:C:32:GLU:HB3	3:C:35:PHE:CD1	2.50	0.45
6:G:41:GLN:HE21	6:G:80:THR:HA	1.80	0.45
1:A:1248:THR:HB	5:F:136:PRO:HG2	1.99	0.45
4:E:41:GLU:O	4:E:44:ASP:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:ASP:O	1:A:450:ASN:ND2	2.34	0.45
2:B:108:ALA:HB3	2:B:279:LEU:HD23	1.98	0.45
3:D:111:THR:HG22	3:D:129:VAL:HG12	1.99	0.45
3:D:133:LEU:HD23	3:D:133:LEU:HA	1.85	0.45
7:H:64:DT:H2"	7:H:65:DA:N7	2.32	0.45
1:A:525:THR:HG21	1:A:687:ARG:HG2	1.97	0.45
1:A:577:VAL:HG23	1:A:661:VAL:O	2.16	0.45
1:A:736:VAL:HG22	1:A:747:GLY:O	2.15	0.45
2:B:495:ASN:HB2	2:B:1247:LYS:HE2	1.97	0.45
2:B:860:ARG:HG2	2:B:861:ASN:N	2.31	0.45
1:A:700:VAL:HG13	1:A:1117:LEU:HD23	1.99	0.45
3:D:59:VAL:HG21	3:D:85:LEU:HD13	1.99	0.45
5:F:34:VAL:HG22	5:F:89:ILE:HD11	1.98	0.45
5:F:35:HIS:CD2	5:F:49:GLU:HG2	2.51	0.45
7:H:17:DG:H2"	7:H:18:DT:H71	1.98	0.45
2:B:253:VAL:CG2	2:B:261:ALA:HB3	2.46	0.45
2:B:381:ILE:HD11	2:B:412:LEU:HD13	1.98	0.45
2:B:513:MET:O	2:B:575:GLY:HA3	2.16	0.45
7:H:60:DT:H2"	7:H:61:DT:H72	1.97	0.45
8:I:43:DT:H2"	8:I:44:DA:C8	2.51	0.45
1:A:356:THR:HB	1:A:361:SER:OG	2.16	0.45
2:B:10:ALA:HB1	6:G:29:LEU:HG	1.98	0.45
2:B:98:ARG:HG2	2:B:247:PRO:HG2	1.99	0.45
2:B:372:MET:HE2	2:B:372:MET:HB3	1.81	0.45
2:B:513:MET:HE2	2:B:579:LEU:HB2	1.99	0.45
2:B:525:MET:HE2	2:B:525:MET:HB3	1.84	0.45
3:D:76:GLU:HB2	3:D:81:ILE:HD11	1.99	0.45
1:A:192:ASP:HB3	1:A:346:TYR:CD1	2.52	0.45
8:I:9:DT:H2"	8:I:10:DC:C6	2.51	0.45
2:B:1186:TYR:HE1	2:B:1188:GLU:HB2	1.82	0.45
1:A:124:MET:CE	1:A:493:ILE:HG21	2.46	0.45
1:A:19:PRO:HA	1:A:1156:ARG:HD3	1.98	0.44
1:A:104:ILE:HG23	1:A:484:LEU:HD13	1.99	0.44
1:A:445:ILE:HD11	7:H:51:DC:H41	1.82	0.44
1:A:727:VAL:HG11	3:C:75:GLN:HE21	1.82	0.44
1:A:1002:LEU:HD23	1:A:1002:LEU:HA	1.88	0.44
2:B:1221:LEU:HD22	2:B:1306:LEU:HB2	1.99	0.44
3:C:45:ARG:HH12	3:D:37:HIS:CB	2.30	0.44
3:D:9:LEU:HD11	3:D:195:ARG:NH1	2.32	0.44
3:D:76:GLU:HG2	3:D:80:GLU:OE1	2.17	0.44
3:C:41:ASN:O	3:C:45:ARG:HG3	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:VAL:HB	1:A:99:LYS:HB3	2.00	0.44
1:A:104:ILE:HD12	1:A:116:ASP:HB3	1.99	0.44
3:D:113:ALA:CB	3:D:126:PRO:HB3	2.46	0.44
7:H:19:DA:H2''	7:H:20:DG:C8	2.52	0.44
1:A:1307:ASN:HB3	1:A:1312:ASN:O	2.17	0.44
2:B:71:LEU:HB2	2:B:90:VAL:HG21	2.00	0.44
2:B:291:ILE:HG13	5:F:27:TYR:HE2	1.82	0.44
2:B:399:LYS:HE2	2:B:403:ARG:HH12	1.81	0.44
3:C:224:LEU:HD23	3:D:228:LEU:HD21	2.00	0.44
1:A:575:LEU:HG	1:A:579:ALA:HB3	1.99	0.44
1:A:633:LEU:HB3	1:A:644:LEU:HD23	1.99	0.44
2:B:32:SER:O	6:G:57:ARG:NH2	2.51	0.44
2:B:781:LYS:HE3	2:B:933:ARG:HD2	1.99	0.44
3:C:103:ASN:N	3:C:103:ASN:OD1	2.50	0.44
1:A:10:ARG:HH21	1:A:791:LEU:HD12	1.82	0.44
1:A:1107:MET:HE2	1:A:1107:MET:HB2	1.81	0.44
5:F:19:TYR:CE2	5:F:78:GLN:HG2	2.53	0.44
1:A:14:ASP:HB3	1:A:1157:GLN:HB2	1.99	0.44
1:A:852:ALA:HB1	1:A:862:LEU:HD11	2.00	0.44
3:C:205:MET:HE2	3:C:207:THR:CG2	2.48	0.44
5:F:19:TYR:CD1	5:F:81:MET:HE3	2.53	0.44
1:A:1172:LEU:O	1:A:1176:LEU:HG	2.18	0.44
2:B:342:LEU:HG	2:B:1352:ILE:HA	2.00	0.44
2:B:1143:ASP:OD1	2:B:1148:ARG:NH1	2.51	0.44
1:A:657:THR:HB	1:A:1187:PHE:HB2	2.00	0.44
1:A:697:LYS:O	1:A:799:ASN:ND2	2.37	0.44
1:A:1278:LEU:HD22	2:B:484:MET:HE1	2.00	0.44
3:C:46:ILE:HD11	3:C:224:LEU:HD13	1.99	0.44
1:A:75:LEU:HD21	1:A:127:ILE:HD12	1.98	0.43
1:A:1090:ASN:O	3:C:182:ARG:NH1	2.51	0.43
2:B:367:GLY:HA3	2:B:448:GLN:HB2	2.00	0.43
3:D:77:ASP:OD2	3:D:77:ASP:N	2.51	0.43
5:F:158:LEU:HD13	5:F:180:MET:HE1	2.00	0.43
7:H:52:DA:H2''	7:H:53:DA:H5'	2.00	0.43
1:A:823:VAL:HG22	1:A:1060:ILE:HG22	2.00	0.43
2:B:531:LYS:HG2	3:D:182:ARG:HD3	1.99	0.43
2:B:1164:SER:HA	2:B:1200:GLU:HG3	2.00	0.43
7:H:47:DA:H2''	7:H:48:DG:OP1	2.18	0.43
8:I:41:DC:H2''	8:I:42:DA:C8	2.53	0.43
1:A:816:ILE:HD13	1:A:1232:MET:HE1	2.00	0.43
1:A:1089:GLU:OE2	1:A:1211:ARG:NH2	2.43	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:GLU:OE1	5:F:53:GLN:HG2	2.17	0.43
2:B:423:LEU:HB3	2:B:466:MET:SD	2.58	0.43
2:B:697:MET:SD	2:B:741:ALA:HB3	2.59	0.43
7:H:43:DA:H1'	7:H:44:DT:O4'	2.18	0.43
8:I:53:DC:H2''	8:I:54:DA:C8	2.54	0.43
1:A:10:ARG:CZ	1:A:697:LYS:HD3	2.48	0.43
1:A:11:ILE:O	1:A:1149:TYR:OH	2.31	0.43
1:A:178:PRO:HA	1:A:397:LEU:HD23	2.01	0.43
1:A:1270:PHE:CD1	1:A:1290:MET:HE2	2.53	0.43
1:A:1275:VAL:HG13	1:A:1287:LEU:HD11	2.01	0.43
1:A:958:LYS:HB3	1:A:958:LYS:HE2	1.88	0.43
2:B:115:TRP:CE2	2:B:1329:THR:HG23	2.54	0.43
3:C:205:MET:HE2	3:C:207:THR:HG21	2.00	0.43
8:I:37:DT:H2'	8:I:38:DT:H71	1.99	0.43
1:A:216:THR:OG1	1:A:217:THR:N	2.52	0.43
1:A:873:ILE:HG13	1:A:944:ARG:HH21	1.82	0.43
2:B:912:GLY:O	2:B:1360:GLY:N	2.46	0.43
5:F:169:ILE:H	5:F:169:ILE:HG12	1.64	0.43
7:H:20:DG:H2''	7:H:21:DA:H8	1.84	0.43
1:A:832:HIS:CD2	1:A:1058:ARG:HD2	2.54	0.43
2:B:7:PHE:HE2	6:G:70:ILE:HD11	1.84	0.43
2:B:134:ASP:OD2	2:B:159:ILE:HD12	2.18	0.43
2:B:356:THR:N	2:B:447:ILE:O	2.50	0.43
2:B:536:LEU:HD21	3:D:152:TYR:CE1	2.54	0.43
2:B:847:ASP:HB3	2:B:856:ILE:HD12	2.00	0.43
2:B:886:VAL:HG21	2:B:1230:THR:HG21	2.00	0.43
4:E:26:ARG:NE	4:E:53:GLU:OE1	2.41	0.43
6:G:70:ILE:HD13	6:G:70:ILE:HA	1.84	0.43
8:I:12:DT:C4	8:I:13:DA:N6	2.87	0.43
1:A:104:ILE:HD13	1:A:484:LEU:HB3	2.01	0.43
1:A:1296:ASP:OD1	1:A:1296:ASP:N	2.51	0.43
7:H:51:DC:H4'	7:H:52:DA:OP2	2.19	0.43
1:A:367:TYR:HD1	1:A:381:ALA:HA	1.84	0.43
1:A:1146:GLN:HB2	1:A:1161:LEU:HD12	2.01	0.43
2:B:135:ILE:HA	2:B:138:VAL:HG12	2.01	0.43
3:C:114:ASP:OD2	3:C:114:ASP:N	2.52	0.43
7:H:27:DT:H2''	7:H:28:DA:C8	2.53	0.43
1:A:722:GLY:HA2	1:A:737:ASN:OD1	2.18	0.42
2:B:233:LYS:HG3	6:G:42:ARG:NH2	2.34	0.42
2:B:269:TYR:O	2:B:273:ILE:HG13	2.19	0.42
2:B:337:ARG:HD3	2:B:337:ARG:HA	1.89	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:53:THR:O	6:G:57:ARG:HG3	2.19	0.42
3:D:86:LYS:HZ1	3:D:174:ASP:HB2	1.78	0.42
2:B:100:GLU:HG2	6:G:20:PRO:HG2	2.02	0.42
2:B:114:ILE:HD12	2:B:114:ILE:HA	1.81	0.42
2:B:317:THR:HG22	2:B:323:PRO:HA	2.00	0.42
