



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:36 PM UTC

PDB ID : 6FLQ / pdb_00006flq
EMDB ID : EMD-4275
Title : CryoEM structure of E.coli RNA polymerase paused elongation complex bound to NusA
Authors : Guo, X.; Weixlbaumer, A.
Deposited on : 2018-01-26
Resolution : 3.60 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:

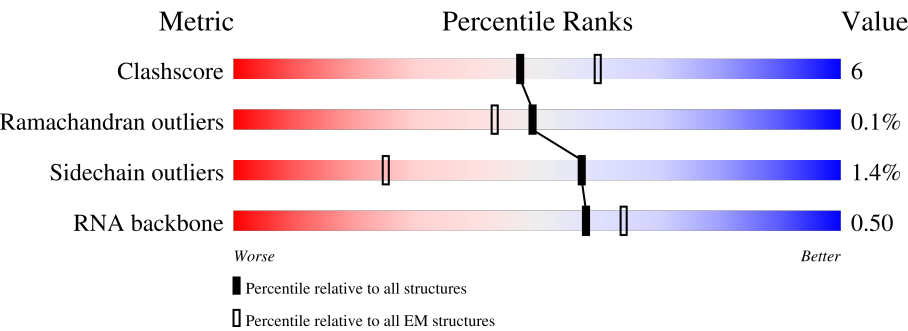
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.60 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

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	88% 79%14%6%
1	B	329	86% 76%14%9%
2	C	1342	85% 82%17%
3	D	1407	81% 80%14%5%
4	E	91	92% 93%5%
5	F	495	100% 95%5%
6	N	31	94% 81%19%

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Mol	Chain	Length	Quality of chain
7	R	21	95% 38% 38% 24%
8	T	39	79% 77% 23%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 30201 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	310	Total	C	N	O	S	0	0
			2168	1339	394	429	6		
1	B	298	Total	C	N	O	S	0	0
			2068	1280	374	408	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1341	Total	C	N	O	S	0	0
			10573	6634	1841	2055	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1334	Total	C	N	O	S	0	0
			10357	6510	1846	1952	49		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	90	Total	C	N	O	S	0	0
			709	430	136	142	1		

- Molecule 5 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	495	Total	C	N	O	0	0
			2447	1457	495	495		

- Molecule 6 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	31	Total	C	N	O	P	0	0
			647	304	131	181	31		

- Molecule 7 is a RNA chain called RNA (5'-R(*CP*CP*UP*GP*AP*UP*CP*AP*GP*GP*CP*GP*AP*UP*GP*UP*GP*UP*GP*CP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	21	Total	C	N	O	P	0	0
			444	199	77	148	20		

- Molecule 8 is a DNA chain called DNA (39-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	39	Total	C	N	O	P	0	0
			785	375	135	236	39		

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

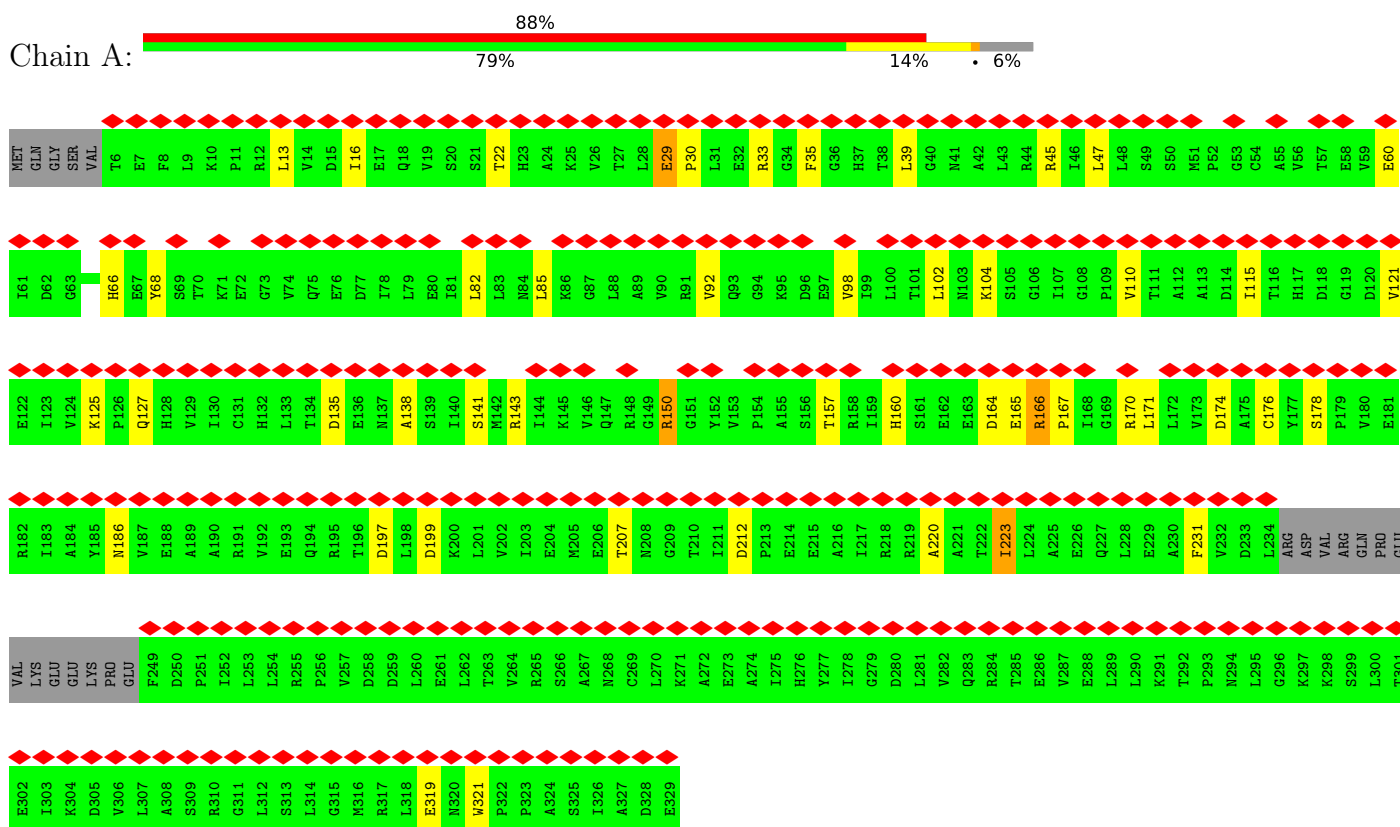
- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

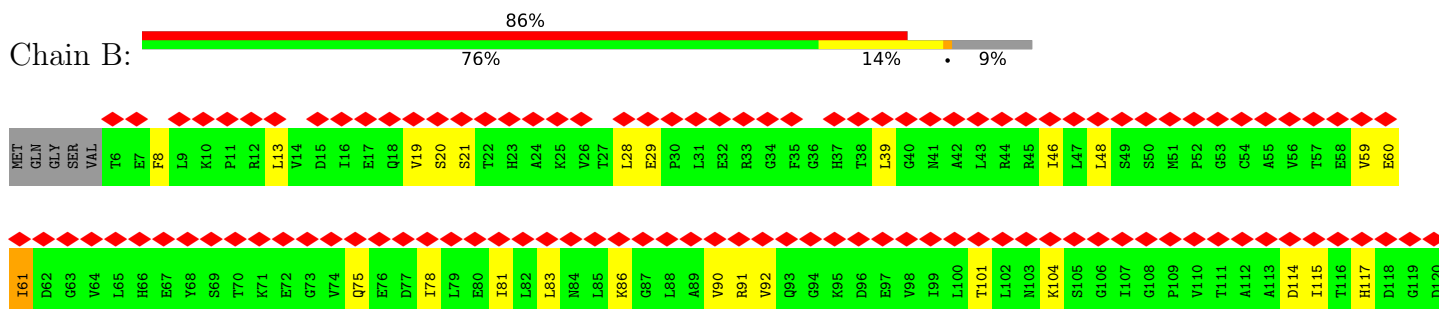
3 Residue-property plots

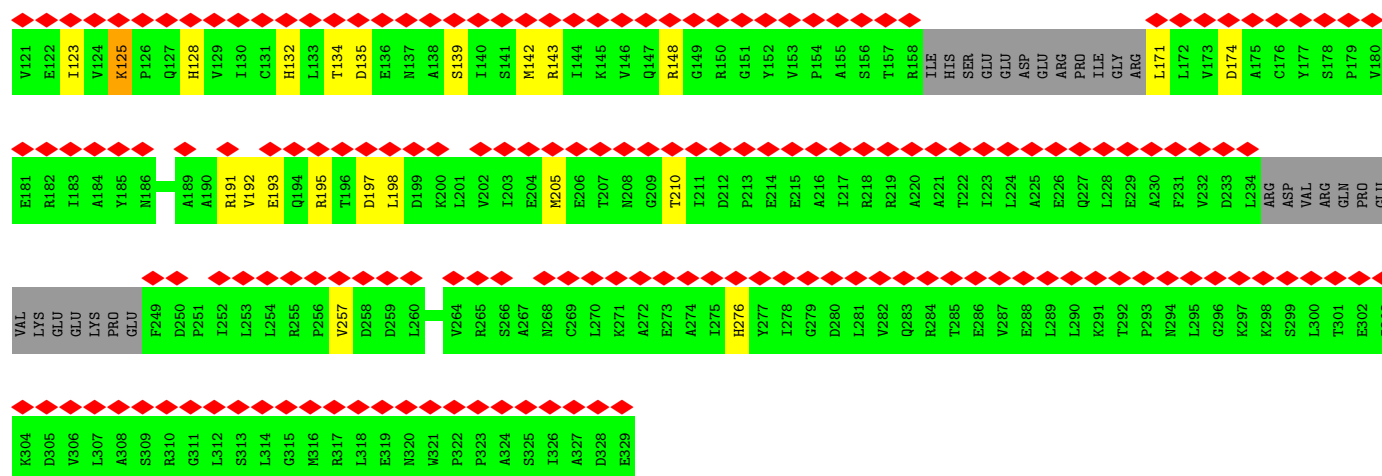
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

