



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 03:20 PM EST

PDB ID : 6C9Y
EMDB ID : EMD-7438
Title : Cryo-EM structure of E. coli RNAP sigma70 holoenzyme
Authors : Narayanan, A.; Vago, F.; Li, K.; Qayyum, M.Z.; Yenool, D.; Jiang, W.; Murakami, K.S.
Deposited on : 2018-01-29
Resolution : 4.25 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

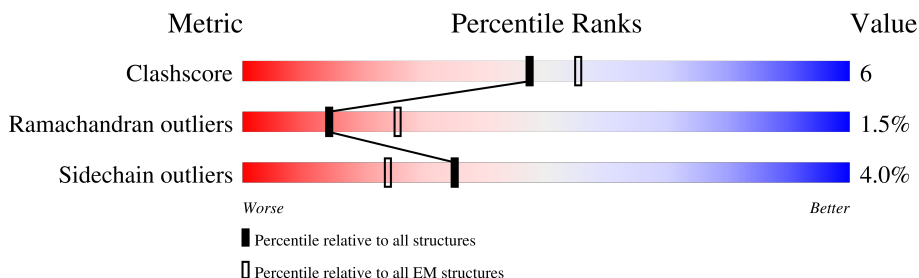
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.25 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 ≥ 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	329	<div> <div>37%</div> <div>55%</div> <div>14%</div> <div>30%</div> </div>
1	B	329	<div> <div>34%</div> <div>52%</div> <div>14%</div> <div>33%</div> </div>
2	C	1342	<div> <div>65%</div> <div>82%</div> <div>16%</div> <div>•</div> </div>
3	D	1407	<div> <div>63%</div> <div>73%</div> <div>21%</div> <div>• •</div> </div>
4	E	91	<div> <div>75%</div> <div>73%</div> <div>10%</div> <div>16%</div> </div>
5	F	613	<div> <div>70%</div> <div>62%</div> <div>13%</div> <div>24%</div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 28920 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 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	230	Total	C	N	O	S	0	0
			1787	1112	317	352	6		
1	B	221	Total	C	N	O	S	0	0
			1708	1067	302	333	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0
			10570	6631	1841	2055	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1350	Total	C	N	O	S	0	0
			10434	6553	1856	1976	49		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	76	Total	C	N	O	S	0	0
			605	368	115	121	1		

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

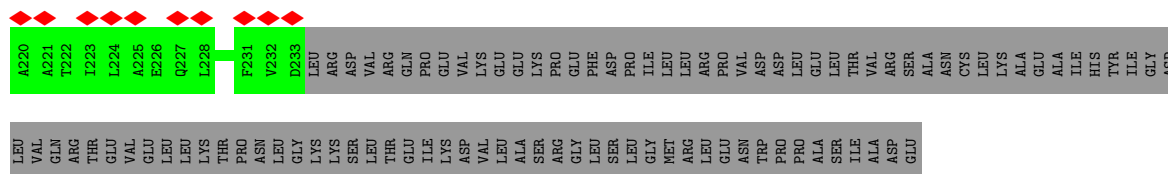
Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	468	Total	C	N	O	S	0	0
			3813	2389	678	723	23		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

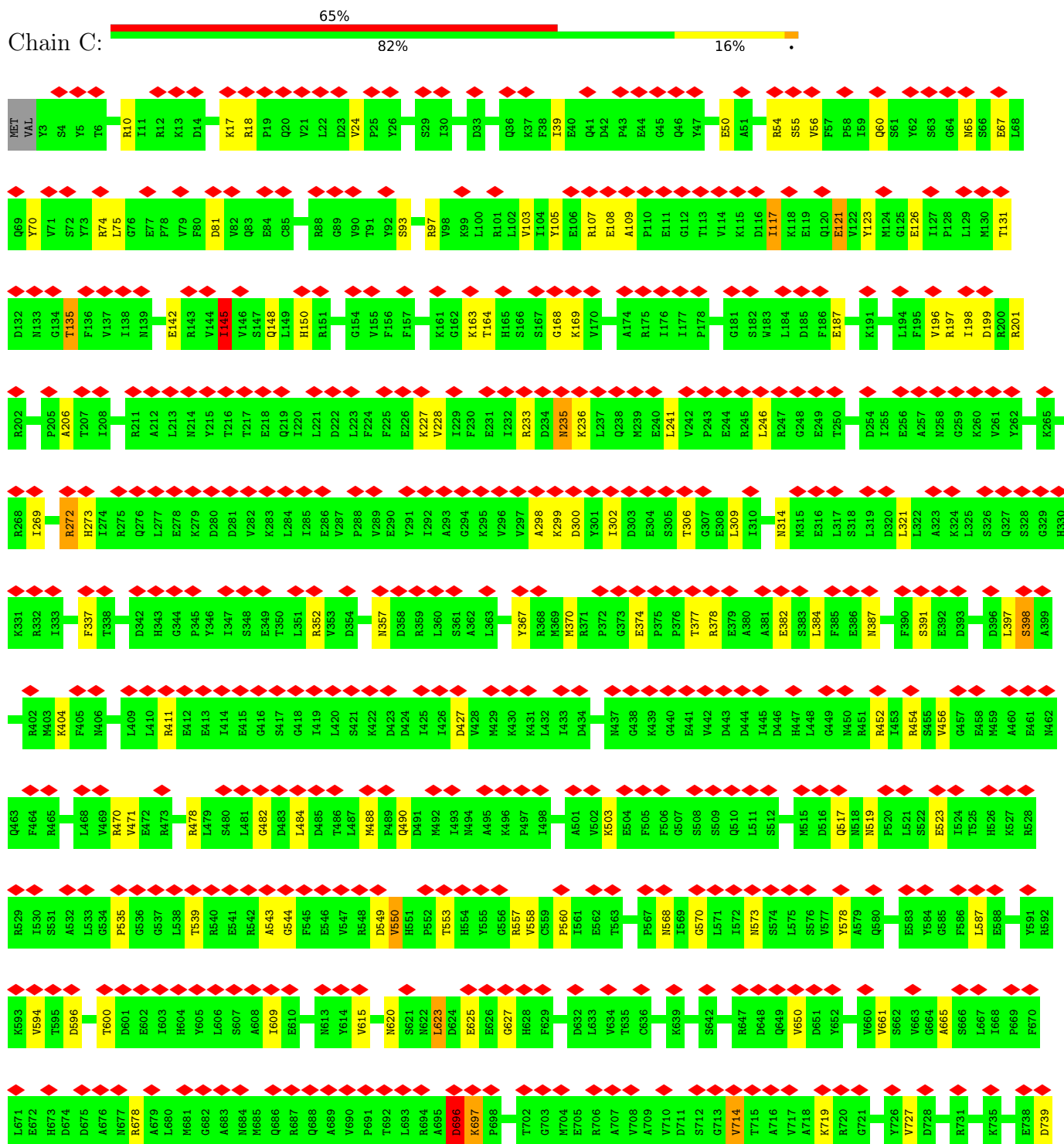
Mol	Chain	Residues	Atoms		AltConf
6	D	1	Total 1	Mg 1	0

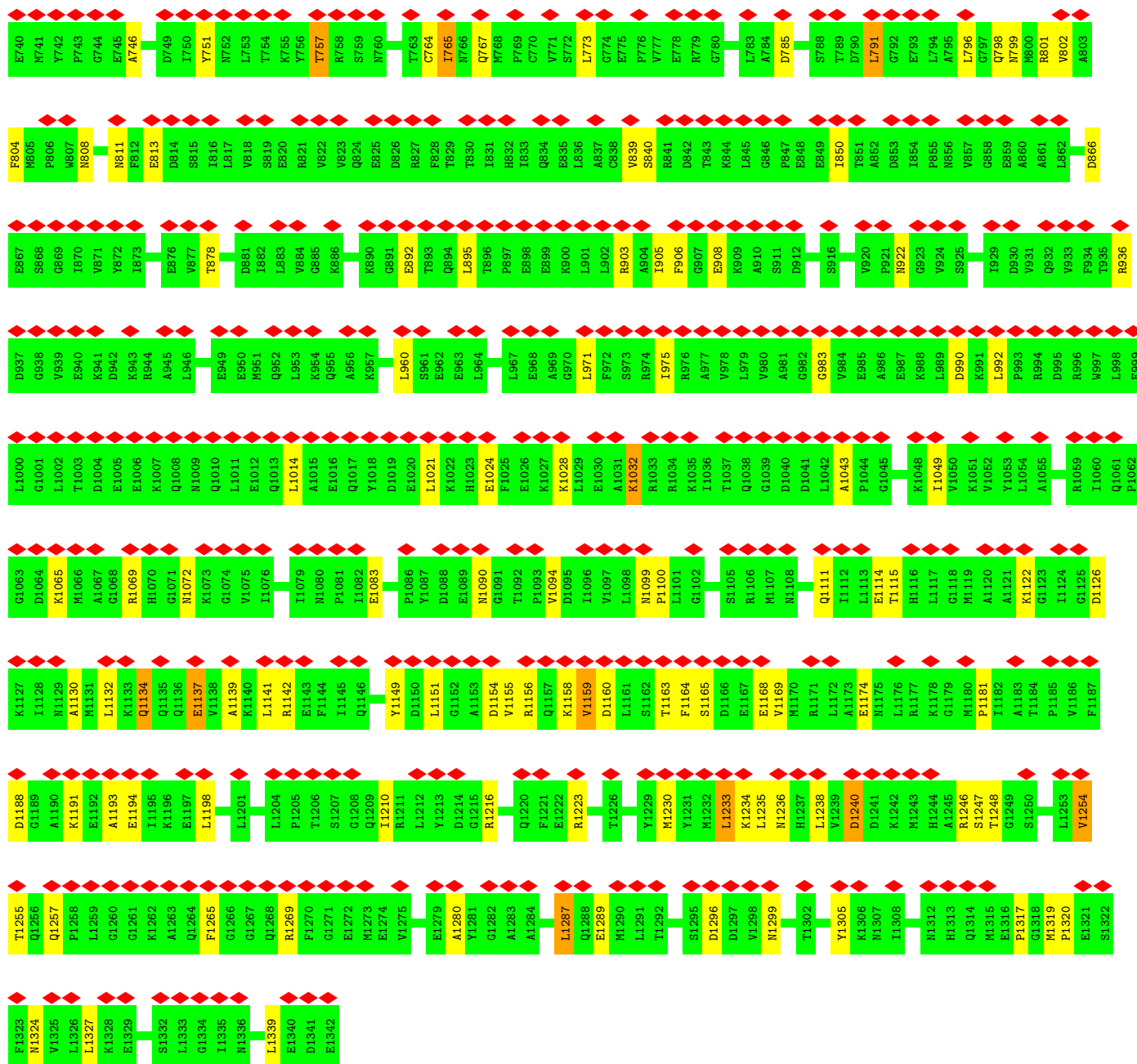
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	D	2	Total 2	Zn 2	0