2:B:395:LYS:HE3	2:B:395:LYS:HB3	1.67	0.42
3:D:100:LEU:HD12	3:D:117:HIS:HA	2.01	0.42
6:G:55:LEU:HG	6:G:66:VAL:HG21	2.00	0.42
1:A:97:ARG:HB3	1:A:121:GLU:HG2	2.02	0.42
1:A:344:GLY:HA3	1:A:346:TYR:CE2	2.55	0.42
1:A:302:ILE:O	1:A:330:HIS:NE2	2.39	0.42
1:A:739:ASP:OD2	1:A:740:GLU:N	2.52	0.42
2:B:1238:GLN:O	2:B:1242:ARG:HB2	2.19	0.42
5:F:19:TYR:HD1	5:F:81:MET:HE3	1.85	0.42
1:A:17:LYS:NZ	1:A:1189:GLY:O	2.53	0.42
1:A:1255:THR:HG21	2:B:341:ASN:CG	2.45	0.42
1:A:1290:MET:HE3	1:A:1290:MET:HB3	1.84	0.42
2:B:152:THR:HG23	2:B:172:PHE:CE1	2.55	0.42
2:B:424:ASN:ND2	2:B:424:ASN:C	2.77	0.42
2:B:1361:THR:HA	4:E:17:PHE:HB3	2.02	0.42
3:D:14:VAL:HG12	3:D:15:ASP:OD1	2.20	0.42
8:I:2:DT:H2"	8:I:3:DA:C8	2.55	0.42
1:A:953:LEU:HD11	1:A:1033:ARG:HG3	2.01	0.42
1:A:1270:PHE:CE1	1:A:1274:GLU:HB3	2.53	0.42
2:B:865:HIS:CE1	2:B:867:GLN:HB3	2.55	0.42
6:G:21:LEU:H	6:G:21:LEU:HG	1.43	0.42
1:A:783:LEU:HD23	1:A:783:LEU:HA	1.79	0.42
2:B:51:PRO:HB3	2:B:57:PHE:O	2.20	0.42
2:B:930:LEU:HD11	2:B:1241:TYR:CE1	2.55	0.42
1:A:100:LEU:HD22	1:A:122:VAL:HG11	2.01	0.42
1:A:125:GLY:HA3	1:A:499:SER:HB2	2.01	0.42
1:A:411:ARG:NH1	1:A:424:ASP:OD1	2.44	0.42
1:A:1333:LEU:HG	2:B:327:LEU:HB3	2.02	0.42
2:B:165:TYR:CE1	2:B:178:ALA:HB3	2.55	0.42
2:B:194:LEU:HD12	2:B:228:VAL:HG23	2.01	0.42
2:B:288:PRO:HD3	5:F:60:TRP:CE2	2.54	0.42
2:B:298:MET:SD	5:F:49:GLU:HB3	2.59	0.42
6:G:27:LYS:HA	6:G:27:LYS:HD2	1.86	0.42
3:C:137:ASN:OD1	3:C:137:ASN:N	2.53	0.42
1:A:213:LEU:HD23	1:A:422:LYS:HG2	2.03	0.41
1:A:459:MET:HE1	1:A:511:LEU:HD12	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1108:ASN:OD1	1:A:1108:ASN:N	2.48	0.41
2:B:122:SER:HB2	2:B:132:LEU:HD13	2.02	0.41
2:B:165:TYR:CE2	2:B:169:LEU:HD11	2.54	0.41
1:A:221:LEU:HD13	1:A:336:LEU:HD21	2.01	0.41
1:A:228:VAL:HG23	1:A:337:PHE:HB2	2.03	0.41
1:A:445:ILE:HD11	7:H:51:DC:N4	2.34	0.41
1:A:672:GLU:HG2	1:A:673:HIS:CD2	2.56	0.41
1:A:1247:SER:O	2:B:348:ASP:HB3	2.20	0.41
1:A:1307:ASN:O	1:A:1312:ASN:N	2.47	0.41
1:A:1336:ASN:ND2	6:G:46:ASN:O	2.53	0.41
2:B:1150:PRO:HD2	2:B:1216:ALA:HB2	2.02	0.41
2:B:1156:LEU:CD2	2:B:1224:ARG:HH21	2.30	0.41
3:C:218:ARG:NE	3:D:231:PHE:O	2.51	0.41
3:C:226:GLU:CG	3:D:10:LYS:HE3	2.43	0.41
3:D:82:LEU:HD13	3:D:173:VAL:HG22	2.02	0.41
5:F:19:TYR:OH	5:F:72:LEU:O	2.36	0.41
5:F:175:GLN:HB3	5:F:180:MET:O	2.20	0.41
1:A:26:TYR:HE2	1:A:32:LEU:HD12	1.85	0.41
1:A:160:ASP:OD1	1:A:164:THR:N	2.44	0.41
1:A:312:ALA:N	1:A:315:MET:SD	2.94	0.41
1:A:1117:LEU:HD21	1:A:1182:ILE:HG21	2.01	0.41
2:B:371:LYS:HD3	2:B:371:LYS:HA	1.74	0.41
2:B:843:VAL:HB	2:B:883:ARG:HD3	2.03	0.41
2:B:1349:GLU:OE1	2:B:1349:GLU:N	2.41	0.41
3:C:182:ARG:HB3	3:C:206:GLU:HB3	2.02	0.41
3:C:136:GLU:CD	3:C:136:GLU:H	2.28	0.41
6:G:31:LYS:O	6:G:35:GLU:HG3	2.20	0.41
7:H:38:DT:H2''	7:H:39:DG:H5'	2.02	0.41
1:A:12:ARG:O	1:A:1157:GLN:NE2	2.48	0.41
3:C:133:LEU:HD11	3:C:140:ILE:HG22	2.01	0.41
6:G:9:LEU:HD12	6:G:16:GLU:HG2	2.02	0.41
7:H:15:DT:H2''	7:H:16:DA:H8	1.84	0.41
7:H:60:DT:H2''	7:H:61:DT:C7	2.50	0.41
8:I:38:DT:H2''	8:I:39:DA:C8	2.56	0.41
1:A:292:ILE:HD12	1:A:292:ILE:HA	1.92	0.41
1:A:811:ASN:HA	1:A:815:SER:HB2	2.03	0.41
1:A:846:GLY:O	1:A:889:PRO:HG2	2.21	0.41
2:B:122:SER:O	2:B:126:LEU:N	2.48	0.41
2:B:133:ARG:HD3	2:B:133:ARG:C	2.45	0.41
3:D:84:ASN:ND2	3:D:129:VAL:O	2.54	0.41
1:A:175:ARG:HG2	1:A:177:ILE:HG12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1109:ILE:HD11	2:B:740:LEU:HD22	2.02	0.41
2:B:847:ASP:OD1	2:B:860:ARG:N	2.45	0.41
6:G:29:LEU:HD11	6:G:48:PHE:CE2	2.56	0.41
1:A:210:LEU:HD23	1:A:210:LEU:HA	1.82	0.41
1:A:241:LEU:HD13	1:A:285:ILE:HD13	2.03	0.41
6:G:25:SER:HA	6:G:29:LEU:HD12	2.03	0.41
1:A:13:LYS:NZ	1:A:1149:TYR:O	2.40	0.41
1:A:972:PHE:HB3	1:A:994:ARG:NH1	2.34	0.41
2:B:349:TYR:HE1	2:B:379:PRO:HG2	1.86	0.41
2:B:725:MET:O	2:B:728:SER:OG	2.39	0.41
2:B:1137:GLY:O	2:B:1141:VAL:HG23	2.20	0.41
3:C:35:PHE:CE2	3:D:46:ILE:HD12	2.56	0.41
3:C:47:LEU:HB3	3:C:183:ILE:HD11	2.02	0.41
3:D:57:THR:HG22	3:D:175:ALA:HB2	2.03	0.41
3:D:85:LEU:CD2	3:D:130:ILE:HD11	2.51	0.41
5:F:175:GLN:HE22	5:F:182:HIS:CD2	2.37	0.41
5:F:206:LYS:H	5:F:206:LYS:HG3	1.60	0.41
1:A:942:ASP:OD1	1:A:942:ASP:N	2.54	0.41
2:B:53:ARG:HH21	2:B:60:ARG:HD2	1.85	0.41
2:B:1144:LEU:HD23	2:B:1237:VAL:HG23	2.02	0.41
3:C:135:ASP:HB3	3:C:138:ALA:HB2	2.02	0.41
3:D:61:ILE:HG12	3:D:142:MET:HB2	2.03	0.41
1:A:288:PRO:HB2	1:A:290:GLU:OE1	2.21	0.40
2:B:83:VAL:O	2:B:92:VAL:HG23	2.21	0.40
2:B:528:THR:HG22	3:D:83:LEU:HG	2.02	0.40
7:H:19:DA:H2''	7:H:20:DG:H8	1.86	0.40
7:H:27:DT:H2''	7:H:28:DA:H8	1.86	0.40
1:A:1098:LEU:HD23	1:A:1098:LEU:HA	1.87	0.40
2:B:511:TYR:HE2	2:B:724:MET:HG2	1.86	0.40
2:B:1318:SER:OG	2:B:1342:ASP:OD2	2.31	0.40
3:D:104:LYS:HD2	3:D:114:ASP:OD2	2.21	0.40
1:A:500:ALA:O	1:A:503:LYS:N	2.55	0.40
2:B:836:ARG:HG3	2:B:869:CYS:HB3	2.03	0.40
3:D:13:LEU:HD11	3:D:16:ILE:HG13	2.03	0.40
5:F:176:LYS:HD3	5:F:176:LYS:HA	1.73	0.40
1:A:732:ILE:HD11	1:A:769:PRO:HB3	2.03	0.40
2:B:1253:ILE:H	2:B:1253:ILE:HG13	1.77	0.40
3:C:28:LEU:HD22	3:D:231:PHE:HE2	1.85	0.40
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.86	0.40
1:A:882:ILE:HD11	1:A:919:ARG:HH21	1.87	0.40
2:B:475:GLU:CD	4:E:28:ARG:HH21	2.29	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1257:VAL:HA	2:B:1260:MET:HE2	2.03	0.40
6:G:77:LYS:HB2	6:G:77:LYS:HE2	1.89	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	1339/1342 (100%)	1315 (98%)	23 (2%)	1 (0%)	48	78
2	B	1163/1407 (83%)	1142 (98%)	21 (2%)	0	100	100
3	C	226/329 (69%)	223 (99%)	3 (1%)	0	100	100
3	D	214/329 (65%)	207 (97%)	7 (3%)	0	100	100
4	E	70/91 (77%)	70 (100%)	0	0	100	100
5	F	206/214 (96%)	191 (93%)	14 (7%)	1 (0%)	24	54
6	G	76/82 (93%)	68 (90%)	7 (9%)	1 (1%)	9	33
All	All	3294/3794 (87%)	3216 (98%)	75 (2%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	76	LYS
6	G	27	LYS
1	A	498	ILE