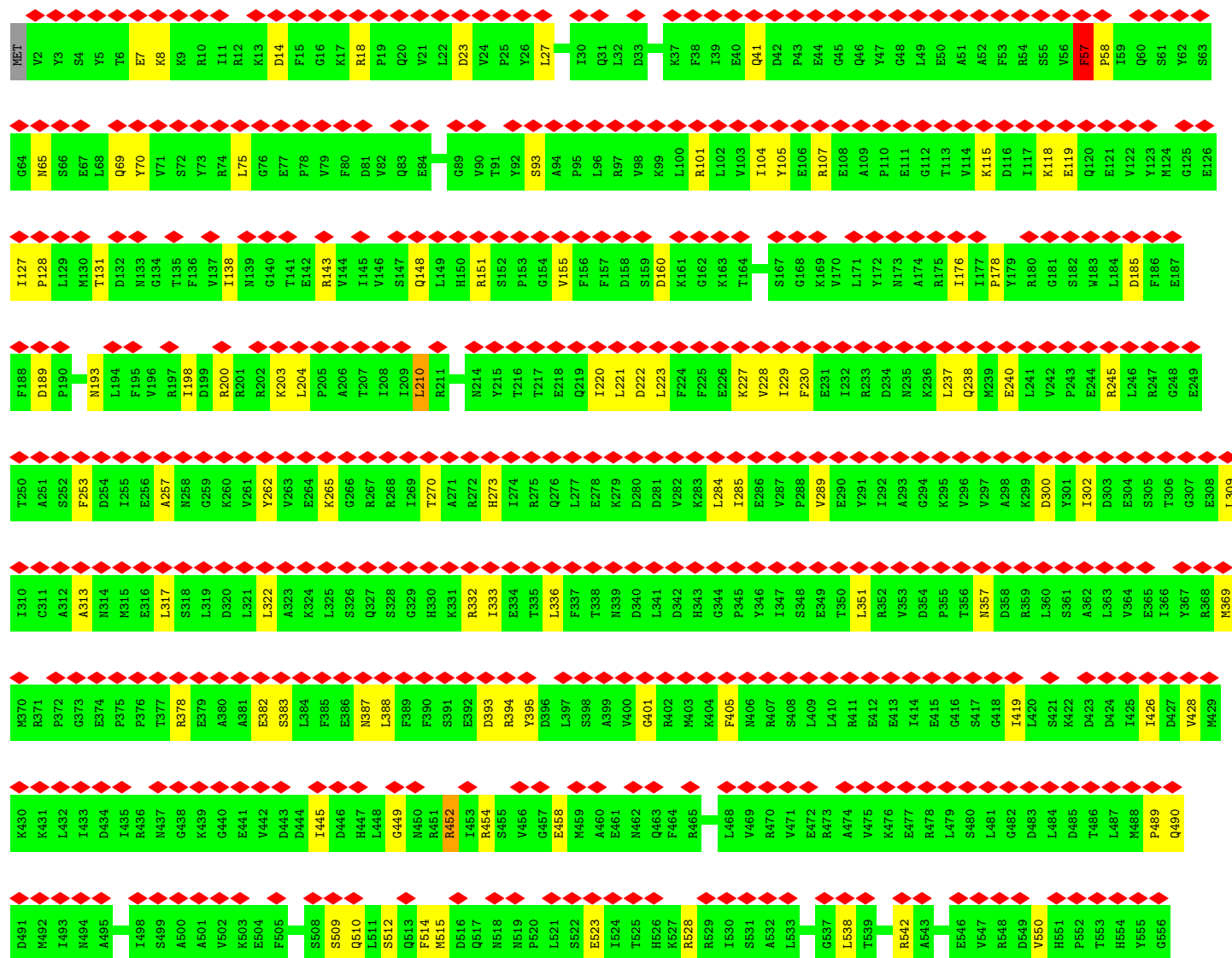
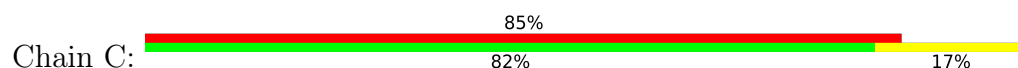


- Molecule 1: DNA-directed RNA polymerase subunit alpha



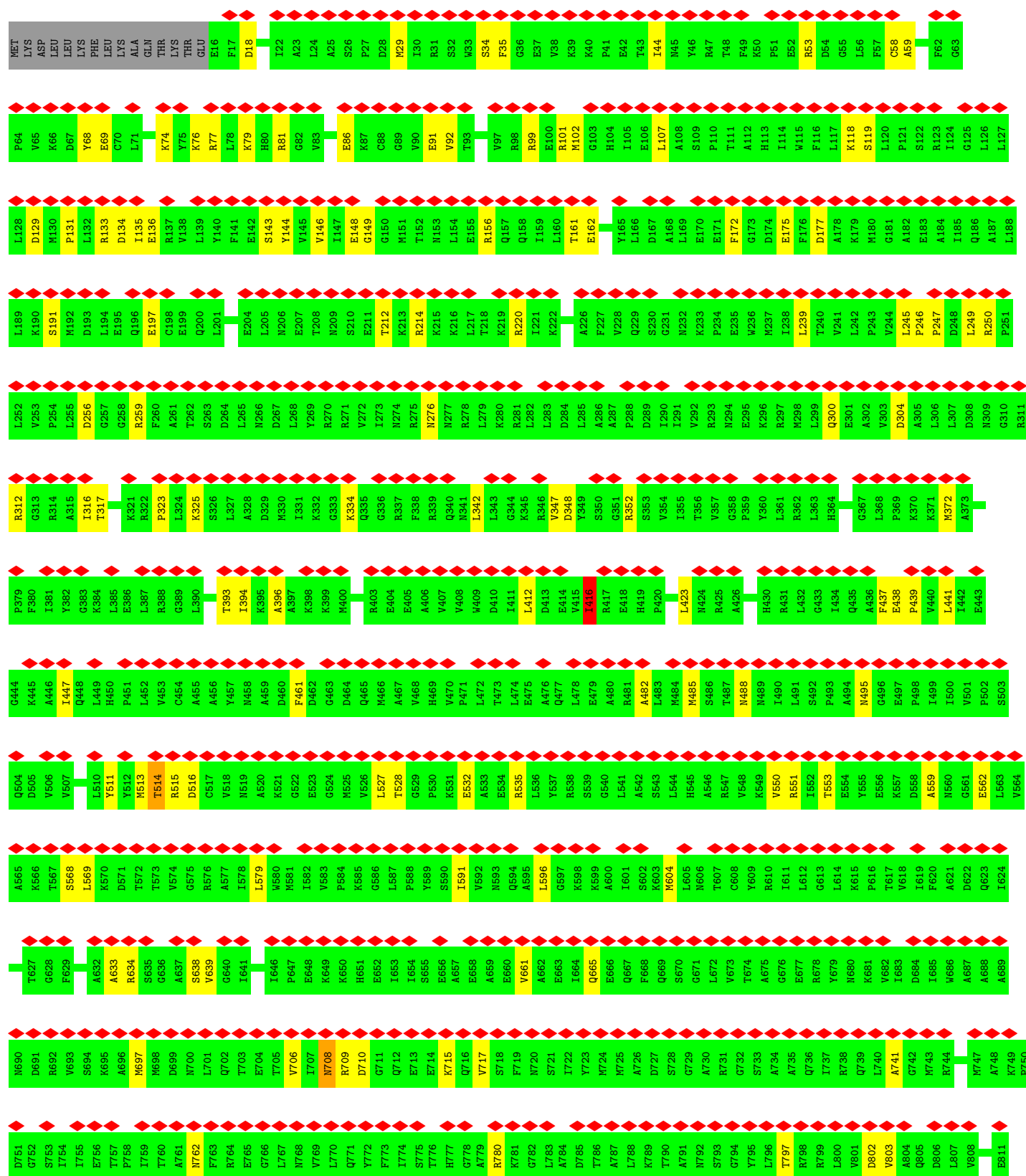
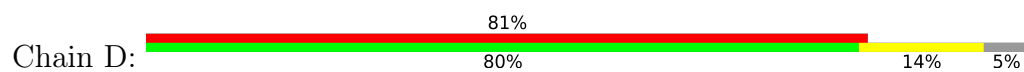


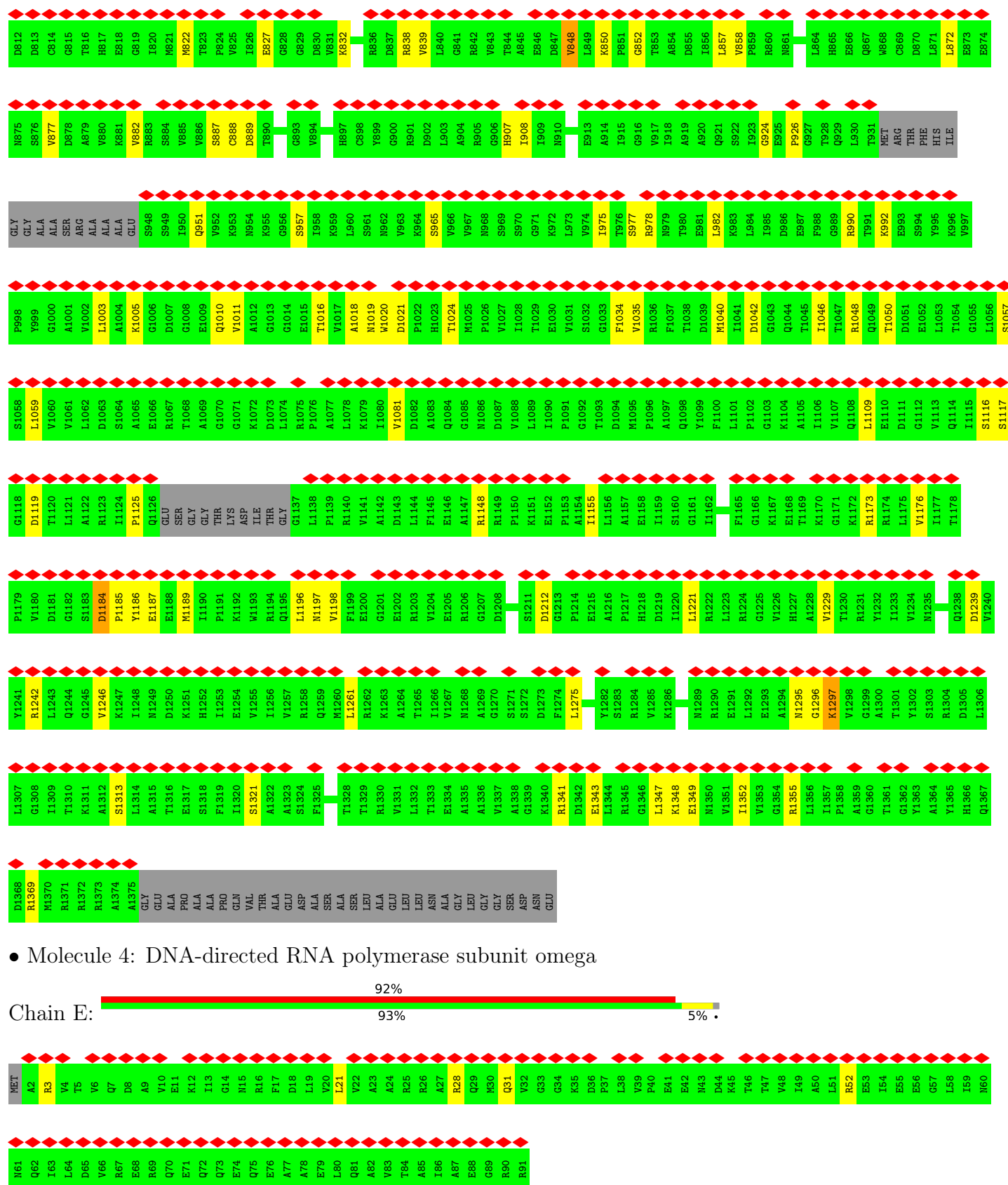
• Molecule 2: DNA-directed RNA polymerase subunit beta