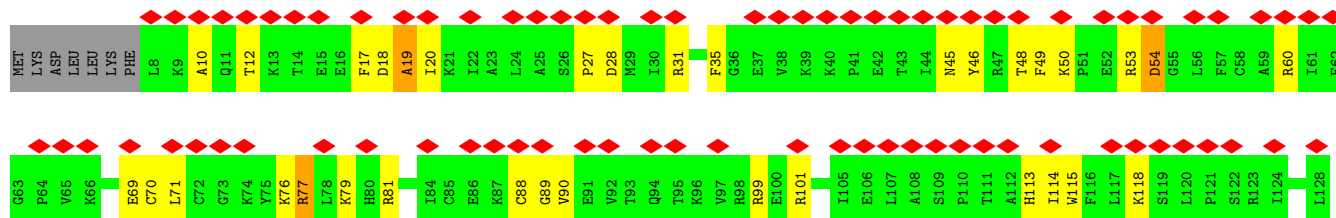
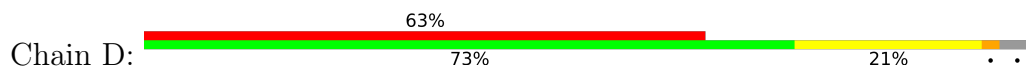


• Molecule 2: DNA-directed RNA polymerase subunit beta

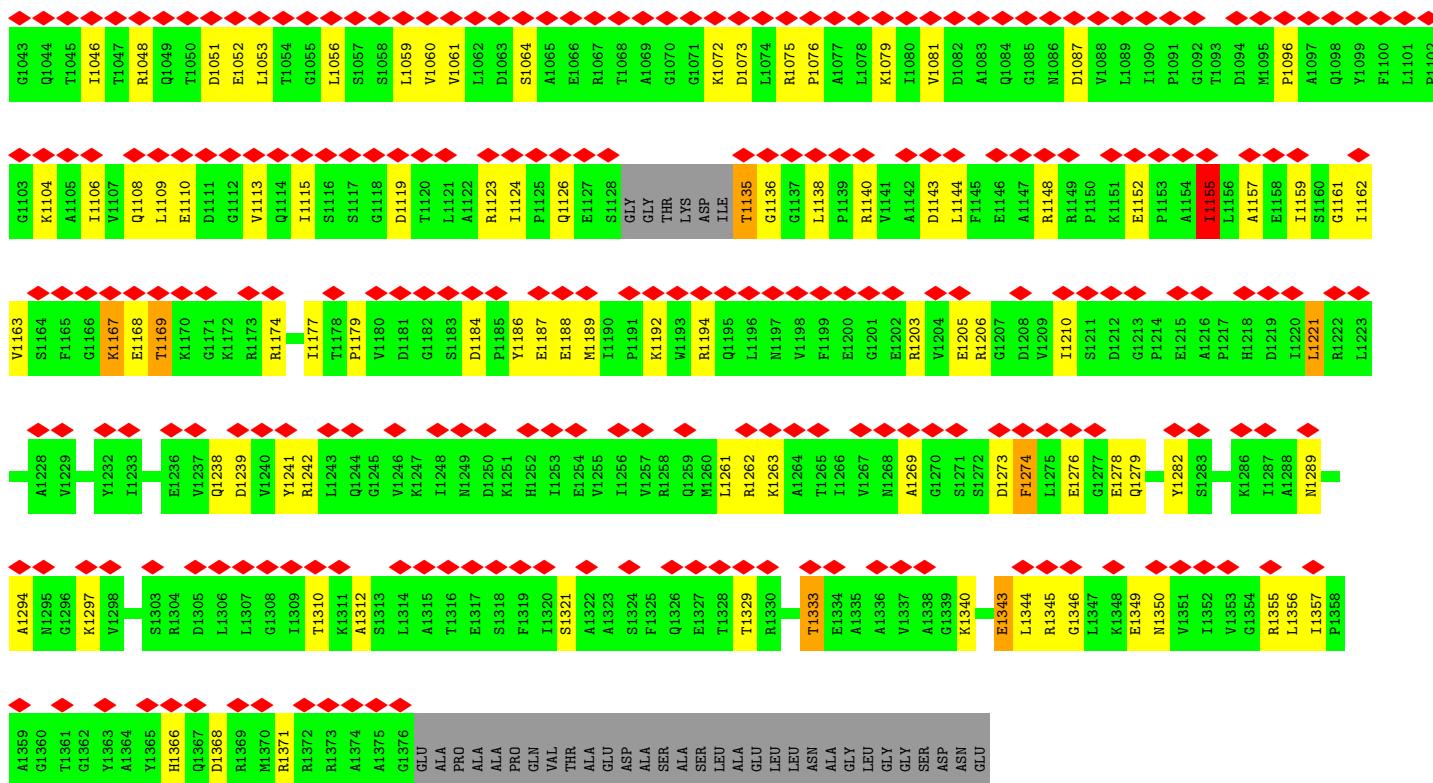




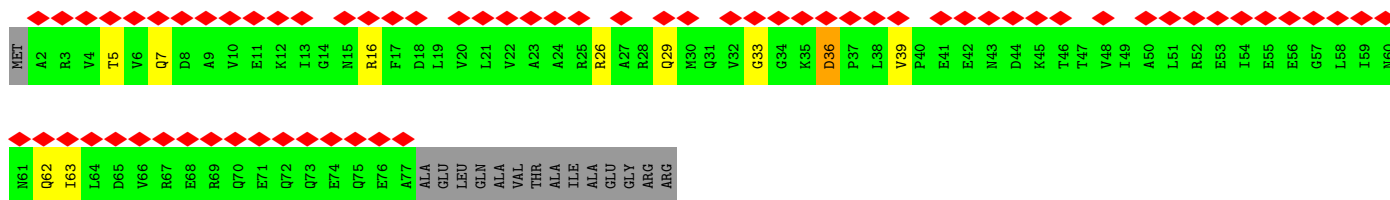
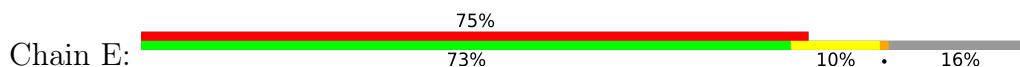
• Molecule 3: DNA-directed RNA polymerase subunit beta'



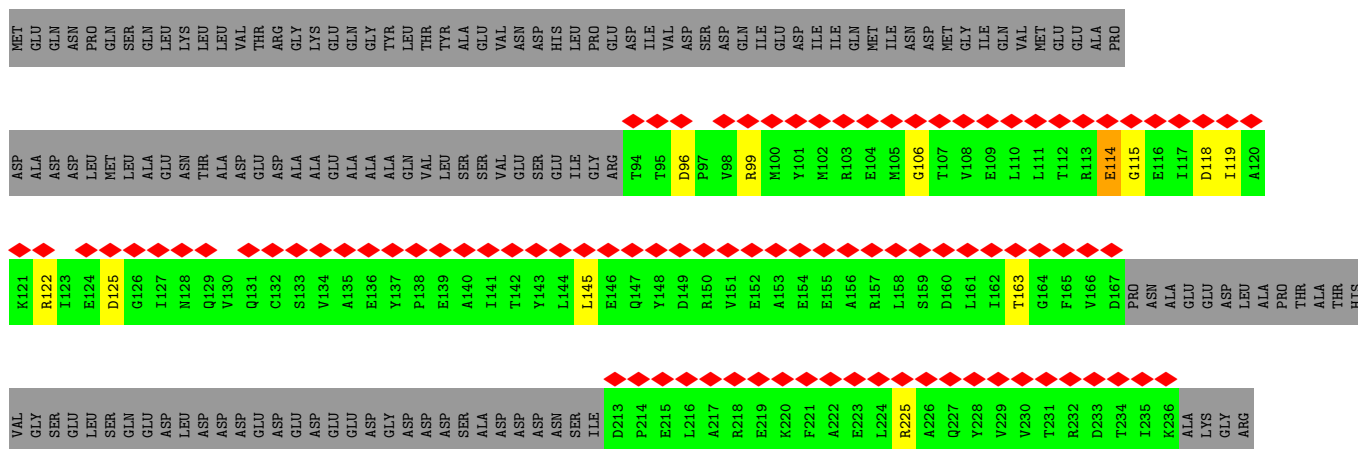




• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor RpoD



V606	L607	R608	S609	F610	L611	D612	ASP	R486	R422	I361	N301
V546	V547	L548	A549	G550	L551	T552	A553	R487	R423	N362	F302
L548	L549	L548	L549	G550	L551	T552	A553	L488	O424	R363	I303
S609	F610	L611	D612	ASP	R486	R422	I361	L489	Y425	R364	T304
L548	L549	G550	L551	T552	A553	R487	R423	L490	K426	N365	L305
L548	L549	G550	L551	T552	A553	R487	R423	L491	F427	F306	F306
L548	L549	G550	L551	T552	A553	R487	R423	L492	T428	T307	T307
L548	L549	G550	L551	T552	A553	R487	R423	L493	T429	G308	G308
L548	L549	G550	L551	T552	A553	R487	R423	L494	Y430	N309	N309
L548	L549	G550	L551	T552	A553	R487	R423	L495	A431	E310	E310
L548	L549	G550	L551	T552	A553	R487	R423	L496	T432	T311	T311
L548	L549	G550	L551	T552	A553	R487	R423	L497	W433	S312	S312
L548	L549	G550	L551	T552	A553	R487	R423	L498	W433	D313	D313
L548	L549	G550	L551	T552	A553	R487	R423	L499	W436	T314	T314
L548	L549	G550	L551	T552	A553	R487	R423	L500	W436	W315	W315
L548	L549	G550	L551	T552	A553	R487	R423	L501	T440	A375	A375
L548	L549	G550	L551	T552	A553	R487	R423	L502	R441	K376	K376
L548	L549	G550	L551	T552	A553	R487	R423	L503	W444	K377	K377
L548	L549	G550	L551	T552	A553	R487	R423	L504	D445	E378	E378
L548	L549	G550	L551	T552	A553	R487	R423	L505	Q446	M379	M379
L548	L549	G550	L551	T552	A553	R487	R423	L506	Q447	V380	V380
L548	L549	G550	L551	T552	A553	R487	R423	L507	A447	E381	E381
L548	L549	G550	L551	T552	A553	R487	R423	L508	W451	A321	A321
L548	L549	G550	L551	T552	A553	R487	R423	L509	I452	M322	M322
L548	L549	G550	L551	T552	A553	R487	R423	L510	P453	N323	N323
L548	L549	G550	L551	T552	A553	R487	R423	L511	W454	K324	K324
L548	L549	G550	L551	T552	A553	R487	R423	L512	G512	P325	P325
L548	L549	G550	L551	T552	A553	R487	R423	L513	D513	W326	W326
L548	L549	G550	L551	T552	A553	R487	R423	L514	D514	S327	S327
L548	L549	G550	L551	T552	A553	R487	R423	L515	E515	E328	E328
L548	L549	G550	L551	T552	A553	R487	R423	L516	D516	K329	K329
L548	L549	G550	L551	T552	A553	R487	R423	L517	S517	L330	L330
L548	L549	G550	L551	T552	A553	R487	R423	L518	H518	H331	H331
L548	L549	G550	L551	T552	A553	R487	R423	L519	T459	D332	D332
L548	L549	G550	L551	T552	A553	R487	R423	L520	I460	K393	K393
L548	L549	G550	L551	T552	A553	R487	R423	L521	M461	Y394	Y394
L548	L549	G550	L551	T552	A553	R487	R423	L522	K462	T395	T395
L548	L549	G550	L551	T552	A553	R487	R423	L523	L463	N396	N396
L548	L549	G550	L551	T552	A553	R487	R423	L524	M464	R397	R397
L548	L549	G550	L551	T552	A553	R487	R423	L525	R465	G398	G398
L548	L549	G550	L551	T552	A553	R487	R423	L526	I466	L399	L399
L548	L549	G550	L551	T552	A553	R487	R423	L527	S467	Q400	Q400
L548	L549	G550	L551	T552	A553	R487	R423	L528	R468	F401	F401
L548	L549	G550	L551	T552	A553	R487	R423	L529	Q469	L402	L402
L548	L549	G550	L551	T552	A553	R487	R423	L530	M470	D403	D403
L548	L549	G550	L551	T552	A553	R487	R423	L531	L471	L404	L404
L548	L549	G550	L551	T552	A553	R487	R423	L532	Q472	L405	L405
L548	L549	G550	L551	T552	A553	R487	R423	L533	E473	Q406	Q406
L548	L549	G550	L551	T552	A553	R487	R423	L534	M474	E407	E407
L548	L549	G550	L551	T552	A553	R487	R423	L535	D533	G408	G408
L548	L549	G550	L551	T552	A553	R487	R423	L536	S534	M409	M409
L548	L549	G550	L551	T552	A553	R487	R423	L537	A535	I410	I410
L548	L549	G550	L551	T552	A553	R487	R423	L538	T536	G411	G411
L548	L549	G550	L551	T552	A553	R487	R423	L539	T537	L412	L412
L548	L549	G550	L551	T552	A553	R487	R423	L540	E538	M413	M413
L548	L549	G550	L551	T552	A553	R487	R423	L541	S539	K414	K414
L548	L549	G550	L551	T552	A553	R487	R423	L542	L540	A415	A415
L548	L549	G550	L551	T552	A553	R487	R423	L543	R541	V416	V416
L548	L549	G550	L551	T552	A553	R487	R423	L544	A542	D417	D417
L548	L549	G550	L551	T552	A553	R487	R423	L545	L483	K418	K418
L548	L549	G550	L551	T552	A553	R487	R423	L546	A484	Y421	Y421
L548	L549	G550	L551	T552	A553	R487	R423	L547	E485		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96067	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.159	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.032	Depositor
Map size (\AA)	315.84, 315.84, 315.84	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.316, 1.316, 1.316	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.40	0/1809	0.82	3/2451 (0.1%)
1	B	0.40	0/1728	0.80	4/2341 (0.2%)
2	C	0.41	1/10739 (0.0%)	0.75	14/14489 (0.1%)
3	D	0.39	0/10591	0.75	11/14307 (0.1%)
4	E	0.34	0/607	0.66	0/817
5	F	0.34	0/3864	0.76	3/5194 (0.1%)
All	All	0.39	1/29338 (0.0%)	0.76	35/39599 (0.1%)