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	1156/1157 (100%)	1148 (99%)	8 (1%)	76	78
2	B	980/1168 (84%)	977 (100%)	3 (0%)	86	84
3	C	196/286 (68%)	195 (100%)	1 (0%)	81	81
3	D	187/286 (65%)	186 (100%)	1 (0%)	81	81
4	E	62/75 (83%)	62 (100%)	0	100	100
5	F	193/198 (98%)	191 (99%)	2 (1%)	68	75
6	G	70/74 (95%)	61 (87%)	9 (13%)	4	16
All	All	2844/3244 (88%)	2820 (99%)	24 (1%)	70	77

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	VAL
1	A	471	VAL
1	A	498	ILE
1	A	878	THR
1	A	893	THR
1	A	1066	MET
1	A	1254	VAL
1	A	1289	GLU
2	B	270	ARG
2	B	424	ASN
2	B	594	GLN
3	C	47	LEU
3	D	96	ASP
5	F	123	LEU
5	F	130	GLN
6	G	6	LEU
6	G	7	GLU
6	G	9	LEU
6	G	10	VAL
6	G	11	GLN
6	G	14	MET
6	G	16	GLU
6	G	18	LYS
6	G	21	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	752	ASN
1	A	798	GLN
1	A	832	HIS
1	A	1209	GLN
1	A	1336	ASN
2	B	335	GLN
2	B	489	ASN
2	B	667	GLN
2	B	1350	ASN
3	C	66	HIS
3	C	93	GLN
3	C	132	HIS
5	F	160	ASN
5	F	175	GLN
5	F	203	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

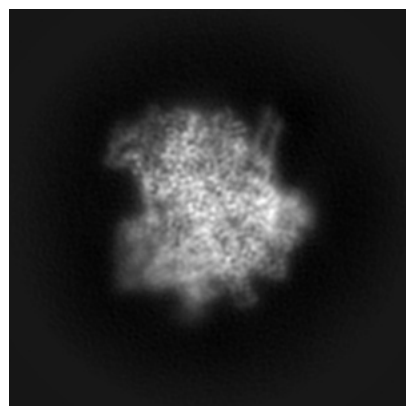
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63697. These allow visual inspection of the internal detail of the map and identification of artifacts.