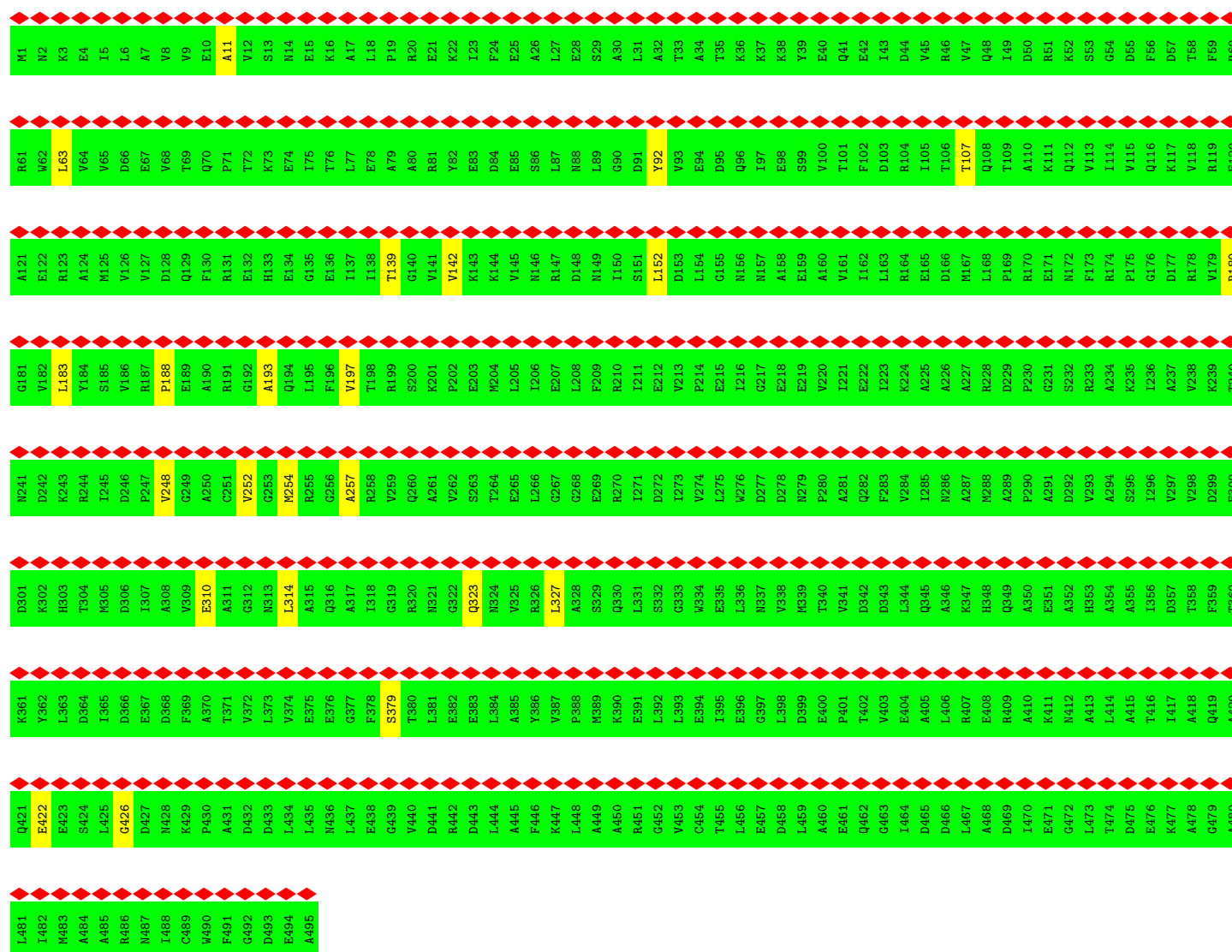
M1304	Y1305	K1306	M1307	I1308	V1309	D1310	G1311	N1312	H1313	Q1314	M1315	P1320	E1321	S1322	P1323	N1324	V1325	L1326	L1327	K1328	E1329	I1330	R1331	S1332	L1333	G1334	I1335	N1336	I1337	E1338	L1339	E1340	D1341	E1342																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
K1242	M1243	H1244	A1245	R1246	S1247	T1248	G1249	S1250	Y1251	L1253	V1254	T1255	Q1256	P1257	P1258	L1259	G1260	G1261	K1262	A1263	Q1264	F1265	G1266	G1267	Q1268	R1269	F1270	I1271	E1272	M1273	E1274	V1275	A1276	L1277	L1278	E1279	A1280	Y1281	G1282	A1283	A1284																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
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- Molecule 3: DNA-directed RNA polymerase subunit beta'

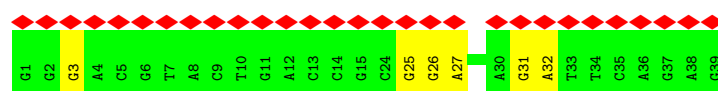
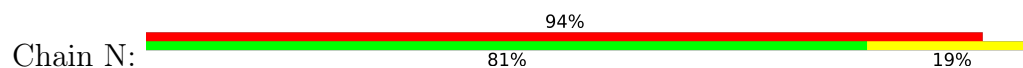




- Molecule 5: Transcription termination/antitermination protein NusA



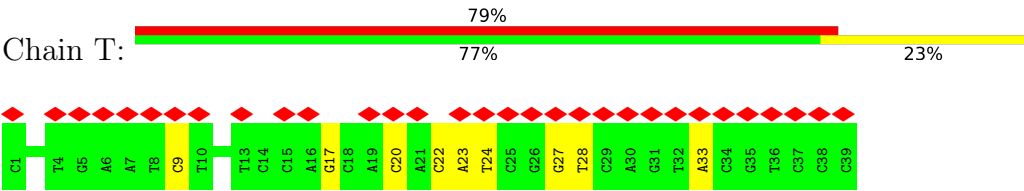
• Molecule 6: DNA (31-MER)



• Molecule 7: RNA (5'-R(*CP*CP*UP*GP*AP*UP*CP*AP*GP*GP*CP*GP*AP*UP*GP*UP*GP*UP*GP*CP*U)-3')



● Molecule 8: DNA (39-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	157100	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 ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.869	Depositor
Minimum map value	-1.326	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.086	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	308.0, 308.0, 308.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.63	0/2189	0.76	1/2981 (0.0%)
1	B	0.58	0/2086	0.83	1/2841 (0.0%)
2	C	0.74	1/10742 (0.0%)	0.81	6/14494 (0.0%)
3	D	0.69	0/10514	0.80	2/14199 (0.0%)
4	E	0.55	0/711	0.70	0/956
5	F	0.23	0/2446	0.63	2/3406 (0.1%)
6	N	0.43	0/728	0.57	0/1121
7	R	0.49	0/494	0.70	0/766
8	T	0.55	0/876	0.61	0/1346
All	All	0.66	1/30786 (0.0%)	0.78	12/42110 (0.0%)

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
1	A	0	4
1	B	0	4
2	C	0	4
3	D	0	5
5	F	0	1
All	All	0	18

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1084	ASP	C-N	-15.66	1.08	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	135	ILE	N-CA-C	-8.60	104.36	112.96
2	C	1084	ASP	CA-C-N	7.11	130.59	120.49
2	C	1084	ASP	C-N-CA	7.11	130.59	120.49
2	C	910	ALA	CA-C-N	5.92	132.35	121.70
2	C	910	ALA	C-N-CA	5.92	132.35	121.70
5	F	11	ALA	CA-C-N	5.74	132.03	121.70
5	F	11	ALA	C-N-CA	5.74	132.03	121.70
2	C	41	GLN	CA-C-N	5.70	141.75	121.59
2	C	41	GLN	C-N-CA	5.70	141.75	121.59
1	B	13	LEU	CA-CB-CG	5.28	134.76	116.30
3	D	982	LEU	CA-CB-CG	5.16	134.37	116.30
1	A	150	ARG	NE-CZ-NH1	-5.11	116.39	121.50