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	C	0	4
3	D	0	2
5	F	0	3
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	550	VAL	C-N	-5.44	1.21	1.34

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	70	TYR	CB-CG-CD1	-9.71	115.17	121.00
2	C	70	TYR	CB-CG-CD2	8.85	126.31	121.00
2	C	1021	LEU	CA-CB-CG	7.09	131.60	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	ARG	CG-CD-NE	-6.80	97.52	111.80
3	D	1221	LEU	CA-CB-CG	6.78	130.89	115.30
2	C	145	ILE	CG1-CB-CG2	-6.78	96.49	111.40
2	C	168	GLY	N-CA-C	-6.72	96.31	113.10
3	D	1343	GLU	C-N-CA	6.66	138.34	121.70
1	A	28	LEU	CA-CB-CG	6.64	130.57	115.30
3	D	709	ARG	NE-CZ-NH1	-6.20	117.20	120.30
3	D	426	ALA	CB-CA-C	5.92	118.98	110.10
2	C	1160	ASP	CB-CA-C	5.88	122.17	110.40
1	B	150	ARG	C-N-CA	-5.84	110.03	122.30
2	C	81	ASP	CB-CG-OD1	5.63	123.36	118.30
3	D	1155	ILE	CG1-CB-CG2	-5.52	99.25	111.40
3	D	77	ARG	CA-CB-CG	5.52	125.55	113.40
1	A	13	LEU	CA-CB-CG	5.48	127.90	115.30
2	C	866	ASP	CB-CG-OD1	5.42	123.18	118.30
3	D	500	ILE	CG1-CB-CG2	-5.42	99.47	111.40
1	B	102	LEU	CA-CB-CG	5.42	127.76	115.30
5	F	471	LEU	CA-CB-CG	5.39	127.71	115.30
3	D	46	TYR	CA-CB-CG	5.38	123.61	113.40
3	D	217	LEU	CA-CB-CG	5.37	127.65	115.30
5	F	586	ARG	NE-CZ-NH1	-5.30	117.65	120.30
3	D	701	LEU	CA-CB-CG	5.29	127.46	115.30
2	C	1158	LYS	CA-CB-CG	5.26	124.97	113.40
5	F	341	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	14	VAL	CA-CB-CG2	5.17	118.66	110.90
2	C	1160	ASP	C-N-CA	5.15	134.58	121.70
2	C	1233	LEU	CA-CB-CG	5.14	127.13	115.30
2	C	233	ARG	C-N-CA	5.12	134.49	121.70
2	C	696	ASP	C-N-CA	5.08	134.39	121.70
3	D	425	ARG	C-N-CA	5.07	134.38	121.70
1	B	48	LEU	CA-CB-CG	5.04	126.88	115.30
2	C	398	SER	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	198	ILE	Peptide
2	C	236	LYS	Peptide
2	C	397	LEU	Peptide
3	D	1184	ASP	Peptide

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Mol	Chain	Res	Type	Group
3	D	901	ARG	Peptide
5	F	569	THR	Peptide
5	F	582	VAL	Peptide
5	F	600	HIS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1787	0	1810	32	0
1	B	1708	0	1741	28	0
2	C	10570	0	10581	115	0
3	D	10434	0	10599	174	0
4	E	605	0	612	6	0
5	F	3813	0	3880	49	0
6	D	1	0	0	0	0
7	D	2	0	0	0	0
All	All	28920	0	29223	373	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 6.