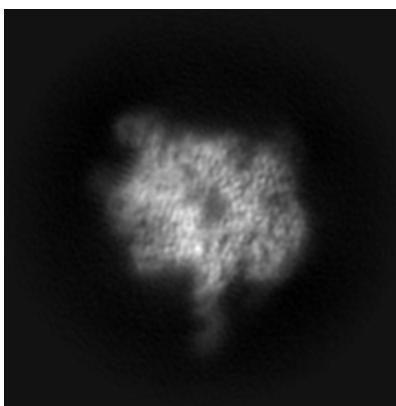
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

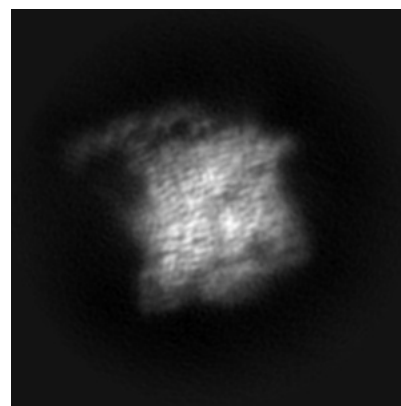
6.1.1 Primary map



X

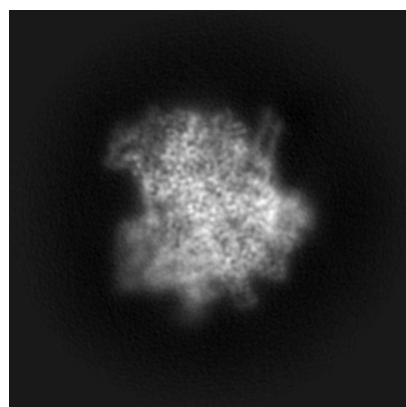


Y

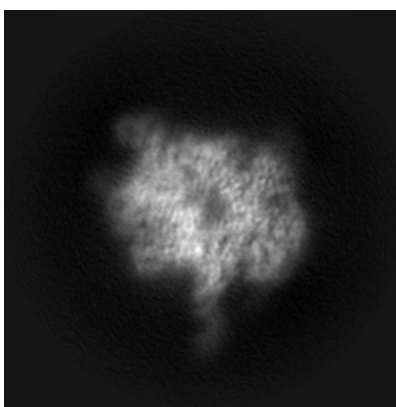


Z

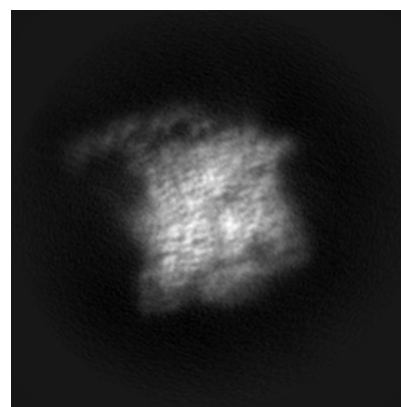
6.1.2 Raw map



X



Y

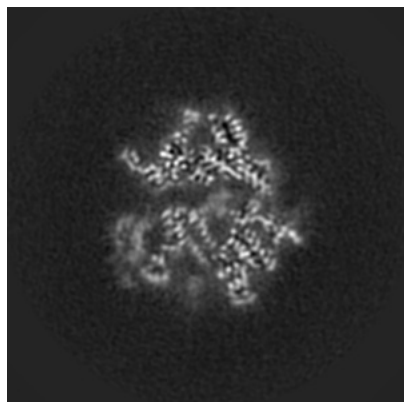


Z

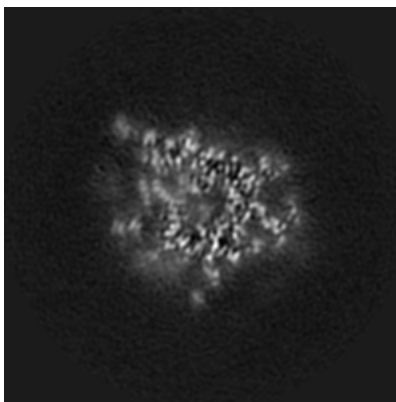
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

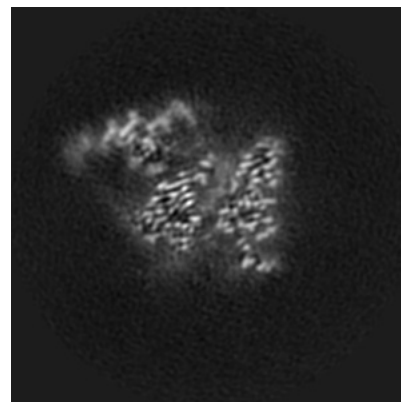
6.2.1 Primary map



X Index: 110

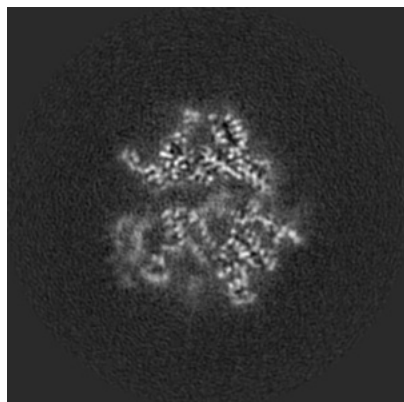


Y Index: 110

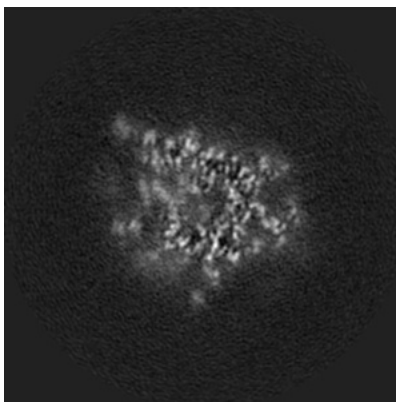


Z Index: 110

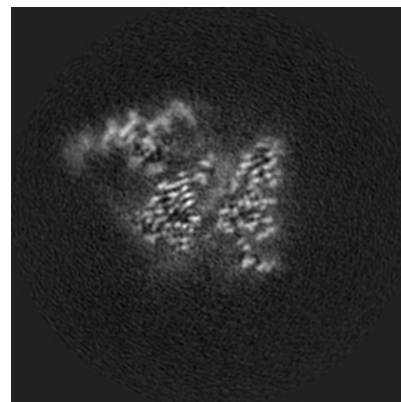
6.2.2 Raw map



X Index: 110



Y Index: 110

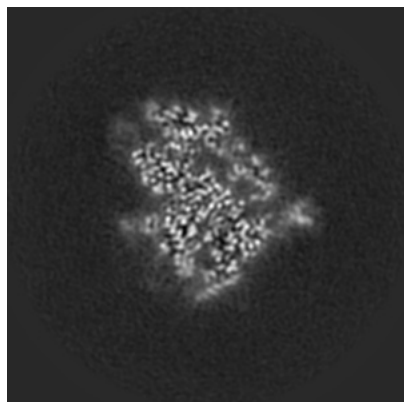


Z Index: 110

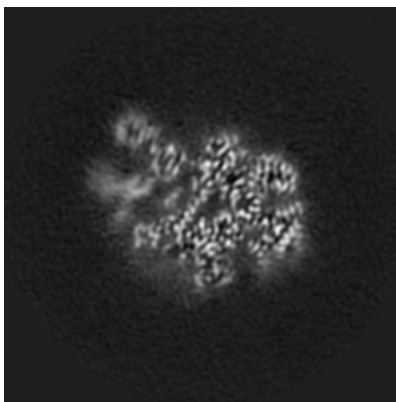
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