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	ARG	Peptide
1	A	29	GLU	Peptide
1	A	319	GLU	Peptide
1	A	321	TRP	Peptide
1	B	134	THR	Peptide
1	B	19	VAL	Peptide
1	B	192	VAL	Peptide
1	B	29	GLU	Peptide
2	C	198	ILE	Peptide
2	C	57	PHE	Peptide
2	C	909	LYS	Peptide
2	C	910	ALA	Peptide
3	D	1184	ASP	Peptide
3	D	119	SER	Peptide
3	D	1297	LYS	Peptide
3	D	416	ILE	Peptide
3	D	53	ARG	Peptide
5	F	379	SER	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	2168	0	1960	31	0
1	B	2068	0	1867	26	0
2	C	10573	0	10584	151	0
3	D	10357	0	10571	138	0
4	E	709	0	719	7	0
5	F	2447	0	1180	11	0
6	N	647	0	347	6	0
7	R	444	0	228	9	0
8	T	785	0	440	8	0
9	D	1	0	0	0	0
10	D	2	0	0	0	0
All	All	30201	0	27896	347	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 (347) 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)
2:C:393:ASP:OD2	2:C:394:ARG:NH1	1.90	1.04
3:D:1341:ARG:NH1	3:D:1343:GLU:OE2	1.98	0.97
3:D:129:ASP:OD2	3:D:220:ARG:NH1	1.98	0.96
1:A:33:ARG:NH1	1:A:199:ASP:OD2	2.02	0.91
3:D:832:LYS:HZ2	3:D:1242:ARG:HH12	1.12	0.90
3:D:68:TYR:OH	3:D:81:ARG:NH1	2.05	0.89
3:D:256:ASP:O	3:D:259:ARG:NH1	2.08	0.87
2:C:452:ARG:NH1	2:C:584:TYR:O	2.08	0.87
2:C:185:ASP:OD2	2:C:200:ARG:NH2	2.07	0.86
2:C:841:ARG:HH12	3:D:259:ARG:NH1	1.74	0.85
2:C:611:GLU:OE2	2:C:637:ARG:NH2	2.12	0.83
3:D:832:LYS:NZ	3:D:1242:ARG:HH12	1.78	0.82
3:D:91:GLU:OE2	3:D:101:ARG:NH2	2.12	0.81
1:A:150:ARG:HH12	1:B:8:PHE:HD1	1.29	0.81
1:A:45:ARG:NH1	2:C:1083:GLU:OE1	2.18	0.77
2:C:452:ARG:NH2	2:C:458:GLU:OE2	2.17	0.77
1:B:60:GLU:OE2	1:B:171:LEU:N	2.18	0.77
3:D:300:GLN:NE2	3:D:304:ASP:OD2	2.20	0.75
3:D:832:LYS:HZ2	3:D:1242:ARG:NH1	1.85	0.73
3:D:1021:ASP:OD2	3:D:1024:THR:OG1	2.07	0.73
3:D:802:ASP:OD1	3:D:1348:LYS:NZ	2.17	0.73
2:C:1314:GLN:HB2	4:E:28:ARG:HH12	1.52	0.72
2:C:563:THR:HG21	3:D:780:ARG:HH12	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:990:ARG:HD2	3:D:992:LYS:HZ3	1.54	0.71
3:D:77:ARG:HG2	3:D:79:LYS:H	1.56	0.71
1:A:60:GLU:OE2	1:A:170:ARG:NE	2.19	0.70
2:C:383:SER:O	2:C:387:ASN:HB2	1.92	0.70
2:C:1069:ARG:NH2	2:C:1114:GLU:OE2	2.20	0.69
3:D:1355:ARG:HH12	3:D:1369:ARG:HH22	1.42	0.67
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.77	0.67
3:D:316:ILE:HB	3:D:323:PRO:HA	1.77	0.66
3:D:709:ARG:NH1	3:D:710:ASP:OD2	2.30	0.65
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.79	0.65
2:C:841:ARG:NH1	3:D:259:ARG:NH1	2.44	0.64
3:D:528:THR:N	3:D:532:GLU:OE2	2.28	0.64
3:D:741:ALA:O	3:D:762:ASN:ND2	2.28	0.64
3:D:857:LEU:HD12	3:D:858:VAL:HG13	1.80	0.64
1:B:90:VAL:HG12	1:B:123:ILE:HG12	1.80	0.64
3:D:1148:ARG:NH1	6:N:27:DA:O3'	2.31	0.64
3:D:58:CYS:SG	3:D:59:ALA:N	2.72	0.63
1:A:164:ASP:HA	1:A:166:ARG:HE	1.63	0.63
1:B:104:LYS:NZ	1:B:114:ASP:OD2	2.20	0.63
2:C:1072:ASN:ND2	2:C:1111:GLN:OE1	2.32	0.62
3:D:156:ARG:NH1	3:D:191:SER:OG	2.31	0.62
1:A:92:VAL:HG12	1:A:121:VAL:HG22	1.81	0.62
3:D:559:ALA:HB3	3:D:562:GLU:HB3	1.81	0.62
1:A:125:LYS:HE2	1:A:127:GLN:HB2	1.82	0.62
2:C:270:THR:H	2:C:273:HIS:HD2	1.48	0.62
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.81	0.62
2:C:841:ARG:HH12	3:D:259:ARG:HH12	1.48	0.61
2:C:229:ILE:HD12	2:C:332:ARG:HH11	1.63	0.61
5:F:142:VAL:HA	5:F:152:LEU:HA	1.81	0.61
2:C:228:VAL:HG22	2:C:245:ARG:HH11	1.66	0.61
1:B:75:GLN:HE22	1:B:132:HIS:HB2	1.65	0.61
2:C:706:ARG:NH2	2:C:793:GLU:OE2	2.33	0.60
2:C:914:LYS:NZ	7:R:17:G:O3'	2.34	0.60
1:B:78:ILE:HD13	1:B:81:ILE:HD13	1.83	0.60
3:D:1355:ARG:HH11	3:D:1369:ARG:HH12	1.49	0.60
2:C:1268:GLN:HE22	3:D:352:ARG:HH11	1.48	0.60
2:C:253:PHE:HA	2:C:265:LYS:HZ2	1.66	0.59
2:C:7:GLU:HG2	2:C:706:ARG:NH1	2.17	0.59
2:C:510:GLN:NE2	7:R:25:G:OP1	2.36	0.59
3:D:1116:SER:N	3:D:1119:ASP:OD2	2.33	0.59
2:C:18:ARG:O	2:C:1156:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:GLU:HG2	1:A:30:PRO:HD3	1.85	0.59
2:C:27:LEU:O	2:C:528:ARG:NH1	2.35	0.59
6:N:31:DG:N2	8:T:9:DC:O2	2.36	0.59
2:C:57:PHE:HD2	2:C:70:TYR:HB2	1.68	0.58
2:C:65:ASN:HB2	2:C:107:ARG:NH1	2.18	0.58
2:C:914:LYS:HZ1	7:R:18:G:P	2.25	0.58
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.37	0.58
1:B:92:VAL:O	1:B:148:ARG:NH2	2.37	0.58
2:C:1142:ARG:NH2	2:C:1165:SER:O	2.36	0.57
2:C:1311:GLY:O	4:E:31:GLN:NE2	2.37	0.57
3:D:1048:ARG:NH2	3:D:1057:SER:O	2.38	0.57
1:A:60:GLU:OE1	1:A:143:ARG:NH2	2.38	0.57
2:C:237:LEU:HD21	2:C:289:VAL:HG23	1.87	0.57
4:E:3:ARG:HH21	4:E:52:ARG:HG2	1.69	0.57
5:F:63:LEU:HA	5:F:92:TYR:HA	1.87	0.57
3:D:822:MET:SD	3:D:838:ARG:NH2	2.78	0.56
1:B:101:THR:HG22	1:B:143:ARG:HG2	1.88	0.56
2:C:1252:SER:OG	2:C:1253:LEU:N	2.36	0.56
3:D:827:GLU:HB3	3:D:832:LYS:HD2	1.86	0.56
3:D:888:CYS:SG	3:D:889:ASP:N	2.78	0.56
3:D:372:MET:HE1	3:D:447:ILE:HD11	1.88	0.56
3:D:638:SER:OG	3:D:639:VAL:N	2.39	0.56
3:D:872:LEU:HD12	3:D:877:VAL:HG11	1.88	0.56
2:C:75:LEU:HD21	2:C:127:ILE:HD11	1.88	0.55
2:C:1246:ARG:NH1	2:C:1258:PRO:HB3	2.20	0.55
3:D:848:VAL:HG22	3:D:858:VAL:HG22	1.87	0.55
1:B:195:ARG:HD2	1:B:198:LEU:HD11	1.89	0.55
2:C:813:GLU:HB2	3:D:461:PHE:HD2	1.72	0.55
3:D:334:LYS:HE3	8:T:17:DG:OP2	2.07	0.55
3:D:591:ILE:HD11	3:D:604:MET:HA	1.89	0.55
3:D:1196:LEU:HD23	3:D:1198:VAL:H	1.71	0.55
2:C:626:GLU:OE1	2:C:628:HIS:ND1	2.40	0.54
2:C:1336:ASN:ND2	3:D:29:MET:SD	2.81	0.54
3:D:416:ILE:HG23	3:D:439:PRO:HG2	1.90	0.54
3:D:977:SER:OG	3:D:978:ARG:N	2.39	0.54
2:C:1080:ASN:HD22	2:C:1085:MET:HE3	1.72	0.54
2:C:528:ARG:NH2	2:C:576:SER:O	2.35	0.54
2:C:638:SER:OG	2:C:639:LYS:N	2.40	0.54
3:D:197:GLU:OE2	3:D:220:ARG:NH2	2.40	0.54
3:D:438:GLU:HG3	3:D:485:MET:HE1	1.90	0.54
2:C:1254:VAL:O	3:D:99:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:PRO:HG2	1:A:170:ARG:HD3	1.91	0.53
1:B:115:ILE:HG21	1:B:123:ILE:HD12	1.90	0.53
3:D:1355:ARG:NH1	3:D:1369:ARG:HH12	2.05	0.53
2:C:221:LEU:HD21	2:C:336:LEU:HD11	1.90	0.53
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.91	0.53
2:C:1250:SER:OG	7:R:19:C:O2	2.27	0.53
3:D:1321:SER:HB2	3:D:1349:GLU:OE2	2.09	0.53
2:C:589:THR:OG1	2:C:659:GLN:NE2	2.40	0.53
2:C:230:PHE:HB2	2:C:333:ILE:HB	1.90	0.52
2:C:767:GLN:HB3	2:C:784:ALA:HB1	1.90	0.52
2:C:160:ASP:OD1	2:C:160:ASP:N	2.40	0.52
2:C:808:ASN:H	3:D:633:ALA:HB2	1.74	0.52
2:C:866:ASP:OD1	2:C:869:GLY:N	2.42	0.52
3:D:1003:LEU:HD23	3:D:1018:ALA:HB2	1.91	0.52
2:C:735:LYS:HA	2:C:748:ILE:HG22	1.91	0.52
2:C:257:ALA:HB3	2:C:262:TYR:HE2	1.74	0.52
3:D:1050:THR:HA	3:D:1057:SER:HA	1.90	0.52
2:C:210:LEU:HD12	2:C:220:ILE:HG12	1.90	0.52
2:C:302:ILE:HA	2:C:309:LEU:HA	1.91	0.52
3:D:1184:ASP:O	3:D:1186:TYR:N	2.40	0.52
3:D:393:THR:HG23	3:D:396:ALA:H	1.75	0.52
2:C:222:ASP:CG	2:C:227:LYS:HZ3	2.17	0.51
2:C:1042:LEU:HD13	2:C:1046:VAL:HG13	1.92	0.51
2:C:1246:ARG:HH21	2:C:1249:GLY:H	1.57	0.51
5:F:139:THR:HA	5:F:180:ARG:HA	1.91	0.51
3:D:516:ASP:OD1	3:D:516:ASP:N	2.41	0.51
2:C:138:ILE:HD12	2:C:143:ARG:HG3	1.93	0.51
3:D:832:LYS:NZ	3:D:1242:ARG:NH1	2.51	0.51
1:A:186:ASN:N	1:A:186:ASN:OD1	2.44	0.51
2:C:148:GLN:OE1	2:C:454:ARG:NH1	2.44	0.51
1:B:191:ARG:NH2	1:B:193:GLU:O	2.44	0.51
1:B:48:LEU:HD11	3:D:535:ARG:HG3	1.93	0.51
2:C:69:GLN:HE21	2:C:101:ARG:CZ	2.24	0.50
2:C:804:PHE:HE1	2:C:1098:LEU:HD12	1.75	0.50
1:A:13:LEU:HD11	1:A:16:ILE:HD11	1.93	0.50
3:D:148:GLU:OE1	3:D:156:ARG:NH2	2.44	0.50
3:D:1221:LEU:HD12	3:D:1229:VAL:HG11	1.94	0.50
2:C:151:ARG:HE	2:C:445:ILE:HG21	1.76	0.50
3:D:706:VAL:HG12	3:D:715:LYS:HG2	1.92	0.50
2:C:18:ARG:HH21	2:C:620:ASN:HA	1.75	0.50
3:D:393:THR:OG1	3:D:394:ILE:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:THR:O	1:A:160:HIS:ND1	2.41	0.50
2:C:959:ASP:OD1	2:C:960:LEU:N	2.45	0.50
3:D:146:VAL:HG12	3:D:149:GLY:H	1.77	0.50
3:D:957:SER:HB3	3:D:1010:GLN:HE22	1.75	0.50
3:D:143:SER:OG	3:D:144:TYR:N	2.45	0.50
2:C:449:GLY:HA3	2:C:609:ILE:HG23	1.94	0.50
2:C:542:ARG:NH2	6:N:25:DG:OP2	2.42	0.50
3:D:514:THR:HG21	3:D:596:LEU:HD12	1.93	0.50
3:D:850:LYS:HG2	3:D:852:GLY:H	1.77	0.50
3:D:69:GLU:HG2	3:D:76:LYS:HG2	1.93	0.49
3:D:511:TYR:OH	3:D:515:ARG:NH1	2.45	0.49
2:C:864:LYS:HB3	2:C:871:VAL:HG23	1.94	0.49
2:C:14:ASP:OD1	2:C:1157:GLN:HB2	2.12	0.49
2:C:452:ARG:HG3	2:C:452:ARG:HH11	1.77	0.49
3:D:803:VAL:HG23	3:D:1313:SER:HB3	1.94	0.49
5:F:323:GLN:O	5:F:327:LEU:CB	2.60	0.49
2:C:1313:HIS:HD2	4:E:31:GLN:HE22	1.60	0.49
3:D:1005:LYS:NZ	3:D:1011:VAL:HA	2.28	0.49
3:D:495:ASN:OD1	3:D:495:ASN:N	2.42	0.49
3:D:1019:ASN:HD22	3:D:1020:TRP:H	1.60	0.49
2:C:1313:HIS:CD2	4:E:31:GLN:HE22	2.31	0.49
3:D:907:HIS:ND1	3:D:908:ILE:O	2.39	0.49
3:D:1024:THR:HG22	3:D:1125:PRO:HA	1.94	0.49
2:C:101:ARG:HD3	2:C:118:LYS:HE2	1.95	0.49
2:C:509:SER:OG	2:C:510:GLN:N	2.46	0.49
2:C:1165:SER:HB2	2:C:1168:GLU:H	1.78	0.48
2:C:930:ASP:OD2	2:C:932:GLN:NE2	2.42	0.48