All (373) 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)
3:D:1140:ARG:HH12	3:D:1144:LEU:HG	1.32	0.94
1:A:233:ASP:HA	1:B:218:ARG:HH12	1.40	0.87
2:C:74:ARG:NH1	2:C:121:GLU:OE2	2.06	0.87
2:C:299:LYS:NZ	2:C:300:ASP:O	2.11	0.81
2:C:719:LYS:HZ3	2:C:751:TYR:HE1	1.28	0.80
1:A:33:ARG:NH2	1:A:197:ASP:OD2	2.13	0.79
3:D:518:VAL:HA	3:D:547:ARG:HH12	1.45	0.79
3:D:1263:LYS:NZ	3:D:1279:GLN:OE1	2.16	0.79
1:A:232:VAL:O	1:B:218:ARG:NH1	2.16	0.77
3:D:866:GLU:OE2	3:D:901:ARG:NH2	2.15	0.76
2:C:17:LYS:NZ	2:C:1194:GLU:OE2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:50:GLU:OE2	2:C:54:ARG:NE	2.20	0.74
3:D:1278:GLU:OE2	3:D:1279:GLN:NE2	2.21	0.73
2:C:411:ARG:NH2	2:C:427:ASP:OD2	2.22	0.72
3:D:77:ARG:HG3	3:D:79:LYS:HG2	1.72	0.71
2:C:1122:LYS:NZ	2:C:1126:ASP:OD1	2.25	0.70
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.74	0.69
5:F:493:LYS:NZ	5:F:496:LYS:NZ	2.41	0.69
2:C:1069:ARG:NH2	2:C:1114:GLU:OE2	2.26	0.68
1:B:211:ILE:HG12	1:B:219:ARG:HH22	1.59	0.68
1:A:49:SER:HB3	2:C:1083:GLU:OE2	1.95	0.67
2:C:97:ARG:HB3	2:C:121:GLU:HB3	1.77	0.66
5:F:490:PRO:HB2	5:F:493:LYS:HG3	1.76	0.66
2:C:378:ARG:NE	2:C:382:GLU:OE2	2.27	0.65
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.78	0.65
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.77	0.65
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.30	0.65
5:F:493:LYS:HZ3	5:F:496:LYS:HZ1	1.43	0.64
5:F:479:THR:HG22	5:F:482:GLU:HG3	1.80	0.64
5:F:587:ILE:HD12	5:F:590:ILE:HD12	1.79	0.64
2:C:60:GLN:HB3	2:C:67:GLU:HG3	1.80	0.64
1:A:63:GLY:O	1:A:71:LYS:NZ	2.29	0.63
3:D:615:LYS:HZ2	4:E:7:GLN:HB3	1.63	0.63
1:B:180:VAL:O	3:D:535:ARG:NH2	2.30	0.63
3:D:214:ARG:HA	3:D:217:LEU:HB3	1.80	0.63
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.31	0.62
3:D:31:ARG:HE	3:D:241:VAL:HG21	1.64	0.62
2:C:517:GLN:HG3	2:C:523:GLU:OE2	1.99	0.62
1:A:107:ILE:HD11	1:A:136:GLU:HG2	1.81	0.62
3:D:1073:ASP:HA	3:D:1168:GLU:HG2	1.80	0.62
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.81	0.62
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.82	0.61
2:C:272:ARG:HD3	2:C:273:HIS:HD2	1.65	0.61
2:C:1072:ASN:ND2	2:C:1111:GLN:OE1	2.34	0.61
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.33	0.61
5:F:493:LYS:NZ	5:F:496:LYS:HZ1	1.98	0.61
3:D:518:VAL:HA	3:D:547:ARG:NH1	2.15	0.61
3:D:741:ALA:O	3:D:762:ASN:ND2	2.32	0.61
2:C:374:GLU:OE1	5:F:99:ARG:NH1	2.34	0.60
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.81	0.60
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.83	0.60
4:E:36:ASP:N	4:E:36:ASP:OD1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:187:GLU:OE2	2:C:197:ARG:NH2	2.34	0.60
3:D:1140:ARG:NH1	3:D:1144:LEU:HG	2.12	0.60
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.83	0.59
3:D:709:ARG:NH1	3:D:710:ASP:HB3	2.16	0.59
2:C:936:ARG:NH2	2:C:1043:ALA:O	2.35	0.59
2:C:960:LEU:HD21	2:C:1032:LYS:NZ	2.18	0.59
3:D:708:ASN:OD1	3:D:708:ASN:N	2.35	0.59
3:D:532:GLU:HB2	3:D:535:ARG:NH1	2.18	0.59
3:D:1238:GLN:HG3	3:D:1242:ARG:HE	1.66	0.59
3:D:832:LYS:NZ	3:D:1242:ARG:NH1	2.51	0.59
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.84	0.59
3:D:1140:ARG:NH1	3:D:1140:ARG:O	2.36	0.59
2:C:93:SER:OG	2:C:126:GLU:OE1	2.13	0.58
5:F:479:THR:HG23	5:F:481:GLU:H	1.68	0.58
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.37	0.58
3:D:45:ASN:ND2	3:D:48:THR:OG1	2.36	0.58
1:A:64:VAL:HG13	1:A:71:LYS:HE2	1.85	0.58
3:D:17:PHE:O	3:D:1355:ARG:NH2	2.36	0.58
3:D:435:GLN:HE21	3:D:486:SER:HA	1.69	0.58
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.68	0.58
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.37	0.57
5:F:115:GLY:HA2	5:F:118:ASP:HB2	1.86	0.57
1:A:135:ASP:HB3	1:A:138:ALA:HB2	1.85	0.57
5:F:371:LYS:HA	5:F:374:ARG:NH1	2.18	0.57
3:D:832:LYS:HZ2	3:D:832:LYS:HB3	1.70	0.57
3:D:905:ARG:HH21	3:D:907:HIS:HB2	1.69	0.57
2:C:557:ARG:HB3	2:C:587:LEU:HD13	1.85	0.57
2:C:719:LYS:NZ	2:C:751:TYR:HE1	2.01	0.57
2:C:714:VAL:O	2:C:767:GLN:NE2	2.37	0.57
3:D:957:SER:HB3	3:D:985:ILE:HB	1.87	0.57
5:F:508:GLU:OE1	5:F:518:HIS:ND1	2.38	0.57
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.87	0.56
3:D:646:ILE:HD11	3:D:764:ARG:HD3	1.86	0.56
3:D:970:SER:HB2	3:D:972:LYS:HZ3	1.70	0.56
2:C:387:ASN:HA	2:C:391:SER:HB2	1.88	0.56
3:D:54:ASP:N	3:D:54:ASP:OD1	2.39	0.56
3:D:473:THR:HG23	3:D:476:ALA:H	1.70	0.56
3:D:538:ARG:NH1	3:D:634:ARG:NH1	2.54	0.56
3:D:437:PHE:HZ	3:D:453:VAL:HG11	1.71	0.56
1:A:233:ASP:HA	1:B:218:ARG:NH1	2.16	0.56
5:F:312:SER:OG	5:F:313:ASP:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.88	0.55
2:C:18:ARG:HE	2:C:620:ASN:HA	1.72	0.55
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.89	0.55
3:D:60:ARG:HA	3:D:90:VAL:HG22	1.90	0.55
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.71	0.55
2:C:227:LYS:NZ	2:C:298:ALA:HB1	2.21	0.54
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.89	0.54
3:D:1321:SER:HB2	3:D:1349:GLU:OE2	2.08	0.54
5:F:274:ARG:NH2	5:F:369:GLU:OE1	2.40	0.54
1:A:104:LYS:HD3	1:A:110:VAL:HG13	1.90	0.54
1:B:95:LYS:NZ	1:B:97:GLU:O	2.40	0.54
3:D:1061:VAL:O	3:D:1104:LYS:N	2.40	0.54
2:C:1142:ARG:HG2	2:C:1169:VAL:HG11	1.90	0.53
5:F:493:LYS:HZ2	5:F:496:LYS:NZ	2.05	0.53
2:C:74:ARG:HH12	2:C:121:GLU:CD	2.11	0.53
3:D:1262:ARG:NH2	3:D:1312:ALA:O	2.42	0.53
3:D:388:ARG:NH2	3:D:414:GLU:OE1	2.42	0.53
5:F:119:ILE:HG23	5:F:375:ALA:HB1	1.91	0.53
2:C:1289:GLU:OE2	3:D:472:LEU:HB2	2.08	0.53
2:C:1269:ARG:HG3	3:D:346:ARG:NH1	2.24	0.53
3:D:1087:ASP:HB3	3:D:1096:PRO:HB3	1.91	0.53
1:A:112:ALA:HB3	1:A:126:PRO:HA	1.91	0.53
3:D:1060:VAL:HG22	3:D:1106:ILE:HG12	1.90	0.53
3:D:615:LYS:NZ	4:E:7:GLN:HB3	2.23	0.53
3:D:1036:ARG:HD2	3:D:1079:LYS:HD3	1.90	0.53
5:F:612:ASP:OD1	5:F:612:ASP:N	2.39	0.53
2:C:478:ARG:NH1	2:C:482:GLY:HA2	2.24	0.52
3:D:1143:ASP:HA	3:D:1148:ARG:NH1	2.23	0.52
2:C:903:ARG:NH2	5:F:612:ASP:OD1	2.43	0.52
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.41	0.52
3:D:694:SER:OG	3:D:738:ARG:NE	2.43	0.52
3:D:1046:ILE:HD12	3:D:1059:LEU:HD22	1.92	0.52
5:F:262:VAL:HG11	5:F:264:LYS:HZ2	1.74	0.52
3:D:930:LEU:HD11	3:D:1241:TYR:HE1	1.75	0.52
5:F:376:LYS:NZ	5:F:417:ASP:HA	2.24	0.52
2:C:367:TYR:HD1	2:C:384:LEU:HD22	1.75	0.52
1:B:182:ARG:NH1	3:D:534:GLU:OE1	2.43	0.51
3:D:1340:LYS:HB2	3:D:1340:LYS:NZ	2.25	0.51
1:B:62:ASP:OD1	1:B:62:ASP:N	2.34	0.51
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.75	0.51
3:D:370:LYS:HA	3:D:441:LEU:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:576:ARG:NH1	3:D:593:ASN:O	2.43	0.51
3:D:709:ARG:O	3:D:711:GLY:N	2.43	0.51
3:D:1109:LEU:HD22	3:D:1113:VAL:HG11	1.93	0.51
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.43	0.51
3:D:1143:ASP:HA	3:D:1148:ARG:HH11	1.76	0.51
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.92	0.51
2:C:739:ASP:OD1	2:C:739:ASP:N	2.43	0.51
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.93	0.51
2:C:1100:PRO:HB3	3:D:639:VAL:HG12	1.92	0.51
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.76	0.51
2:C:148:GLN:NE2	2:C:535:PRO:O	2.38	0.50
3:D:69:GLU:HG3	3:D:76:LYS:HG2	1.93	0.50
3:D:909:ILE:HD11	3:D:913:GLU:HG2	1.92	0.50
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.93	0.50
2:C:905:ILE:HG23	5:F:595:LEU:HD13	1.93	0.50
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.93	0.50
3:D:843:VAL:HG13	3:D:883:ARG:HD3	1.94	0.50
1:B:125:LYS:NZ	1:B:125:LYS:HB3	2.26	0.50
3:D:1002:VAL:N	3:D:1019:ASN:O	2.42	0.50
1:A:58:GLU:HG2	1:A:145:LYS:HE3	1.94	0.49
3:D:1051:ASP:HB2	3:D:1056:LEU:HB2	1.93	0.49
3:D:1034:PHE:N	3:D:1081:VAL:O	2.44	0.49
1:A:59:VAL:HG13	1:A:144:ILE:HG12	1.94	0.49
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.93	0.49
2:C:1240:ASP:N	2:C:1240:ASP:OD1	2.45	0.49
1:A:167:PRO:HB2	1:A:170:ARG:HG2	1.95	0.49
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.94	0.49
1:B:44:ARG:HG3	1:B:183:ILE:HD13	1.94	0.49
3:D:48:THR:O	3:D:50:LYS:N	2.43	0.49
2:C:1269:ARG:HB3	3:D:343:LEU:HD22	1.95	0.49
5:F:554:ARG:HH21	5:F:587:ILE:HD13	1.76	0.49
5:F:454:VAL:HA	5:F:457:ILE:HD12	1.94	0.49
3:D:1329:THR:O	3:D:1333:THR:OG1	2.27	0.48
2:C:272:ARG:HD3	2:C:273:HIS:CD2	2.47	0.48
3:D:621:ALA:HA	3:D:624:ILE:HD12	1.95	0.48
3:D:1059:LEU:HG	3:D:1110:GLU:OE2	2.14	0.48
3:D:824:PRO:HD3	3:D:835:LEU:HD13	1.96	0.48
1:B:14:VAL:HB	1:B:28:LEU:HD13	1.95	0.48
3:D:1186:TYR:OH	3:D:1188:GLU:OE1	2.23	0.48
3:D:549:LYS:NZ	3:D:569:LEU:O	2.46	0.48
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:352:ARG:NH1	3:D:465:GLN:OE1	2.47	0.48
1:A:102:LEU:HD23	1:A:115:ILE:HG12	1.95	0.47
3:D:1159:ILE:HD12	3:D:1206:ARG:HD2	1.96	0.47
1:A:16:ILE:HG12	1:A:26:VAL:HG12	1.96	0.47
3:D:1064:SER:O	3:D:1072:LYS:NZ	2.47	0.47
5:F:122:ARG:HA	5:F:125:ASP:HB2	1.97	0.47
1:B:16:ILE:HB	1:B:26:VAL:HG13	1.96	0.47
2:C:201:ARG:HG3	2:C:201:ARG:HH11	1.79	0.47
2:C:201:ARG:HH12	2:C:370:MET:HA	1.78	0.47
1:B:133:LEU:HD23	1:B:138:ALA:HB1	1.97	0.47
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.96	0.47