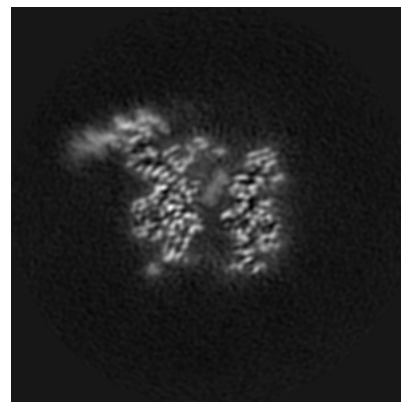
6.3.1 Primary map



X Index: 98

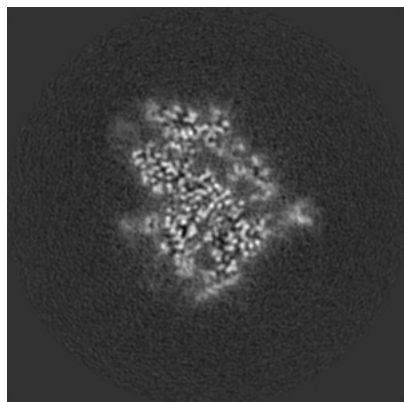


Y Index: 100

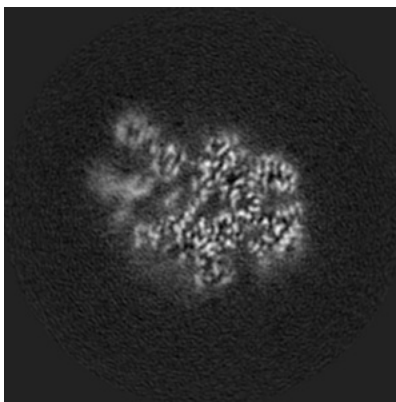


Z Index: 115

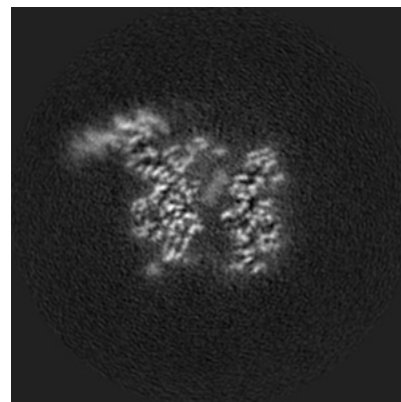
6.3.2 Raw map



X Index: 98



Y Index: 100

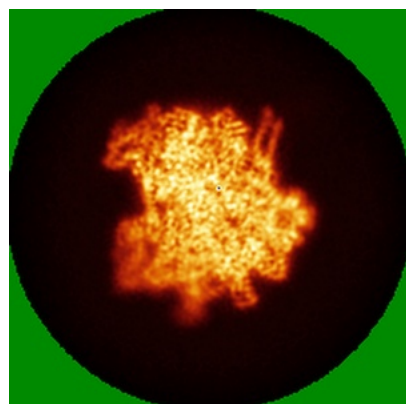


Z Index: 115

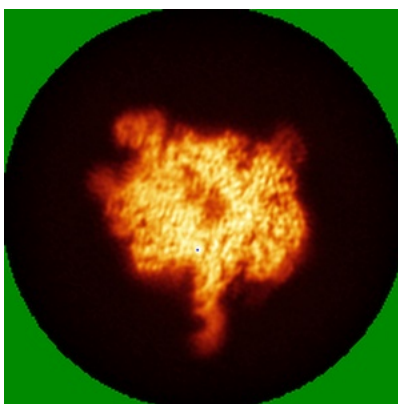
The images above show the largest variance slices of the map in three orthogonal directions.

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

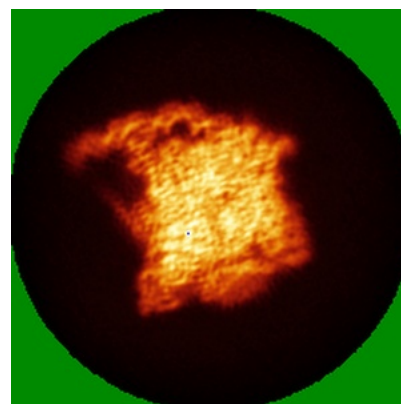
6.4.1 Primary map



X

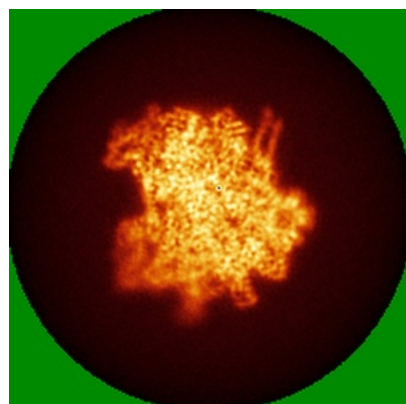


Y

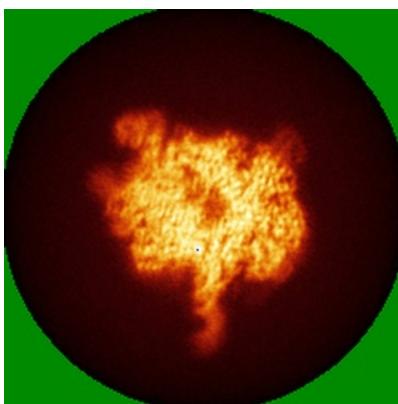


Z

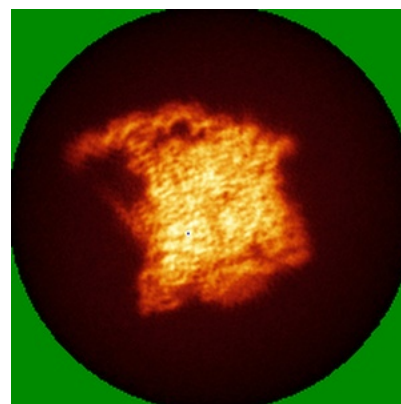
6.4.2 Raw map



X



Y

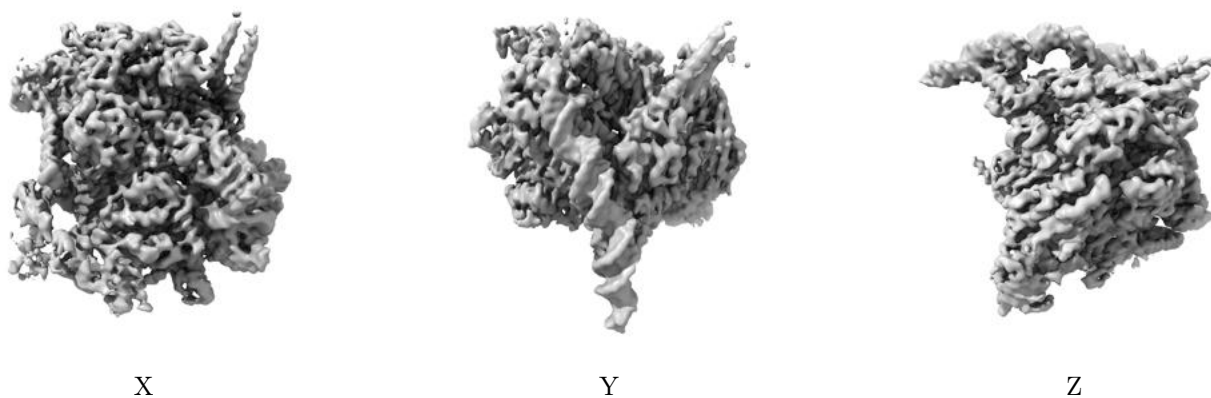


Z

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 0.015. 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.