5:F:183:LEU:HA	5:F:197:VAL:HA	1.95	0.48
2:C:1142:ARG:HE	2:C:1169:VAL:HG21	1.77	0.48
3:D:1040:MET:HB3	3:D:1046:ILE:HD13	1.94	0.48
6:N:3:DG:OP2	6:N:3:DG:H2'	2.14	0.48
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.95	0.48
2:C:1219:GLU:OE1	3:D:634:ARG:NH1	2.44	0.48
3:D:550:VAL:O	3:D:569:LEU:HA	2.14	0.47
1:A:68:TYR:HB3	2:C:756:TYR:HD2	1.78	0.47
3:D:1034:PHE:HB2	3:D:1081:VAL:O	2.14	0.47
2:C:731:ARG:HH21	2:C:750:ILE:HD11	1.79	0.47
1:A:223:ILE:HG12	1:B:8:PHE:HZ	1.80	0.47
3:D:172:PHE:HB3	3:D:175:GLU:OE2	2.15	0.47
8:T:23:DA:H2'	8:T:24:DT:H71	1.96	0.47
1:A:135:ASP:HB3	1:A:138:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1146:GLN:HE21	2:C:1161:LEU:HB2	1.79	0.47
2:C:979:LEU:HD21	2:C:1000:LEU:HD23	1.97	0.47
3:D:118:LYS:NZ	3:D:312:ARG:HH11	2.12	0.47
5:F:248:VAL:O	5:F:252:VAL:CB	2.62	0.47
3:D:423:LEU:HD13	3:D:437:PHE:HD2	1.80	0.47
2:C:802:VAL:HG23	2:C:1096:ILE:HB	1.96	0.47
3:D:1197:ASN:ND2	3:D:1212:ASP:OD2	2.48	0.47
2:C:1279:GLU:OE2	3:D:1347:LEU:HB3	2.15	0.47
2:C:1321:GLU:OE2	3:D:99:ARG:NH2	2.48	0.47
2:C:119:GLU:OE1	2:C:490:GLN:N	2.47	0.46
2:C:512:SER:O	2:C:512:SER:OG	2.33	0.46
5:F:310:GLU:O	5:F:314:LEU:N	2.47	0.46
1:A:174:ASP:OD1	1:A:174:ASP:N	2.43	0.46
2:C:357:ASN:OD1	2:C:357:ASN:N	2.48	0.46
2:C:228:VAL:HG22	2:C:245:ARG:NH1	2.31	0.46
2:C:238:GLN:HE21	2:C:284:LEU:HD21	1.81	0.46
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.49	0.46
3:D:1295:ASN:OD1	3:D:1297:LYS:N	2.48	0.46
3:D:246:PRO:O	3:D:250:ARG:NH1	2.49	0.46
3:D:1173:ARG:O	3:D:1189:MET:HA	2.16	0.46
2:C:733:VAL:HG22	2:C:750:ILE:HG13	1.98	0.46
2:C:222:ASP:OD1	2:C:227:LYS:NZ	2.46	0.45
3:D:342:LEU:HD23	3:D:1352:ILE:HG23	1.96	0.45
2:C:189:ASP:OD2	2:C:193:ASN:HB2	2.16	0.45
3:D:1005:LYS:HZ3	3:D:1011:VAL:HG12	1.82	0.45
1:B:135:ASP:N	1:B:135:ASP:OD1	2.48	0.45
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.98	0.45
3:D:149:GLY:HA3	3:D:177:ASP:H	1.82	0.45
1:A:47:LEU:HD13	1:A:220:ALA:HB2	1.98	0.45
1:A:66:HIS:HD2	1:A:68:TYR:HB2	1.82	0.45
2:C:563:THR:HG21	3:D:780:ARG:NH1	2.27	0.45
3:D:325:LYS:NZ	7:R:22:U:OP1	2.49	0.45
2:C:562:GLU:OE1	2:C:662:SER:OG	2.30	0.45
3:D:161:THR:OG1	3:D:162:GLU:N	2.50	0.45
1:A:102:LEU:HD23	1:A:115:ILE:HD13	1.98	0.45
3:D:1005:LYS:HZ3	3:D:1011:VAL:HA	1.82	0.45
3:D:990:ARG:CD	3:D:992:LYS:HZ3	2.27	0.44
2:C:712:SER:OG	2:C:713:GLY:N	2.43	0.44
2:C:799:ASN:HB3	2:C:1231:TYR:HD1	1.82	0.44
3:D:926:PRO:HB3	3:D:1246:VAL:HG11	1.98	0.44
3:D:1005:LYS:NZ	3:D:1011:VAL:HG12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:254:MET:O	5:F:257:ALA:HB2	2.17	0.44
1:B:83:LEU:HD11	3:D:528:THR:HA	2.00	0.44
2:C:1268:GLN:NE2	3:D:352:ARG:HH11	2.15	0.44
3:D:528:THR:HG23	3:D:532:GLU:OE2	2.17	0.44
3:D:661:VAL:O	3:D:665:GLN:N	2.50	0.44
2:C:23:ASP:N	2:C:23:ASP:OD1	2.47	0.44
2:C:104:ILE:HD13	2:C:115:LYS:HB3	1.98	0.44
2:C:538:LEU:H	2:C:538:LEU:HD23	1.82	0.44
2:C:632:ASP:OD1	2:C:632:ASP:N	2.38	0.44
2:C:203:LYS:NZ	8:T:9:DC:OP2	2.49	0.44
1:A:231:PHE:HE1	1:B:28:LEU:HD13	1.83	0.44
3:D:697:MET:HE3	3:D:697:MET:HB2	1.86	0.44
2:C:176:ILE:HD11	2:C:428:VAL:HG11	2.00	0.44
2:C:942:ASP:OD2	2:C:944:ARG:HB3	2.18	0.44
3:D:708:ASN:OD1	3:D:708:ASN:N	2.37	0.44
2:C:189:ASP:OD1	2:C:189:ASP:N	2.49	0.44
3:D:245:LEU:O	3:D:250:ARG:NH1	2.51	0.44
1:B:61:ILE:HG23	1:B:142:MET:HE3	2.00	0.43
2:C:229:ILE:HB	2:C:240:GLU:OE2	2.17	0.43
2:C:270:THR:H	2:C:273:HIS:CD2	2.30	0.43
2:C:1033:ARG:O	2:C:1037:THR:OG1	2.29	0.43
2:C:1247:SER:OG	2:C:1248:THR:N	2.50	0.43
3:D:513:MET:HE3	3:D:579:LEU:HB2	2.00	0.43
2:C:378:ARG:NE	2:C:382:GLU:OE2	2.51	0.43
3:D:551:ARG:HA	3:D:568:SER:O	2.19	0.43
2:C:317:LEU:HD13	2:C:322:LEU:HD11	1.99	0.43
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.83	0.43
3:D:568:SER:OG	3:D:569:LEU:N	2.52	0.43
8:T:22:DC:H2''	8:T:23:DA:H8	1.83	0.43
3:D:131:PRO:HG2	3:D:134:ASP:OD2	2.18	0.43
3:D:247:PRO:HA	3:D:250:ARG:NH1	2.33	0.43
6:N:31:DG:H2''	6:N:32:DA:H5''	2.00	0.43
3:D:951:GLN:HA	3:D:1016:THR:HA	2.00	0.43
1:B:125:LYS:HZ3	1:B:128:HIS:HB2	1.83	0.43
2:C:223:LEU:HD21	2:C:426:ILE:HD13	2.00	0.43
2:C:934:PHE:O	2:C:1048:LYS:HA	2.18	0.43
3:D:107:LEU:HA	3:D:276:ASN:HD21	1.83	0.43
7:R:23:G:H2'	7:R:24:U:C6	2.53	0.43
1:B:197:ASP:OD1	1:B:197:ASP:N	2.51	0.43
3:D:1042:ASP:HA	3:D:1046:ILE:HG13	2.00	0.43
4:E:3:ARG:HD3	4:E:3:ARG:HA	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:988:LYS:HZ3	2:C:991:LYS:HZ1	1.65	0.43
2:C:1030:GLU:OE2	2:C:1033:ARG:NH2	2.52	0.43
3:D:1035:VAL:HG21	3:D:1109:LEU:HD21	2.00	0.43
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.86	0.42
1:B:20:SER:OG	1:B:21:SER:N	2.52	0.42
2:C:143:ARG:NH1	2:C:514:PHE:HE1	2.17	0.42
7:R:25:G:H5'	7:R:26:U:OP2	2.19	0.42
8:T:33:DA:OP2	8:T:33:DA:H2'	2.19	0.42
1:A:176:CYS:O	1:A:178:SER:N	2.52	0.42
3:D:717:VAL:H	3:D:717:VAL:HG22	1.59	0.42
5:F:422:GLU:O	5:F:426:GLY:N	2.52	0.42
2:C:401:GLY:O	2:C:405:PHE:HB2	2.20	0.42
2:C:714:VAL:HB	2:C:787:PRO:HD2	2.01	0.42
3:D:214:ARG:HH12	3:D:1275:LEU:HD22	1.84	0.42
6:N:26:DG:H2''	6:N:27:DA:C8	2.54	0.42
3:D:316:ILE:HG13	3:D:317:THR:H	1.84	0.42
3:D:965:SER:HA	3:D:975:ILE:HA	2.02	0.42
3:D:1116:SER:OG	3:D:1117:SER:N	2.52	0.42
7:R:20:G:H2'	7:R:21:A:C8	2.54	0.42
1:A:197:ASP:OD1	1:A:197:ASP:N	2.41	0.42
1:B:257:VAL:N	1:B:276:HIS:O	2.34	0.42
2:C:515:MET:HE2	2:C:523:GLU:HG2	2.01	0.42
1:A:22:THR:OG1	1:A:207:THR:O	2.34	0.42
1:A:35:PHE:HE1	1:B:46:ILE:HD13	1.83	0.42
1:B:205:MET:HB2	1:B:205:MET:HE3	1.73	0.42
1:A:212:ASP:OD1	1:A:212:ASP:N	2.39	0.42
2:C:119:GLU:OE2	2:C:490:GLN:HB2	2.19	0.42
3:D:74:LYS:NZ	3:D:86:GLU:HG3	2.35	0.42
3:D:527:LEU:HD22	3:D:532:GLU:HG3	2.02	0.42
1:B:91:ARG:NH1	1:B:210:THR:O	2.53	0.41
2:C:801:ARG:HG2	2:C:1229:TYR:CE1	2.55	0.41
4:E:21:LEU:HD12	4:E:21:LEU:HA	1.85	0.41
2:C:119:GLU:HB2	2:C:489:PRO:HD2	2.02	0.41
7:R:15:C:H2'	7:R:16:A:H8	1.84	0.41
2:C:93:SER:HA	2:C:128:PRO:HA	2.02	0.41
2:C:1262:LYS:NZ	2:C:1262:LYS:HB3	2.35	0.41
3:D:1196:LEU:HD21	3:D:1198:VAL:HG12	2.02	0.41
1:A:82:LEU:HD11	1:A:171:LEU:HD23	2.02	0.41
1:A:104:LYS:HG2	1:A:110:VAL:HG22	2.02	0.41
1:B:86:LYS:HE2	1:B:174:ASP:HB2	2.02	0.41
2:C:1196:LYS:HD2	2:C:1206:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:27:DG:H2"	8:T:28:DT:OP2	2.20	0.41
1:B:104:LYS:O	1:B:139:SER:HA	2.20	0.41
2:C:1246:ARG:HH12	2:C:1258:PRO:HB3	1.85	0.41
2:C:1255:THR:O	2:C:1257:GLN:N	2.54	0.41
2:C:151:ARG:HH21	2:C:445:ILE:HG12	1.86	0.41
2:C:800:MET:HE3	2:C:800:MET:HB2	1.79	0.41
2:C:1325:VAL:HG22	3:D:249:LEU:HD11	2.02	0.41
3:D:34:SER:OG	3:D:35:PHE:N	2.53	0.41
3:D:1176:VAL:HG22	3:D:1187:GLU:HG2	2.03	0.41
3:D:1355:ARG:NH1	3:D:1369:ARG:HH22	2.11	0.41
2:C:1066:MET:SD	2:C:1076:ILE:HD11	2.61	0.41
1:A:102:LEU:O	1:A:141:SER:HA	2.21	0.41
2:C:454:ARG:HH11	2:C:454:ARG:HD2	1.65	0.41
3:D:887:SER:O	3:D:887:SER:OG	2.37	0.41
3:D:1046:ILE:HB	3:D:1059:LEU:HD21	2.02	0.41
2:C:204:LEU:HD22	2:C:369:MET:HE1	2.02	0.41
2:C:300:ASP:OD1	2:C:313:ALA:N	2.54	0.41
2:C:906:PHE:HE2	5:F:107:THR:HA	1.85	0.41
2:C:1261:GLY:HA2	8:T:20:DC:OP2	2.20	0.41
3:D:347:VAL:HG12	3:D:348:ASP:O	2.21	0.41
3:D:412:LEU:HD22	3:D:441:LEU:HD21	2.02	0.41
2:C:624:ASP:OD1	2:C:624:ASP:N	2.54	0.41
3:D:553:THR:O	3:D:553:THR:OG1	2.30	0.41
2:C:8:LYS:HG3	2:C:1164:PHE:HE1	1.86	0.40
2:C:1005:GLU:HB3	2:C:1007:LYS:H	1.85	0.40
2:C:1122:LYS:HG2	2:C:1229:TYR:CZ	2.56	0.40
2:C:302:ILE:HG13	2:C:309:LEU:HB3	2.03	0.40
2:C:1326:LEU:HD12	2:C:1326:LEU:HA	1.84	0.40
3:D:482:ALA:O	3:D:488:ASN:ND2	2.55	0.40
3:D:1295:ASN:OD1	3:D:1296:GLY:N	2.55	0.40
2:C:1341:ASP:OD1	3:D:18:ASP:HB2	2.21	0.40
3:D:102:MET:HB2	3:D:102:MET:HE3	1.86	0.40
5:F:188:PRO:HA	5:F:193:ALA:HB2	2.04	0.40
2:C:178:PRO:HB3	2:C:395:TYR:CZ	2.56	0.40
2:C:222:ASP:HA	2:C:227:LYS:NZ	2.37	0.40
3:D:133:ARG:O	3:D:136:GLU:HB2	2.22	0.40
1:A:165:GLU:OE2	1:A:170:ARG:HG2	2.22	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	306/329 (93%)	262 (86%)	44 (14%)	0	100	100
1	B	292/329 (89%)	243 (83%)	47 (16%)	2 (1%)	18	51
2	C	1339/1342 (100%)	1190 (89%)	147 (11%)	2 (0%)	48	79
3	D	1328/1407 (94%)	1191 (90%)	136 (10%)	1 (0%)	48	79
4	E	88/91 (97%)	82 (93%)	6 (7%)	0	100	100
5	F	493/495 (100%)	458 (93%)	35 (7%)	0	100	100
All	All	3846/3993 (96%)	3426 (89%)	415 (11%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	57	PHE
2	C	58	PRO
1	B	61	ILE
1	B	117	HIS
3	D	1185	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/286 (68%)	191 (98%)	3 (2%)	57	70
1	B	183/286 (64%)	180 (98%)	3 (2%)	55	69
2	C	1155/1157 (100%)	1135 (98%)	20 (2%)	53	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	1114/1168 (95%)	1102 (99%)	12 (1%)	65	74
4	E	74/75 (99%)	74 (100%)	0	100	100
All	All	2720/2972 (92%)	2682 (99%)	38 (1%)	57	71