3:D:322:ARG:NH1	3:D:322:ARG:HB2	2.29	0.47
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.97	0.47
5:F:145:LEU:O	5:F:225:ARG:NH2	2.47	0.47
1:B:90:VAL:HG11	1:B:146:VAL:HG11	1.96	0.47
2:C:314:ASN:O	2:C:352:ARG:NH1	2.43	0.47
3:D:35:PHE:CD2	3:D:101:ARG:HD3	2.50	0.46
2:C:107:ARG:HA	2:C:108:GLU:HA	1.56	0.46
3:D:495:ASN:O	3:D:497:GLU:N	2.48	0.46
2:C:785:ASP:OD2	2:C:791:LEU:N	2.48	0.46
2:C:906:PHE:HE2	5:F:607:LEU:HB3	1.81	0.46
3:D:356:THR:OG1	3:D:357:VAL:N	2.48	0.46
3:D:832:LYS:HZ2	3:D:1242:ARG:NH1	2.13	0.46
1:B:158:ARG:NH1	1:B:172:LEU:HD13	2.30	0.46
3:D:1036:ARG:HH21	3:D:1081:VAL:HG21	1.80	0.46
2:C:145:ILE:HG21	2:C:456:VAL:HG13	1.98	0.46
5:F:493:LYS:NZ	5:F:496:LYS:HZ2	2.12	0.46
2:C:488:MET:O	2:C:490:GLN:N	2.46	0.46
3:D:370:LYS:HD3	3:D:443:GLU:OE2	2.16	0.46
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.51	0.46
3:D:1203:ARG:NH1	3:D:1205:GLU:OE2	2.45	0.46
3:D:342:LEU:HA	3:D:343:LEU:HA	1.76	0.46
3:D:1356:LEU:HD23	3:D:1356:LEU:HA	1.76	0.46
4:E:26:ARG:NH1	4:E:29:GLN:OE1	2.48	0.46
5:F:262:VAL:HG11	5:F:264:LYS:NZ	2.31	0.45
1:B:60:GLU:HB3	1:B:170:ARG:HG2	1.99	0.45
1:B:155:ALA:N	1:B:174:ASP:OD1	2.50	0.45
2:C:1149:TYR:HB3	2:C:1159:VAL:HG21	1.99	0.45
3:D:1161:GLY:HA3	3:D:1179:PRO:HA	1.98	0.45
5:F:559:LEU:HD12	5:F:559:LEU:HA	1.77	0.45
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:962:ASN:O	3:D:980:THR:OG1	2.34	0.45
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.51	0.45
5:F:280:VAL:HG22	5:F:347:ILE:HG21	1.99	0.45
1:B:215:GLU:CD	1:B:219:ARG:HH12	2.19	0.45
3:D:53:ARG:HA	3:D:54:ASP:HA	1.58	0.45
3:D:425:ARG:HH12	3:D:464:ASP:CG	2.19	0.45
3:D:609:TYR:HE1	3:D:614:LEU:HD12	1.82	0.45
3:D:947:GLU:O	3:D:1020:TRP:NE1	2.49	0.45
3:D:977:SER:OG	3:D:980:THR:OG1	2.34	0.45
2:C:990:ASP:OD1	2:C:990:ASP:N	2.49	0.45
2:C:1132:LEU:HD11	2:C:1174:GLU:OE2	2.17	0.45
1:A:43:LEU:HD13	1:A:217:ILE:HD11	1.99	0.45
1:A:45:ARG:HG2	1:B:38:THR:HB	1.98	0.45
2:C:568:ASN:OD1	2:C:568:ASN:N	2.50	0.45
3:D:953:LYS:HB2	3:D:993:GLU:OE2	2.16	0.45
1:B:215:GLU:OE2	1:B:219:ARG:NH1	2.50	0.45
2:C:549:ASP:OD1	2:C:550:VAL:N	2.49	0.45
3:D:638:SER:OG	3:D:639:VAL:N	2.47	0.45
5:F:558:VAL:HA	5:F:576:VAL:HG11	1.98	0.45
1:A:9:LEU:HB2	1:A:32:GLU:HG2	1.98	0.44
2:C:1024:GLU:HG2	2:C:1028:LYS:HD3	1.98	0.44
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	1.98	0.44
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.99	0.44
3:D:1023:HIS:ND1	3:D:1126:GLN:O	2.32	0.44
1:A:14:VAL:HG22	1:A:15:ASP:H	1.82	0.44
2:C:1247:SER:OG	2:C:1248:THR:N	2.50	0.44
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.48	0.44
5:F:525:ASP:OD2	5:F:528:LEU:HG	2.16	0.44
2:C:150:HIS:CD2	2:C:454:ARG:HE	2.35	0.44
2:C:560:PRO:O	3:D:780:ARG:NH2	2.45	0.44
2:C:623:LEU:HD12	2:C:627:GLY:HA2	1.99	0.44
3:D:416:ILE:HD13	3:D:416:ILE:HA	1.80	0.44
3:D:1075:ARG:HD2	3:D:1076:PRO:HD2	2.00	0.44
5:F:395:THR:OG1	5:F:396:ASN:N	2.51	0.44
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.99	0.44
5:F:470:MET:HB2	5:F:478:PRO:HG3	2.00	0.44
5:F:592:ALA:O	5:F:595:LEU:HB2	2.17	0.44
2:C:1130:ALA:O	2:C:1134:GLN:NE2	2.51	0.44
2:C:1319:MET:HA	2:C:1320:PRO:HD3	1.92	0.44
2:C:678:ARG:HA	2:C:678:ARG:HD3	1.79	0.44
2:C:808:ASN:OD1	2:C:1216:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:975:ILE:HD11	2:C:1014:LEU:HB3	2.00	0.44
3:D:19:ALA:HA	3:D:1343:GLU:HA	2.00	0.44
3:D:88:CYS:O	3:D:90:VAL:N	2.51	0.44
3:D:275:ARG:NH1	3:D:298:MET:HB3	2.33	0.44
3:D:885:VAL:HG12	3:D:894:VAL:HG11	2.00	0.44
2:C:55:SER:OG	2:C:56:VAL:N	2.51	0.44
3:D:1174:ARG:HG2	3:D:1189:MET:HG2	2.00	0.44
2:C:503:LYS:HD3	2:C:503:LYS:HA	1.84	0.43
2:C:1164:PHE:HB2	2:C:1168:GLU:HG3	2.01	0.43
3:D:70:CYS:SG	3:D:71:LEU:N	2.90	0.43
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.98	0.43
3:D:1269:ALA:HB2	3:D:1274:PHE:HD1	1.84	0.43
3:D:18:ASP:N	3:D:18:ASP:OD1	2.47	0.43
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.84	0.43
3:D:832:LYS:HD3	3:D:1242:ARG:HH12	1.84	0.43
3:D:848:VAL:HG12	3:D:858:VAL:HG22	2.00	0.43
3:D:1108:GLN:OE1	3:D:1123:ARG:NH1	2.51	0.43
5:F:270:VAL:HG13	5:F:365:MET:HE3	1.99	0.43
1:B:181:GLU:HA	3:D:535:ARG:HH22	1.83	0.43
2:C:357:ASN:OD1	2:C:357:ASN:N	2.49	0.43
3:D:959:LYS:NZ	3:D:985:ILE:HG13	2.34	0.43
1:A:43:LEU:HD23	1:A:43:LEU:HA	1.86	0.43
2:C:1083:GLU:H	2:C:1083:GLU:HG3	1.55	0.43
2:C:1339:LEU:HA	3:D:20:ILE:HG12	2.00	0.43
3:D:516:ASP:HB3	3:D:573:THR:HG21	2.00	0.43
3:D:667:GLN:HG2	3:D:672:LEU:HD22	2.00	0.43
5:F:114:GLU:H	5:F:114:GLU:HG3	1.57	0.43
1:B:67:GLU:OE1	1:B:67:GLU:N	2.49	0.43
2:C:404:LYS:HD2	2:C:404:LYS:HA	1.81	0.43
2:C:908:GLU:OE2	5:F:611:LEU:HB3	2.18	0.43
3:D:1163:VAL:HG23	3:D:1177:ILE:HG22	2.01	0.43
2:C:1280:ALA:HB1	3:D:918:ILE:HG22	2.01	0.43
1:A:12:ARG:NH1	1:A:13:LEU:O	2.51	0.43
3:D:27:PRO:O	3:D:31:ARG:HG3	2.19	0.43
3:D:294:ASN:HD22	5:F:406:GLN:NE2	2.16	0.43
3:D:1344:LEU:O	3:D:1346:GLY:N	2.44	0.43
3:D:118:LYS:HB3	3:D:118:LYS:HE2	1.92	0.43
1:A:71:LYS:HD3	1:A:71:LYS:HA	1.90	0.42
2:C:1065:LYS:HD3	2:C:1235:LEU:HD12	2.01	0.42
2:C:696:ASP:HB3	2:C:697:LYS:H	1.54	0.42
1:B:196:THR:HG23	3:D:443:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:802:VAL:HG11	2:C:1230:MET:HB3	2.00	0.42
2:C:971:LEU:HG	2:C:1014:LEU:HD23	2.00	0.42
3:D:1273:ASP:HB2	3:D:1276:GLU:HB2	2.01	0.42
2:C:24:VAL:HG22	2:C:578:TYR:HE1	1.83	0.42
3:D:222:LYS:HA	3:D:222:LYS:HD2	1.85	0.42
3:D:511:TYR:HE2	3:D:724:MET:HG2	1.85	0.42
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.88	0.42
3:D:429:LEU:HD13	3:D:429:LEU:HA	1.92	0.42
3:D:304:ASP:OD2	3:D:312:ARG:NH2	2.44	0.42
3:D:1021:ASP:HB3	3:D:1024:THR:HB	2.00	0.42
3:D:1157:ALA:HB3	3:D:1206:ARG:HA	2.02	0.42
5:F:106:GLY:O	5:F:385:ARG:NH2	2.53	0.42
1:A:35:PHE:HD1	1:A:35:PHE:HA	1.70	0.42
2:C:39:ILE:HD11	2:C:75:LEU:HG	2.01	0.42
3:D:510:LEU:HD22	3:D:601:ILE:HD11	2.00	0.42
2:C:1254:VAL:O	3:D:99:ARG:NH2	2.40	0.42
2:C:543:ALA:HA	2:C:544:GLY:HA3	1.80	0.42
2:C:570:GLY:O	2:C:573:ASN:ND2	2.45	0.42
3:D:1203:ARG:NH1	3:D:1205:GLU:HG2	2.35	0.42
5:F:387:VAL:HG21	5:F:412:LEU:HD22	2.01	0.42
5:F:476:ARG:HB3	5:F:477:GLU:H	1.62	0.42
1:A:9:LEU:HD23	1:A:9:LEU:HA	1.89	0.41
1:B:112:ALA:HB3	1:B:126:PRO:HA	2.02	0.41
2:C:1137:GLU:HG3	2:C:1139:ALA:H	1.84	0.41
1:A:165:GLU:OE2	1:A:172:LEU:HD11	2.20	0.41
3:D:863:LEU:HD11	3:D:901:ARG:HB3	2.02	0.41
3:D:1152:GLU:OE2	3:D:1194:ARG:HG2	2.21	0.41
5:F:484:ALA:HB1	5:F:491:GLU:HB2	2.02	0.41
1:A:90:VAL:HG21	1:A:146:VAL:HG21	2.02	0.41
2:C:1305:TYR:HE2	5:F:535:ALA:HB2	1.85	0.41
5:F:495:ARG:HD3	5:F:495:ARG:H	1.86	0.41
1:B:71:LYS:HA	1:B:71:LYS:HD3	1.84	0.41
2:C:117:ILE:H	2:C:117:ILE:HG12	1.64	0.41
2:C:661:VAL:HB	2:C:665:ALA:HB3	2.03	0.41
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.88	0.41
2:C:549:ASP:OD2	3:D:750:PRO:HB3	2.20	0.41
2:C:594:VAL:HG11	2:C:650:VAL:HG23	2.03	0.41
3:D:538:ARG:HA	3:D:538:ARG:HD2	1.93	0.41
2:C:135:THR:HG21	2:C:142:GLU:OE2	2.20	0.41
3:D:1115:ILE:HB	3:D:1119:ASP:HB2	2.02	0.41
5:F:309:ASN:HB3	5:F:310:GLU:H	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1025:MET:HB3	3:D:1124:ILE:HB	2.03	0.41
3:D:1174:ARG:NH2	3:D:1187:GLU:OE2	2.54	0.41
3:D:148:GLU:H	3:D:156:ARG:HG3	1.84	0.41
3:D:1167:LYS:HE3	3:D:1167:LYS:HB3	1.85	0.41
2:C:269:ILE:HA	2:C:273:HIS:ND1	2.36	0.41
2:C:799:ASN:OD1	2:C:799:ASN:N	2.54	0.41
3:D:139:LEU:HD23	3:D:139:LEU:HA	1.84	0.41
1:B:26:VAL:O	1:B:203:ILE:N	2.47	0.41
1:B:118:ASP:HB2	1:B:121:VAL:HB	2.03	0.41
3:D:813:ASP:HB2	3:D:897:HIS:CE1	2.56	0.41
1:A:96:ASP:OD1	1:A:148:ARG:NH1	2.54	0.40
2:C:17:LYS:N	2:C:1188:ASP:OD2	2.54	0.40
3:D:161:THR:HG22	3:D:164:GLN:HB2	2.03	0.40
3:D:242:LEU:HA	3:D:243:PRO:HD3	1.90	0.40
3:D:278:ARG:HD3	5:F:407:GLU:OE2	2.20	0.40
3:D:587:LEU:HD23	3:D:591:ILE:HG21	2.02	0.40
3:D:1052:GLU:HG2	3:D:1053:LEU:H	1.86	0.40
4:E:63:ILE:HD13	4:E:63:ILE:HA	1.92	0.40
2:C:804:PHE:HE2	2:C:1115:THR:HG21	1.85	0.40
3:D:832:LYS:HZ2	3:D:1242:ARG:HH11	1.69	0.40
3:D:1155:ILE:HD12	3:D:1210:ILE:HB	2.02	0.40
5:F:589:GLN:O	5:F:593:LYS:N	2.49	0.40
1:A:171:LEU:HD13	1:A:171:LEU:HA	1.91	0.40
2:C:123:TYR:OH	2:C:126:GLU:HG3	2.21	0.40
2:C:227:LYS:HZ3	2:C:298:ALA:HB1	1.84	0.40
3:D:371:LYS:HA	3:D:371:LYS:HD2	1.95	0.40
3:D:1036:ARG:HB3	3:D:1079:LYS:HB3	2.03	0.40
2:C:228:VAL:HG23	2:C:337:PHE:HB2	2.03	0.40
2:C:1255:THR:O	2:C:1257:GLN:N	2.55	0.40
3:D:839:VAL:HG12	3:D:864:LEU:HD12	2.03	0.40
5:F:505:ILE:HD12	5:F:505:ILE:HA	1.95	0.40
2:C:727:VAL:HG23	2:C:773:LEU:HD23	2.03	0.40
2:C:1236:ASN:HA	2:C:1238:LEU:HD12	2.04	0.40
3:D:1282:TYR:HD1	3:D:1282:TYR:HA	1.77	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	228/329 (69%)	204 (90%)	24 (10%)	0	100	100
1	B	217/329 (66%)	196 (90%)	18 (8%)	3 (1%)	11	47
2	C	1338/1342 (100%)	1209 (90%)	109 (8%)	20 (2%)	10	46
3	D	1344/1407 (96%)	1212 (90%)	105 (8%)	27 (2%)	7	40
4	E	74/91 (81%)	70 (95%)	3 (4%)	1 (1%)	11	47
5	F	462/613 (75%)	430 (93%)	27 (6%)	5 (1%)	14	52
All	All	3663/4111 (89%)	3321 (91%)	286 (8%)	56 (2%)	14	46