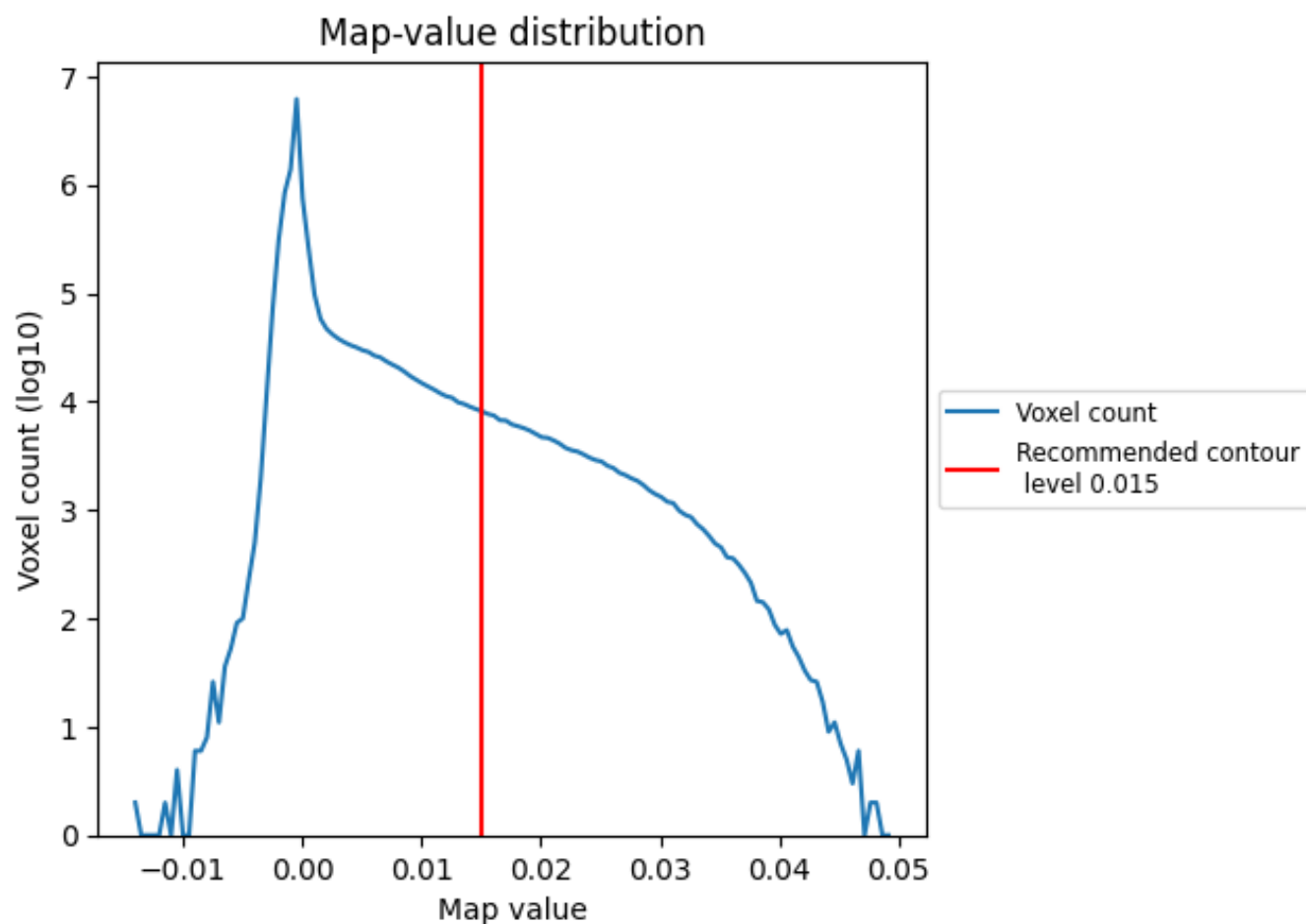
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

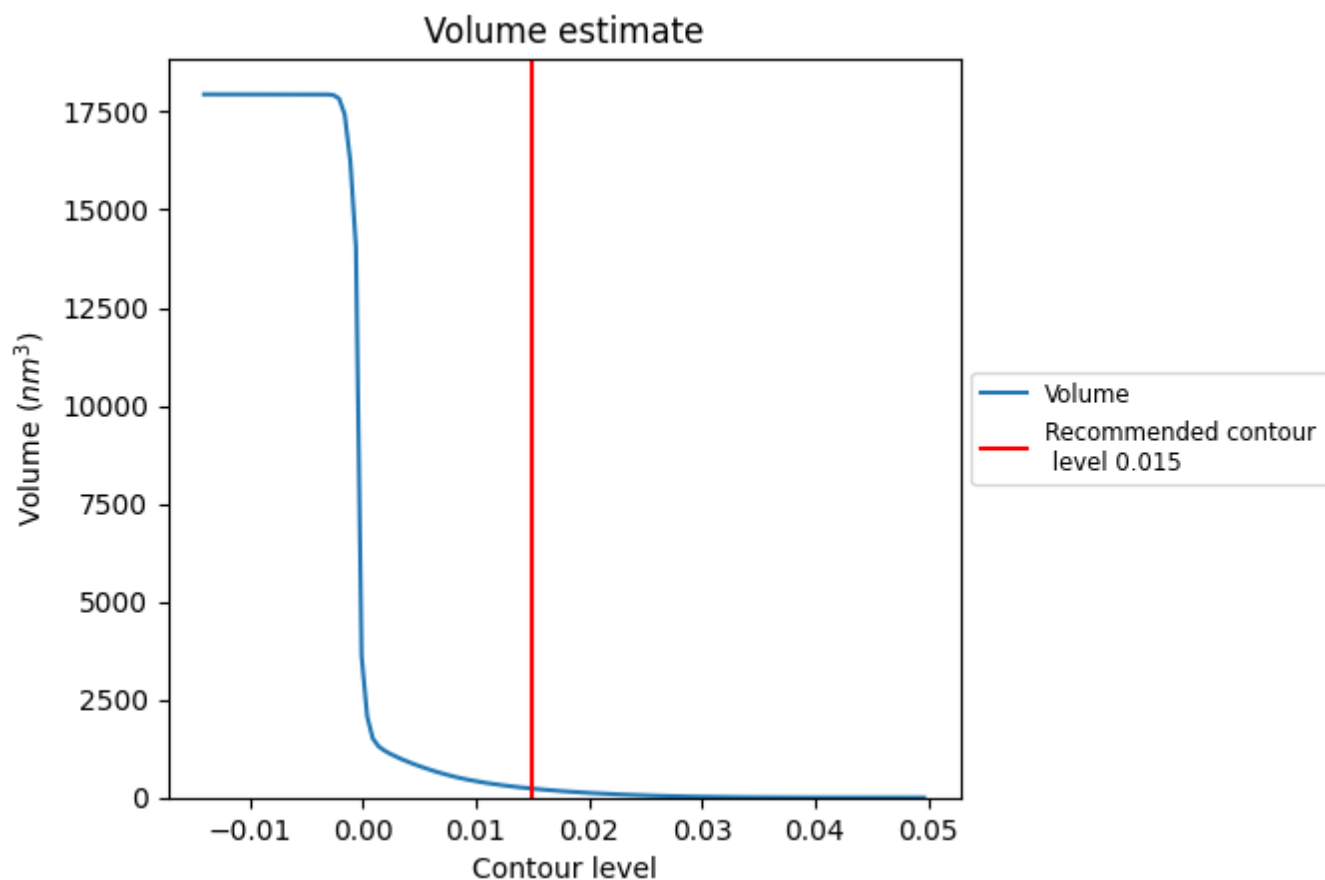
This section contains the results of statistical analysis of the map.

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.