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	98	VAL
1	A	223	ILE
1	B	39	LEU
1	B	59	VAL
1	B	125	LYS
2	C	131	THR
2	C	155	VAL
2	C	210	LEU
2	C	285	ILE
2	C	351	LEU
2	C	388	LEU
2	C	419	ILE
2	C	452	ARG
2	C	550	VAL
2	C	615	VAL
2	C	967	LEU
2	C	1042	LEU
2	C	1082	ILE
2	C	1117	LEU
2	C	1198	LEU
2	C	1253	LEU
2	C	1254	VAL
2	C	1297	ASP
2	C	1301	ARG
2	C	1327	LEU
3	D	44	ILE
3	D	92	VAL
3	D	212	THR
3	D	239	LEU
3	D	416	ILE
3	D	514	THR
3	D	708	ASN
3	D	839	VAL

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Mol	Chain	Res	Type
3	D	848	VAL
3	D	882	VAL
3	D	1155	ILE
3	D	1261	LEU

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	66	HIS
1	A	84	ASN
1	B	66	HIS
1	B	128	HIS
2	C	273	HIS
2	C	387	ASN
2	C	604	HIS
2	C	1237	HIS
2	C	1256	GLN
2	C	1268	GLN
2	C	1299	ASN
2	C	1313	HIS
3	D	153	ASN
3	D	419	HIS
3	D	469	HIS
3	D	867	GLN
3	D	1010	GLN
3	D	1019	ASN
3	D	1023	HIS
3	D	1235	ASN
3	D	1252	HIS
3	D	1259	GLN
3	D	1366	HIS
3	D	1367	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	R	19/21 (90%)	6 (31%)	1 (5%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	R	18	G
7	R	19	C
7	R	20	G
7	R	21	A
7	R	25	G
7	R	29	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	R	20	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	N	1
7	R	1
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	15:DG	O3'	24:DC	P	28.78
1	R	5:A	O3'	14:U	P	17.75
1	C	1084:ASP	C	1085:MET	N	1.08

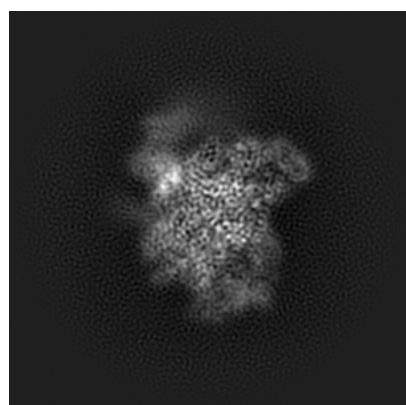
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4275. These allow visual inspection of the internal detail of the map and identification of artifacts.