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	21	SER
1	B	193	GLU
2	C	398	SER
2	C	484	LEU
2	C	697	LYS
3	D	10	ALA
3	D	49	PHE
3	D	426	ALA
3	D	496	GLY
3	D	710	ASP
3	D	712	GLN
3	D	745	GLY
3	D	805	GLN
3	D	826	ILE
3	D	831	VAL
3	D	860	ARG
3	D	1169	THR
3	D	1294	ALA
4	E	33	GLY
5	F	490	PRO

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Mol	Chain	Res	Type
5	F	566	ASP
2	C	121	GLU
2	C	596	ASP
2	C	746	ALA
2	C	1137	GLU
2	C	1154	ASP
2	C	1165	SER
3	D	89	GLY
3	D	1167	LYS
5	F	569	THR
1	B	13	LEU
2	C	696	ASP
2	C	892	GLU
2	C	1317	PRO
3	D	19	ALA
2	C	163	LYS
2	C	199	ASP
2	C	235	ASN
2	C	813	GLU
3	D	173	GLY
3	D	314	ARG
3	D	417	ARG
3	D	585	LYS
2	C	625	GLU
3	D	230	SER
3	D	1274	PHE
3	D	1345	ARG
2	C	169	LYS
2	C	983	GLY
2	C	1223	ARG
3	D	152	THR
3	D	1297	LYS
3	D	357	VAL
5	F	96	ASP
5	F	361	ILE
3	D	828	GLY

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	198/286 (69%)	195 (98%)	3 (2%)	65	80
1	B	189/286 (66%)	182 (96%)	7 (4%)	34	59
2	C	1155/1157 (100%)	1104 (96%)	51 (4%)	28	54
3	D	1115/1168 (96%)	1067 (96%)	48 (4%)	29	55
4	E	65/75 (87%)	61 (94%)	4 (6%)	18	46
5	F	417/540 (77%)	406 (97%)	11 (3%)	46	67
All	All	3139/3512 (89%)	3015 (96%)	124 (4%)	35	57

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	13	LEU
1	A	124	VAL
1	B	9	LEU
1	B	62	ASP
1	B	64	VAL
1	B	71	LYS
1	B	124	VAL
1	B	183	ILE
1	B	191	ARG
2	C	103	VAL
2	C	117	ILE
2	C	131	THR
2	C	135	THR
2	C	145	ILE
2	C	164	THR
2	C	235	ASN
2	C	272	ARG
2	C	306	THR
2	C	321	LEU
2	C	377	THR
2	C	452	ARG
2	C	470	ARG
2	C	471	VAL
2	C	539	THR
2	C	553	THR
2	C	558	VAL

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Mol	Chain	Res	Type
2	C	600	THR
2	C	609	ILE
2	C	615	VAL
2	C	623	LEU
2	C	714	VAL
2	C	757	THR
2	C	764	CYS
2	C	765	ILE
2	C	791	LEU
2	C	878	THR
2	C	895	LEU
2	C	922	ASN
2	C	992	LEU
2	C	1032	LYS
2	C	1090	ASN
2	C	1134	GLN
2	C	1141	LEU
2	C	1151	LEU
2	C	1155	VAL
2	C	1156	ARG
2	C	1159	VAL
2	C	1163	THR
2	C	1198	LEU
2	C	1210	ILE
2	C	1233	LEU
2	C	1234	LYS
2	C	1240	ASP
2	C	1254	VAL
2	C	1265	PHE
2	C	1287	LEU
2	C	1296	ASP
2	C	1299	ASN
2	C	1324	ASN
2	C	1327	LEU
3	D	12	THR
3	D	54	ASP
3	D	81	ARG
3	D	175	GLU
3	D	252	LEU
3	D	269	TYR
3	D	292	VAL
3	D	320	ASN

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Mol	Chain	Res	Type
3	D	324	LEU
3	D	343	LEU
3	D	386	GLU
3	D	392	THR
3	D	394	ILE
3	D	416	ILE
3	D	425	ARG
3	D	429	LEU
3	D	431	ARG
3	D	505	ASP
3	D	514	THR
3	D	515	ARG
3	D	536	LEU
3	D	545	HIS
3	D	569	LEU
3	D	573	THR
3	D	639	VAL
3	D	678	ARG
3	D	680	ASN
3	D	701	LEU
3	D	707	ILE
3	D	708	ASN
3	D	744	ARG
3	D	753	SER
3	D	754	ILE
3	D	801	VAL
3	D	810	THR
3	D	853	THR
3	D	903	LEU
3	D	1019	ASN
3	D	1048	ARG
3	D	1135	THR
3	D	1155	ILE
3	D	1162	ILE
3	D	1221	LEU
3	D	1261	LEU
3	D	1289	ASN
3	D	1310	THR
3	D	1333	THR
3	D	1366	HIS
4	E	5	THR
4	E	36	ASP

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Mol	Chain	Res	Type
4	E	39	VAL
4	E	62	GLN
5	F	114	GLU
5	F	163	THR
5	F	261	LEU
5	F	305	LEU
5	F	465	ARG
5	F	491	GLU
5	F	495	ARG
5	F	526	THR
5	F	527	THR
5	F	558	VAL
5	F	606	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	147	GLN
1	B	117	HIS
1	B	132	HIS
2	C	235	ASN
2	C	276	GLN
2	C	330	HIS
2	C	554	HIS
2	C	922	ASN
2	C	1090	ASN
2	C	1116	HIS
2	C	1134	GLN
2	C	1299	ASN
2	C	1324	ASN
3	D	45	ASN
3	D	294	ASN
3	D	320	ASN
3	D	430	HIS
3	D	435	GLN
3	D	680	ASN
3	D	1010	GLN
3	D	1019	ASN
3	D	1289	ASN
5	F	227	GLN

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 [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

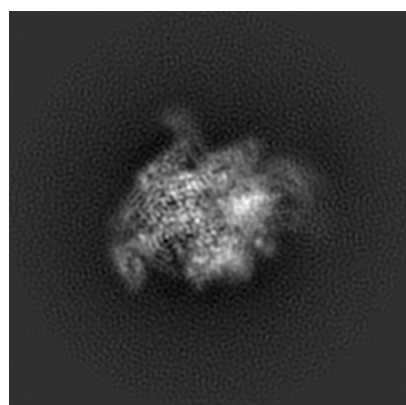
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7438. These allow visual inspection of the internal detail of the map and identification of artifacts.

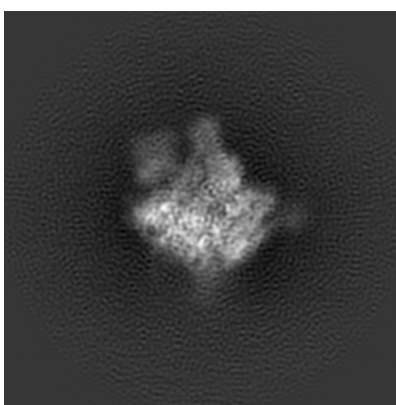
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

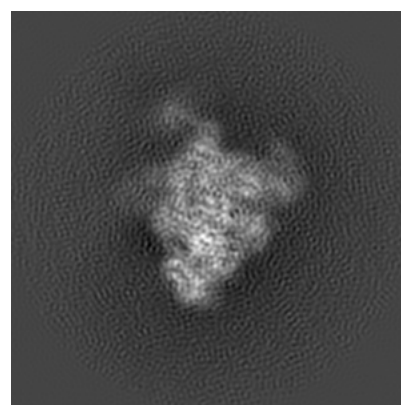
6.1.1 Primary map



X



Y

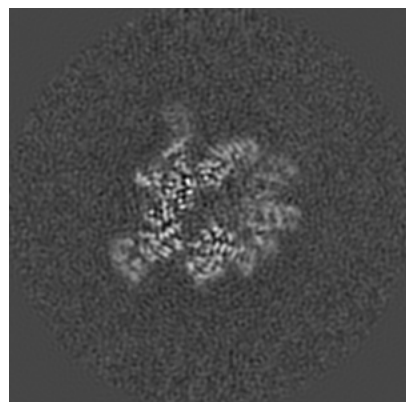


Z

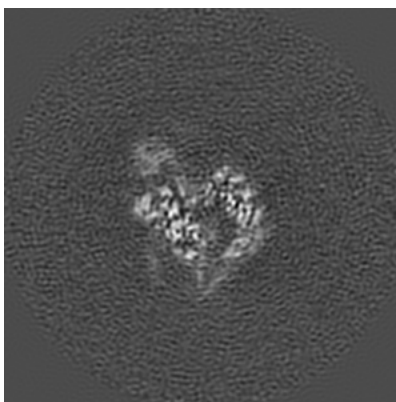
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

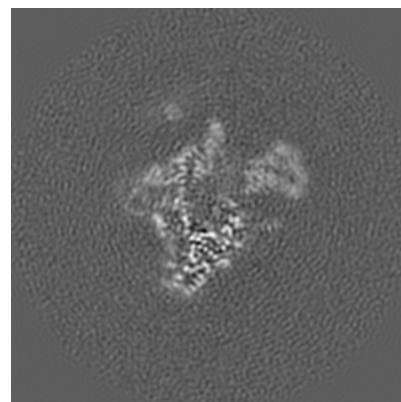
6.2.1 Primary map



X Index: 120



Y Index: 120

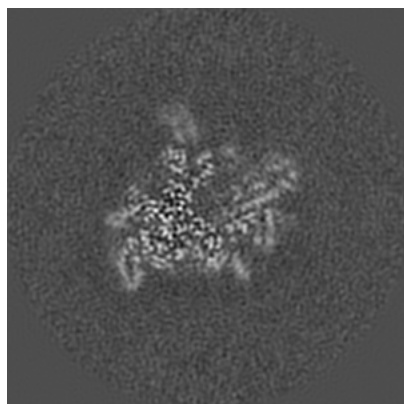


Z Index: 120

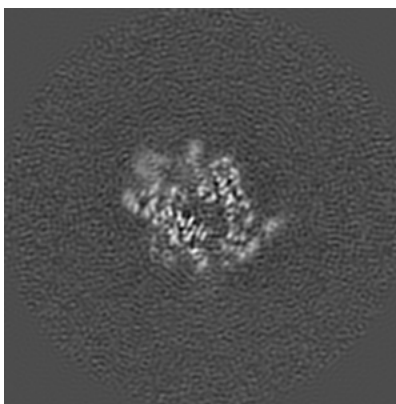
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