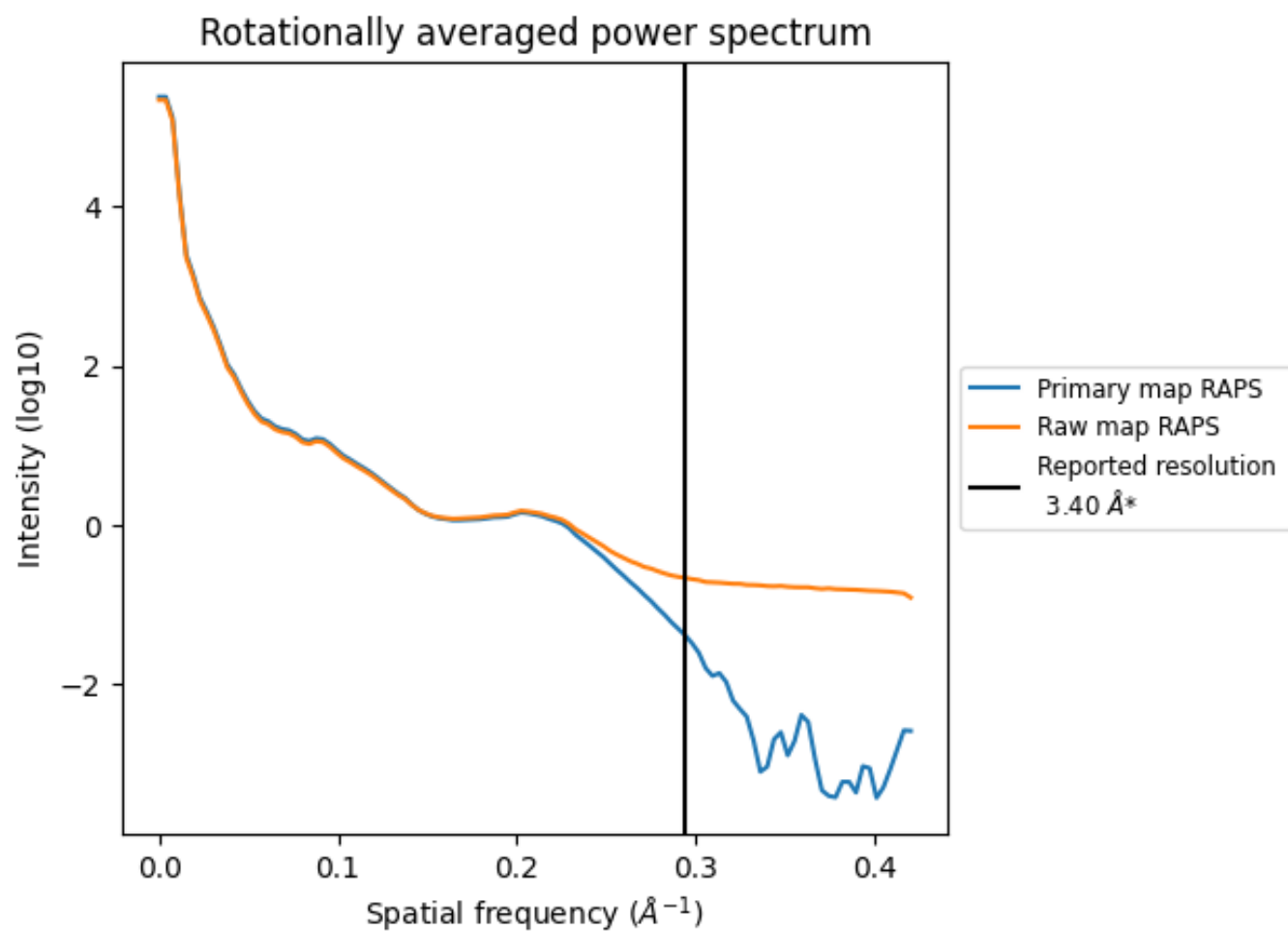
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 229 nm³; this corresponds to an approximate mass of 207 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 ⓘ

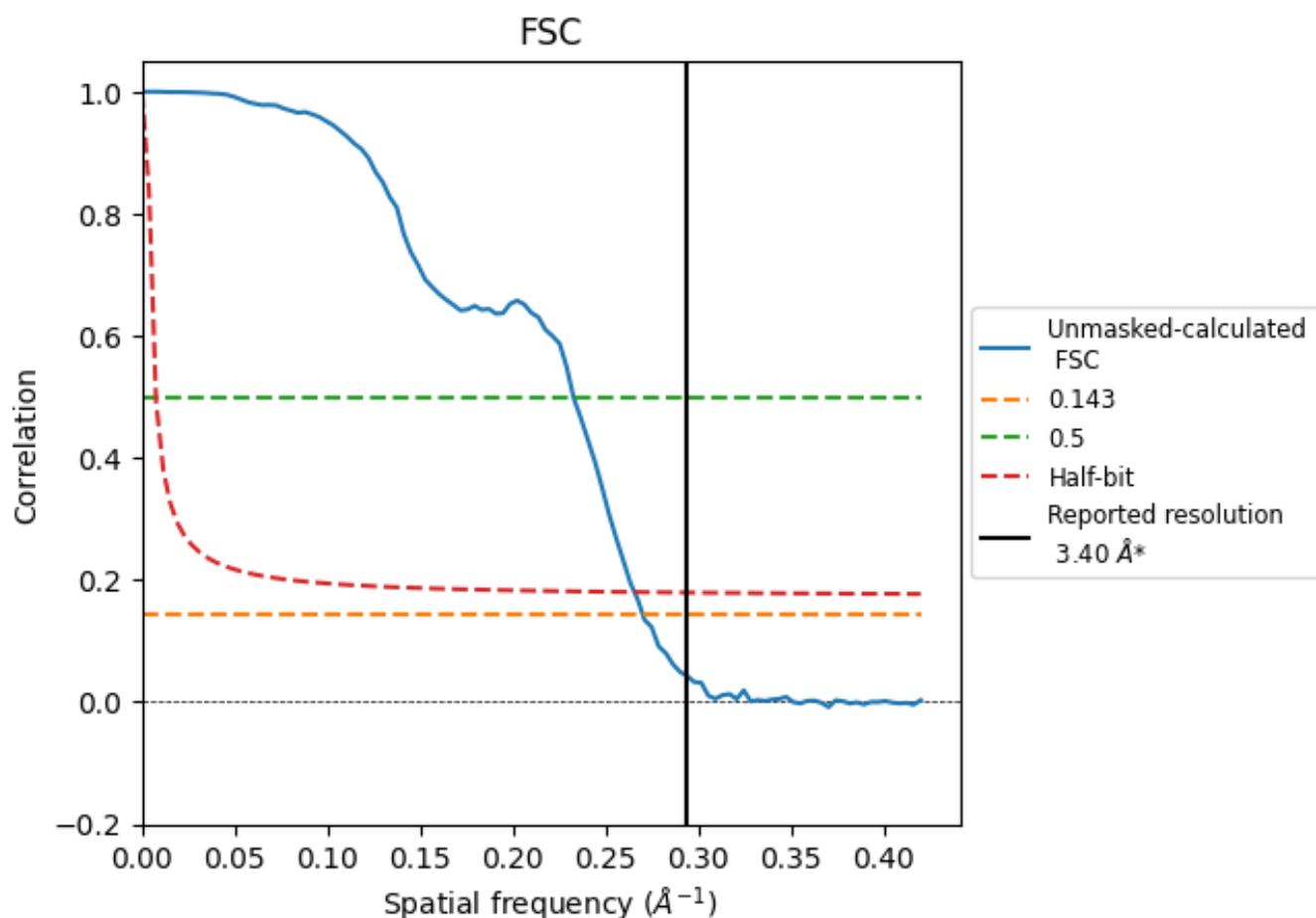


*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

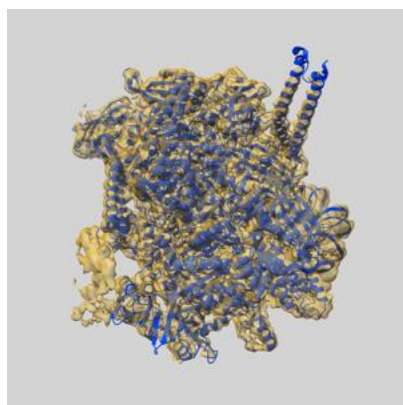
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.70	4.30	3.76

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

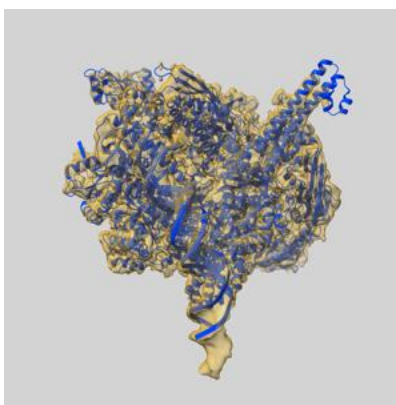
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63697 and PDB model 9M7Y. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