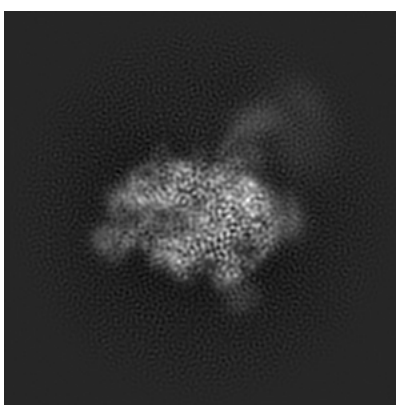
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

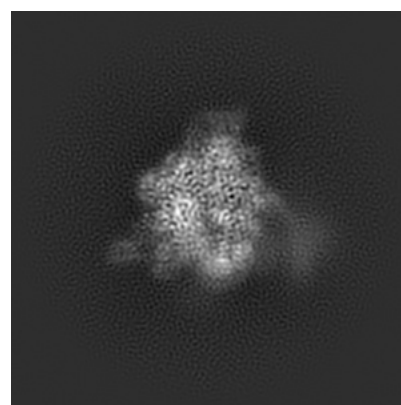
6.1.1 Primary map



X



Y

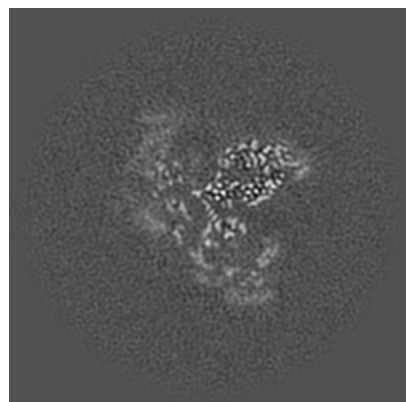


Z

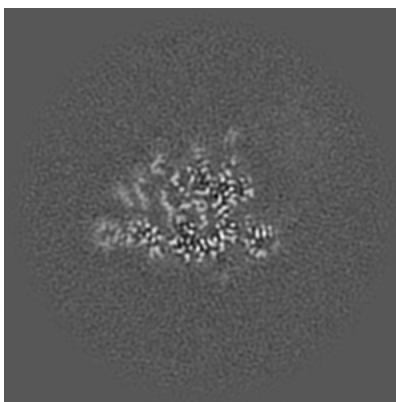
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

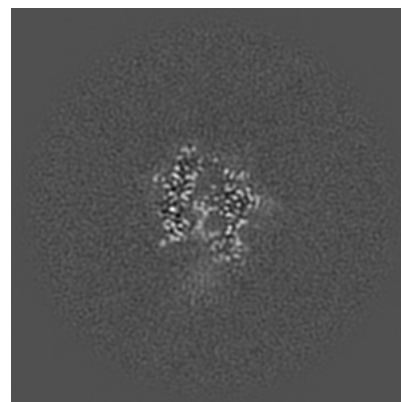
6.2.1 Primary map



X Index: 140



Y Index: 140

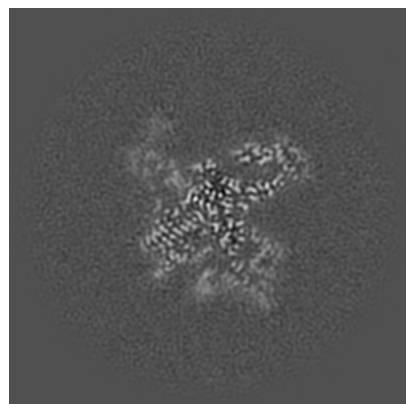


Z Index: 140

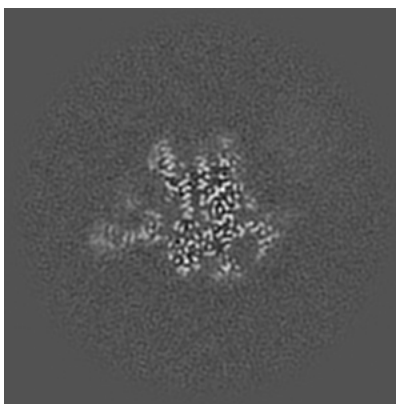
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

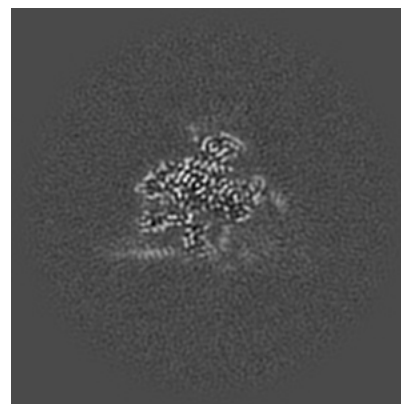
6.3.1 Primary map



X Index: 150



Y Index: 147

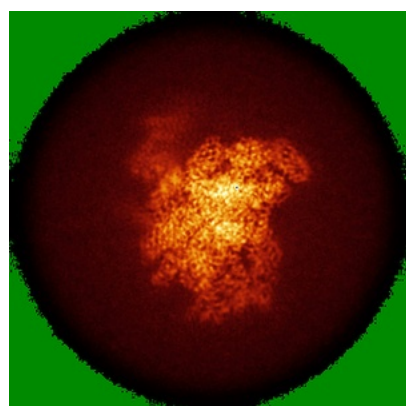


Z Index: 156

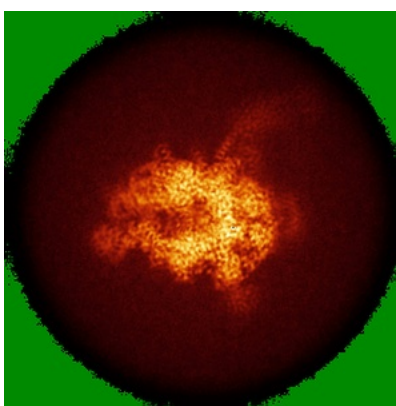
The images above show the largest variance slices of the map in three orthogonal directions.

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

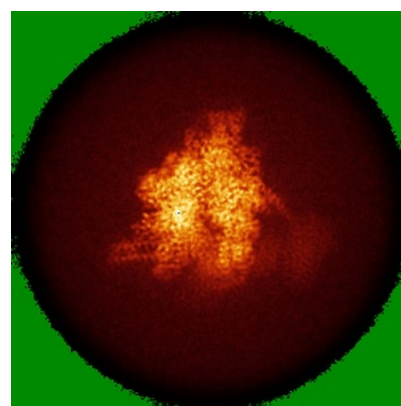
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

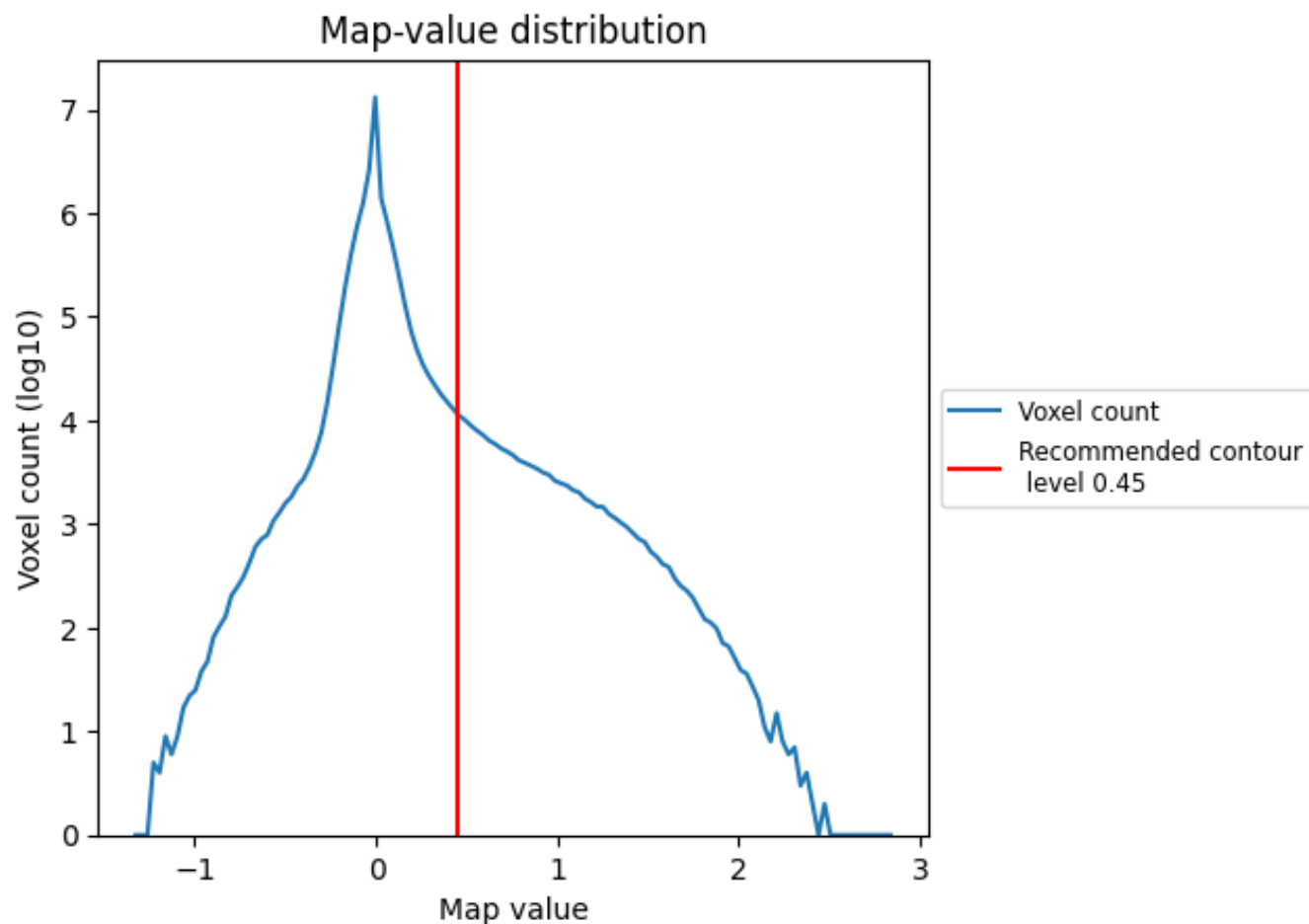
6.6 Mask visualisation

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

7 Map analysis [i](#)

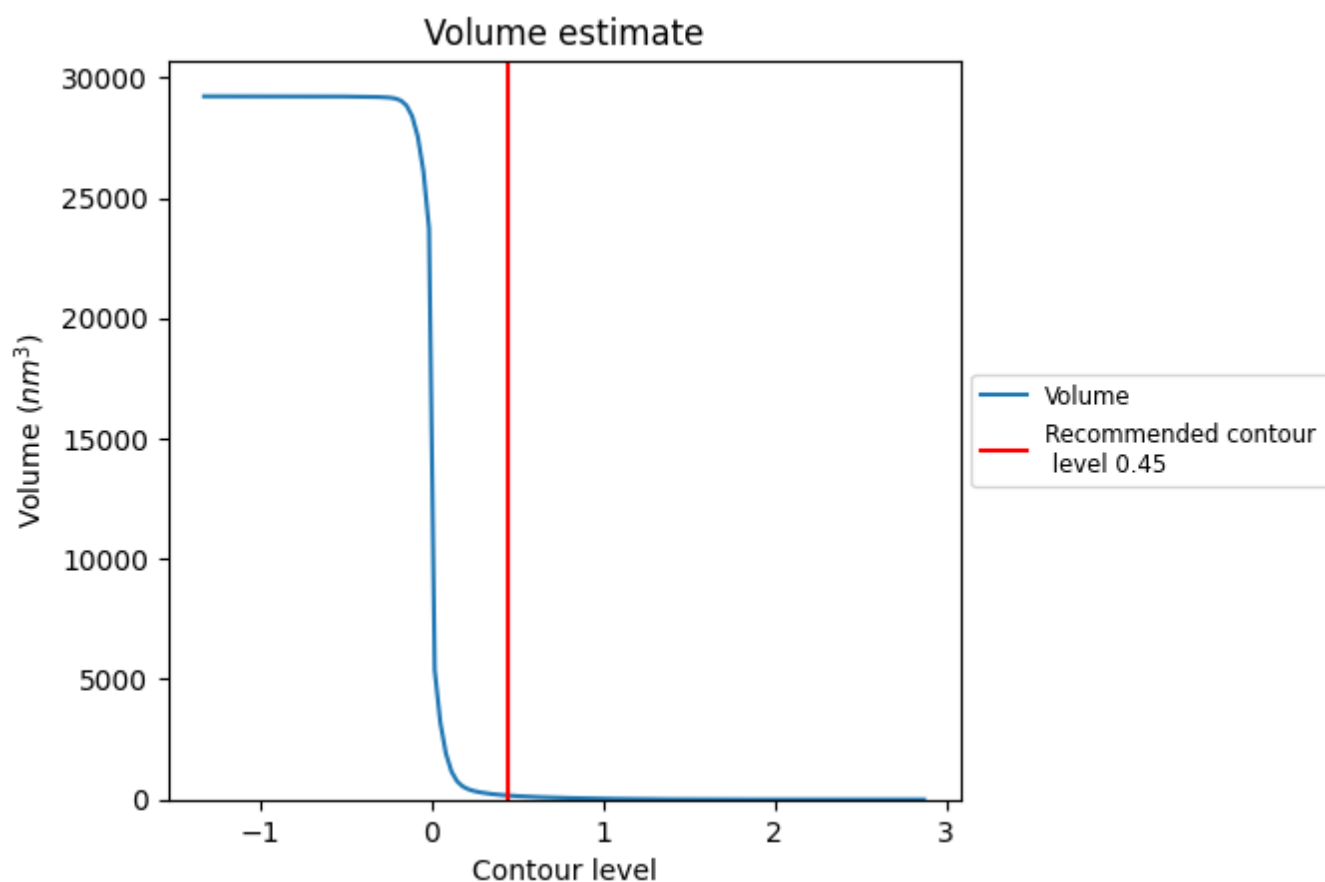
This section contains the results of statistical analysis of the map.