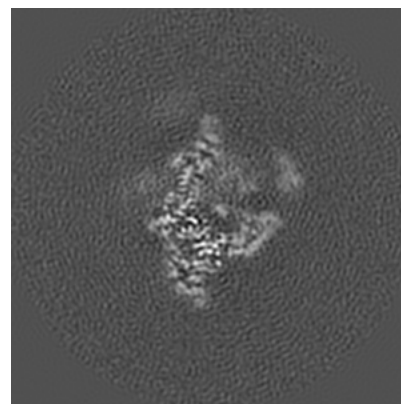
6.3.1 Primary map



X Index: 114



Y Index: 114



Z Index: 114

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

6.4 Orthogonal surface views [i](#)

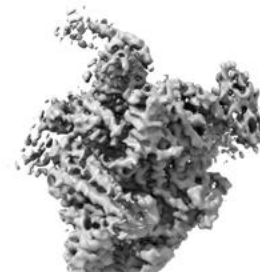
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

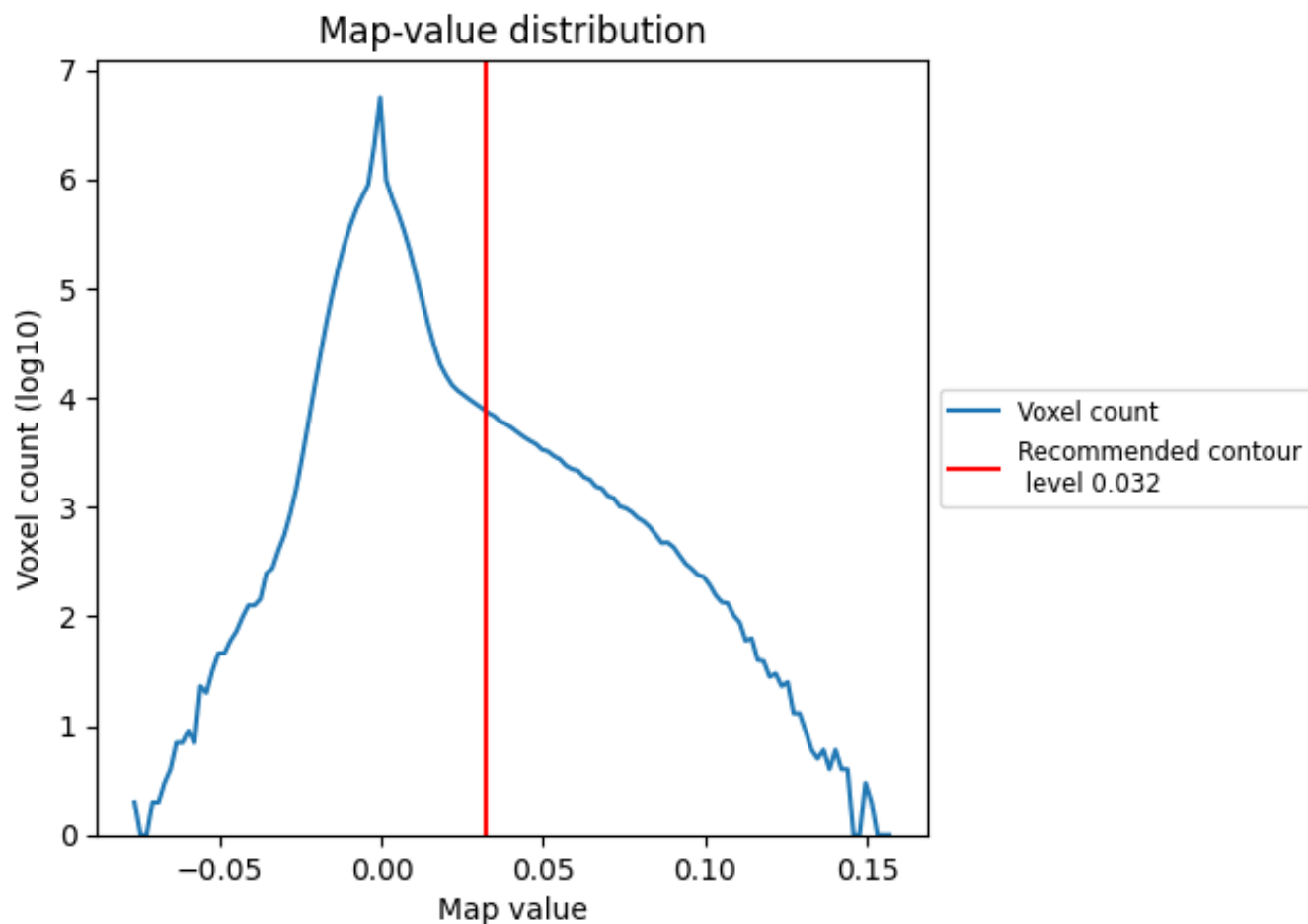
6.5 Mask visualisation

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

7 Map analysis [i](#)

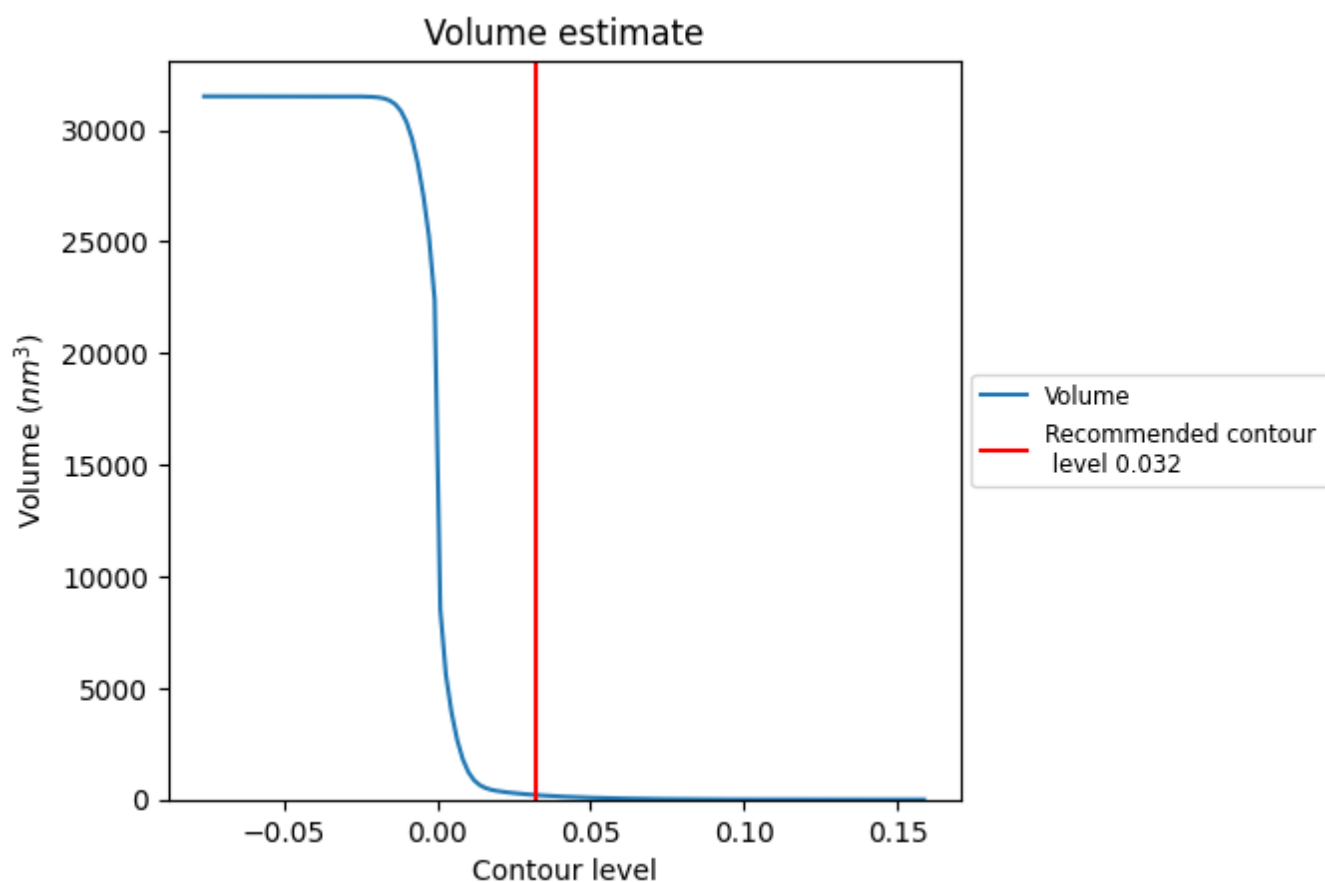
This section contains the results of statistical analysis of the map.

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.

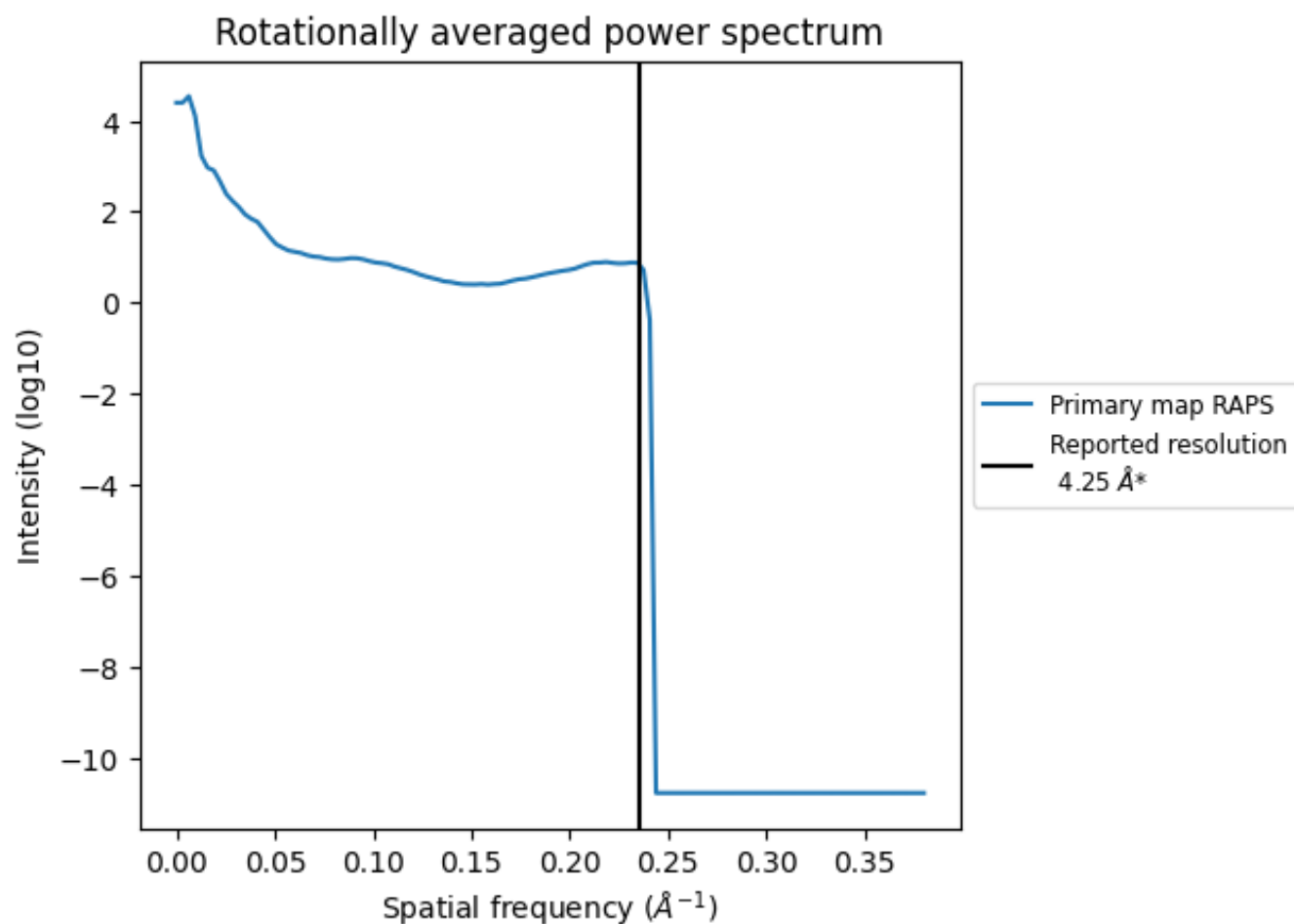
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 206 nm³; this corresponds to an approximate mass of 186 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 0.235 Å⁻¹