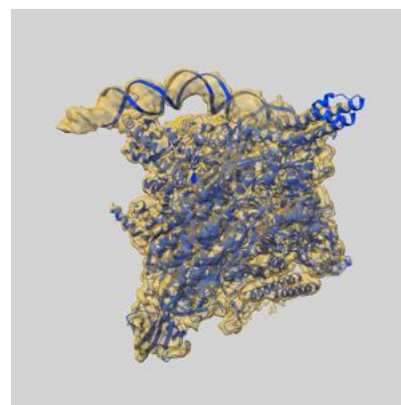
9.1 Map-model overlay [i](#)



X



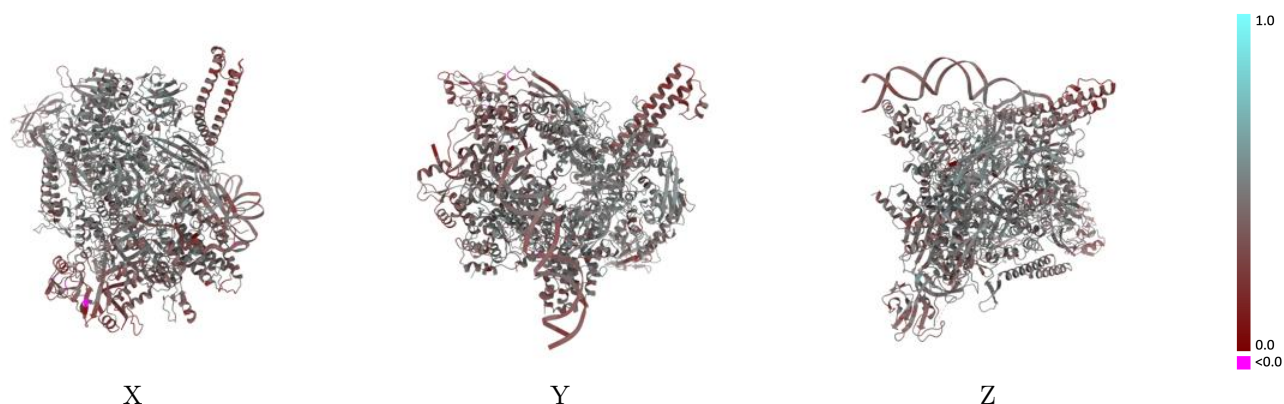
Y



Z

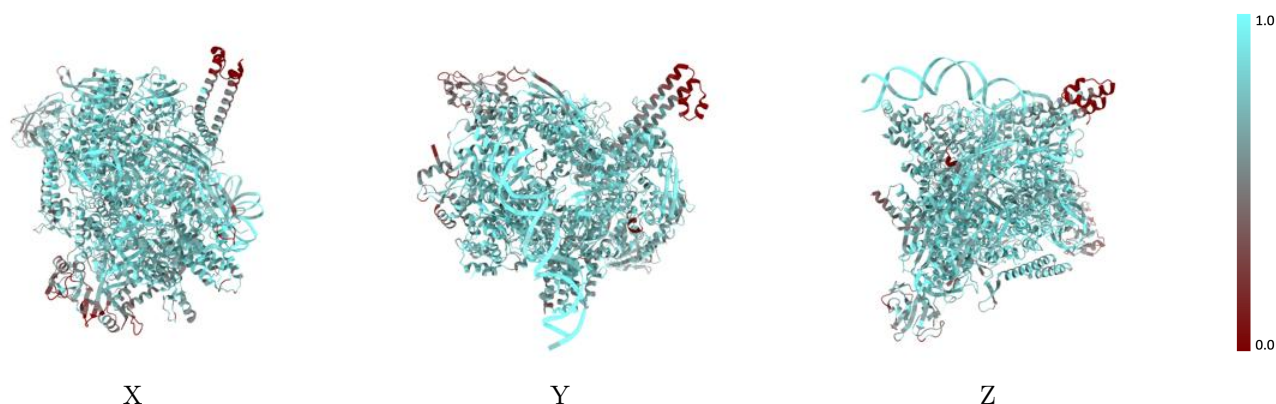
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



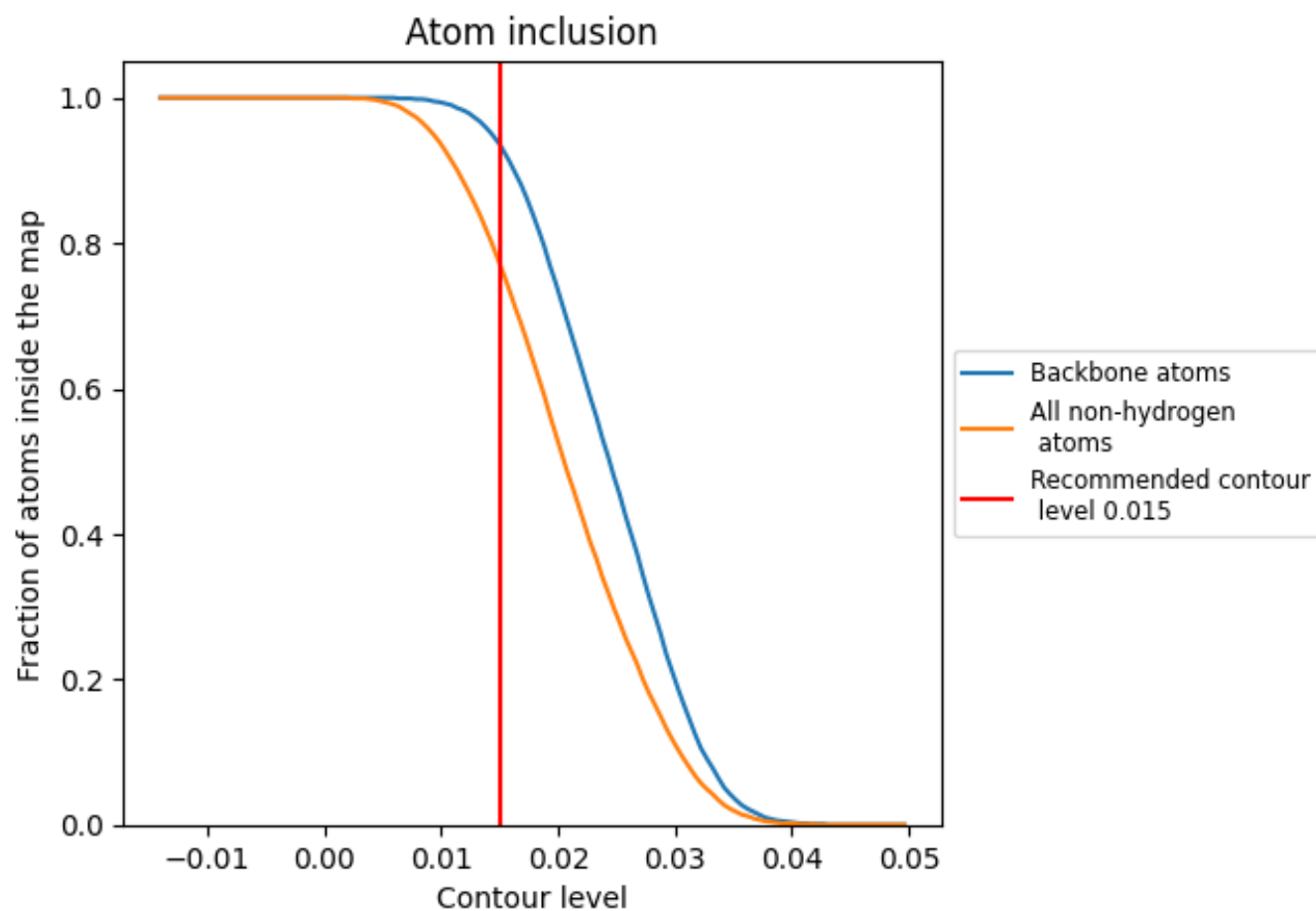
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7720	0.4270
A	0.7540	0.4320
B	0.8010	0.4450
C	0.7550	0.4500
D	0.6890	0.4080
E	0.6520	0.4360
F	0.7780	0.4000
G	0.7550	0.3880
H	0.8520	0.3370
I	0.8500	0.3560

1.0

0.0

<0.0