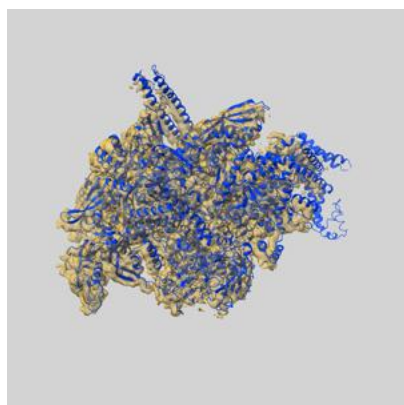
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

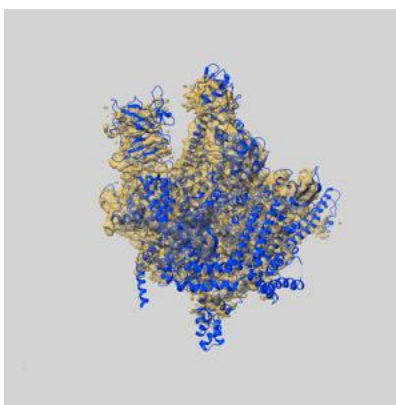
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7438 and PDB model 6C9Y. Per-residue inclusion information can be found in section [3](#) on page [5](#).

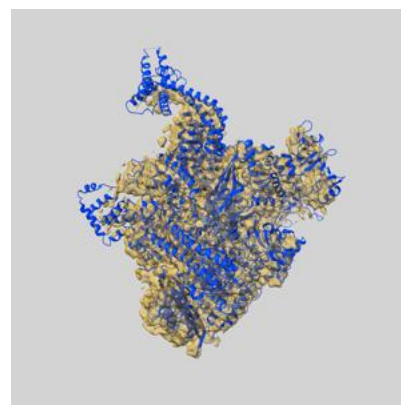
9.1 Map-model overlay [i](#)



X



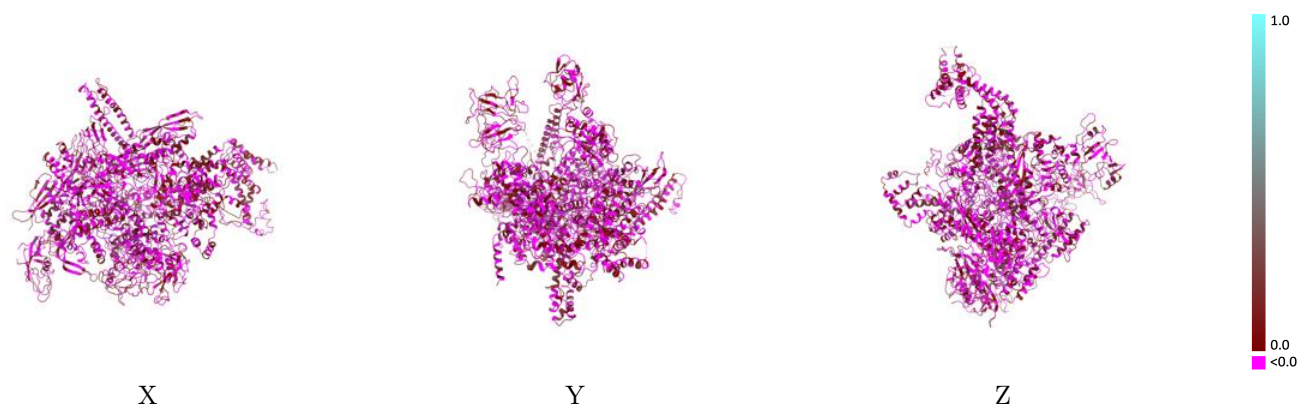
Y



Z

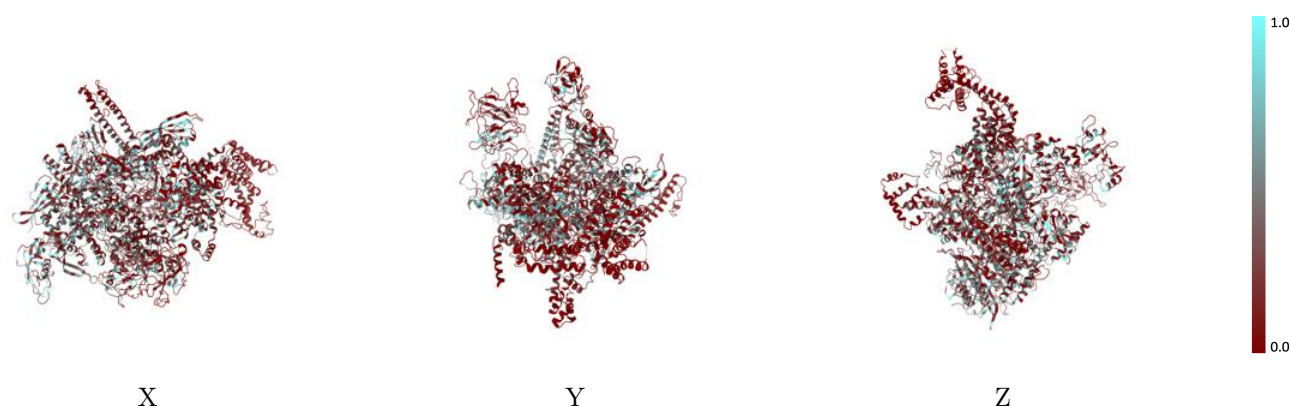
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



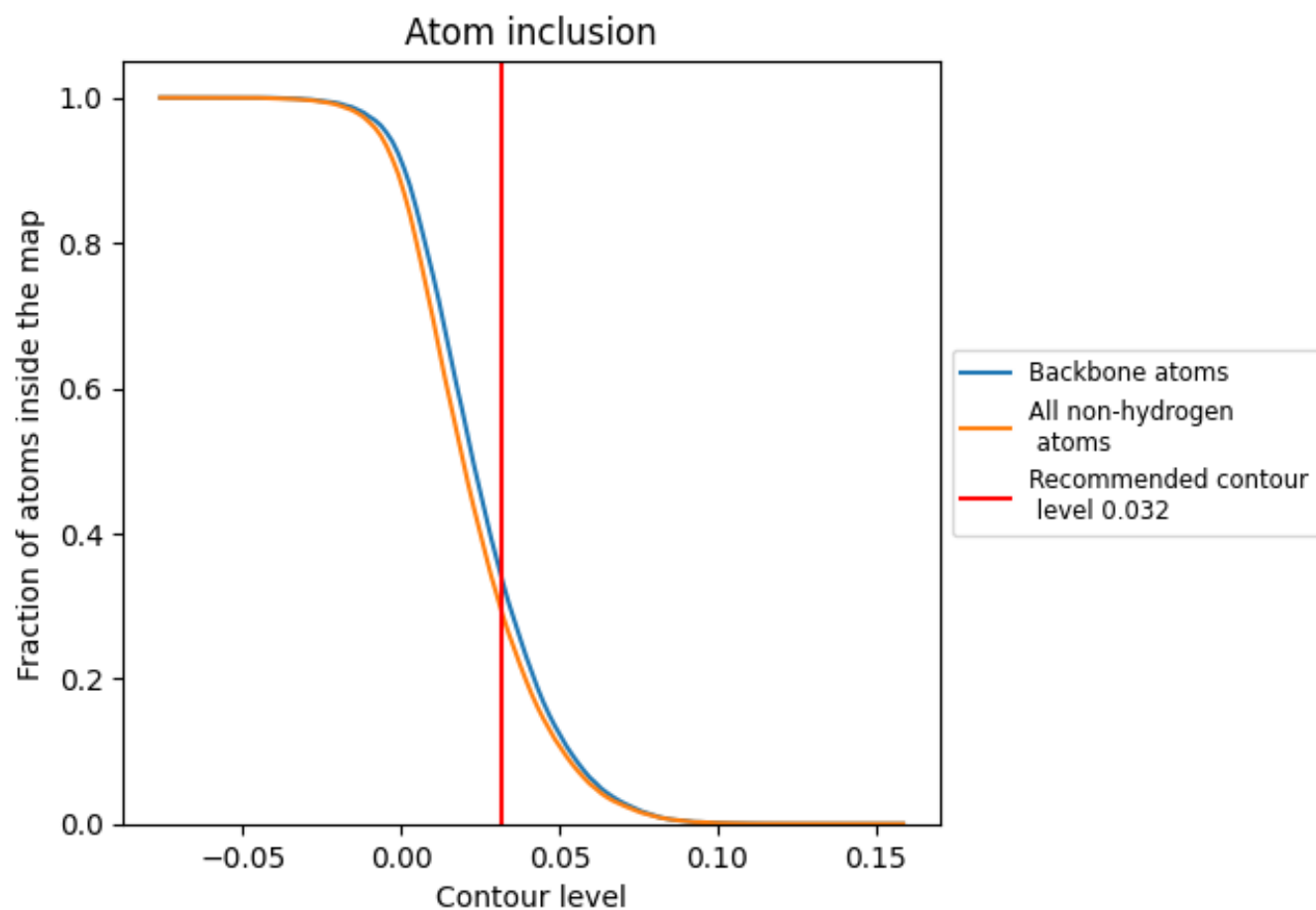
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.032).

9.4 Atom inclusion [i](#)



At the recommended contour level, 34% of all backbone atoms, 29% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.2898	<div></div> -0.0160
A	<div></div> 0.4002	<div></div> -0.0020
B	<div></div> 0.4188	<div></div> -0.0130
C	<div></div> 0.3114	<div></div> -0.0300
D	<div></div> 0.3098	<div></div> -0.0120
E	<div></div> 0.1138	<div></div> -0.0490
F	<div></div> 0.0924	<div></div> 0.0030

1.0
0.0
-0.0