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.

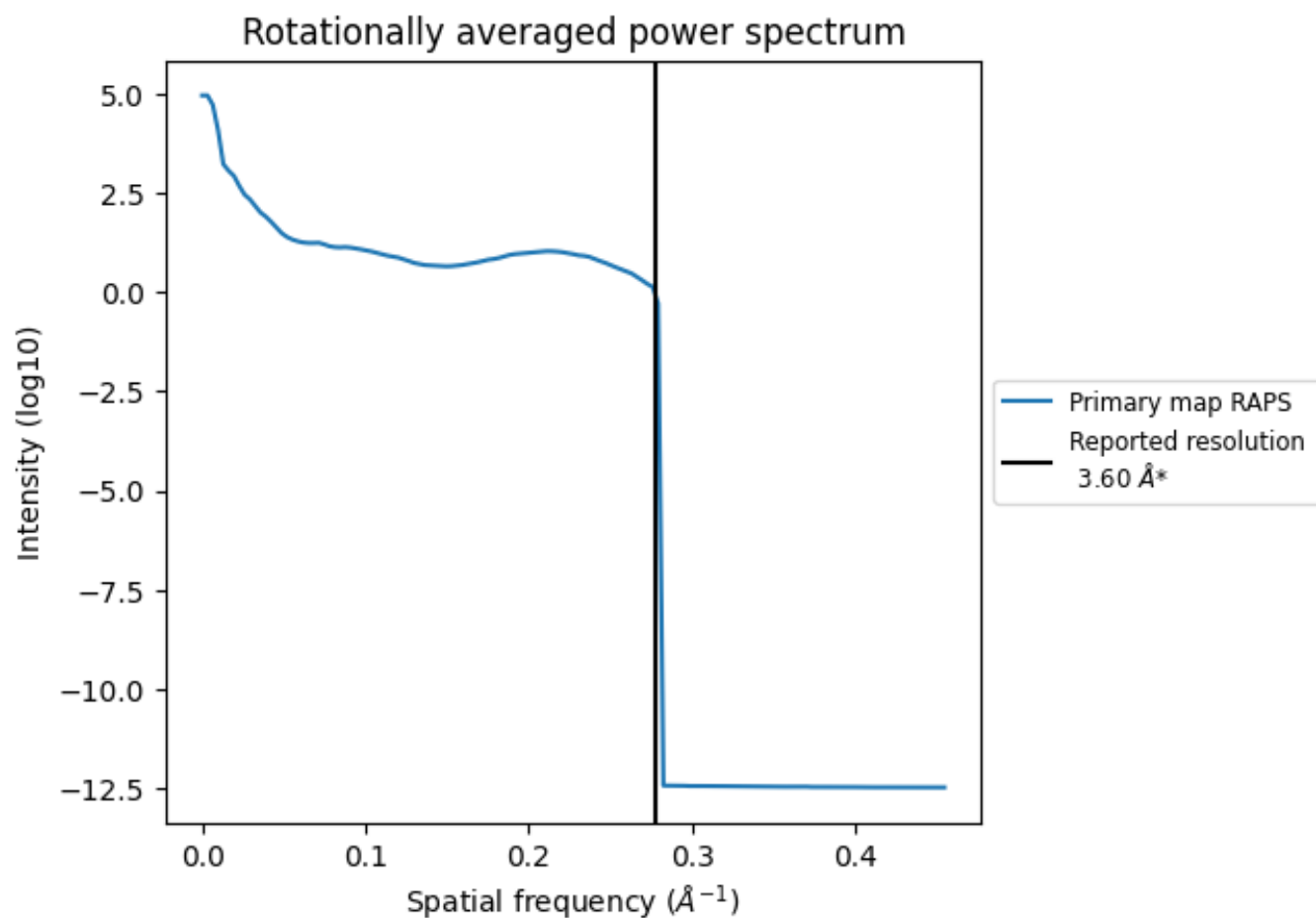
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 166 nm³; this corresponds to an approximate mass of 150 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 0.278 Å⁻¹

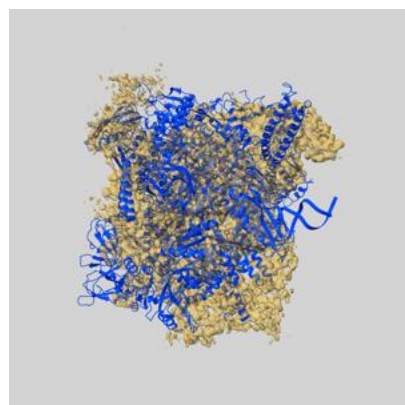
8 Fourier-Shell correlation

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

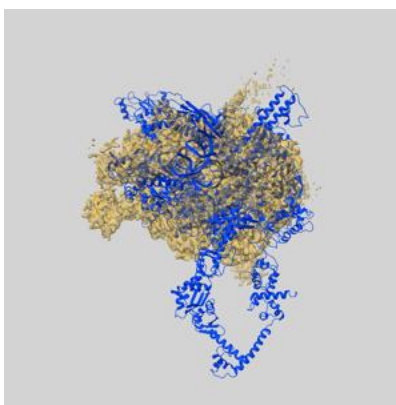
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4275 and PDB model 6FLQ. Per-residue inclusion information can be found in section 3 on page 6.

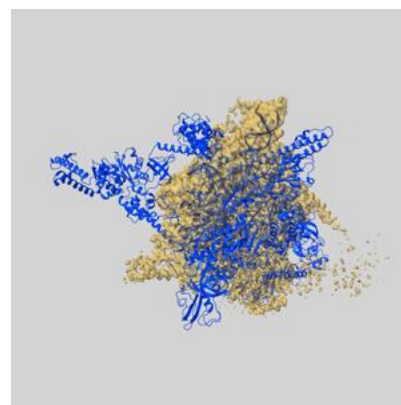
9.1 Map-model overlay [i](#)



X



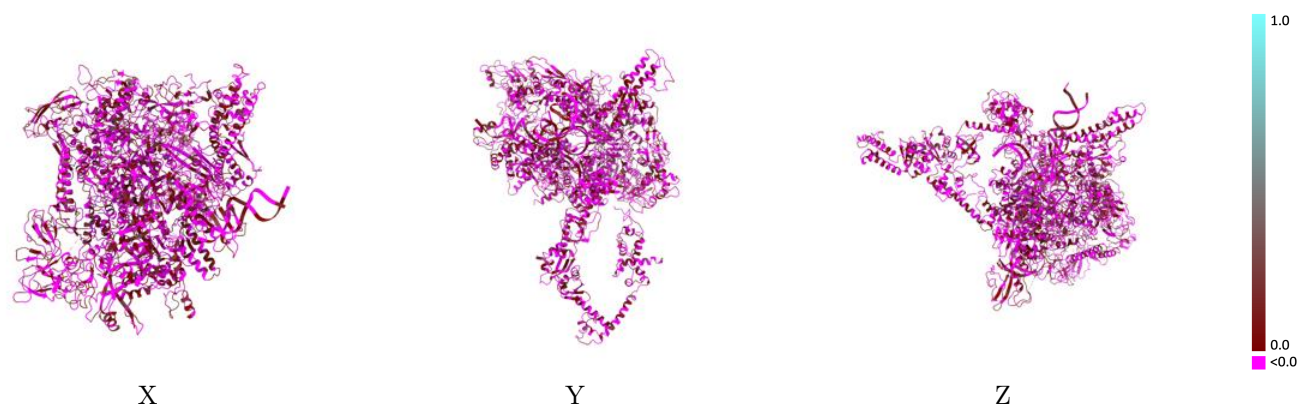
Y



Z

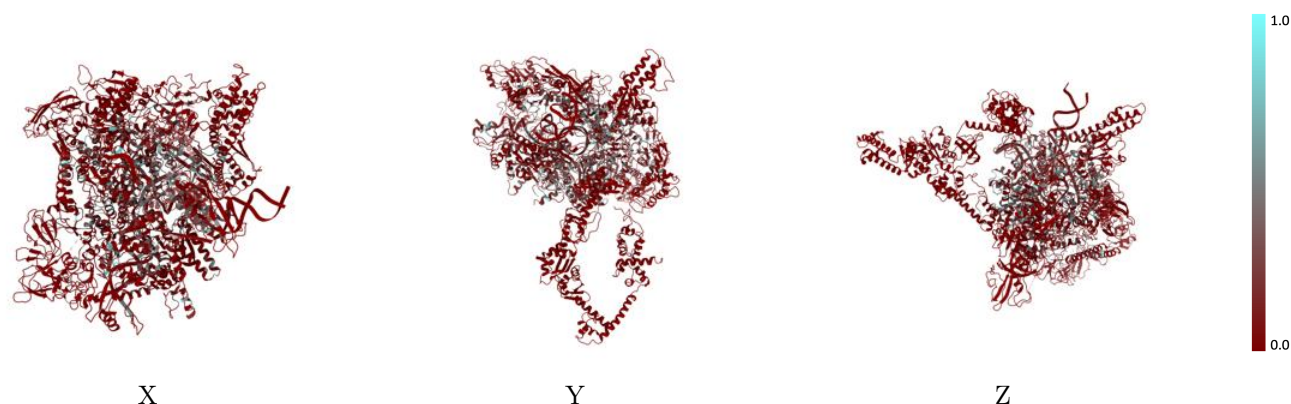
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



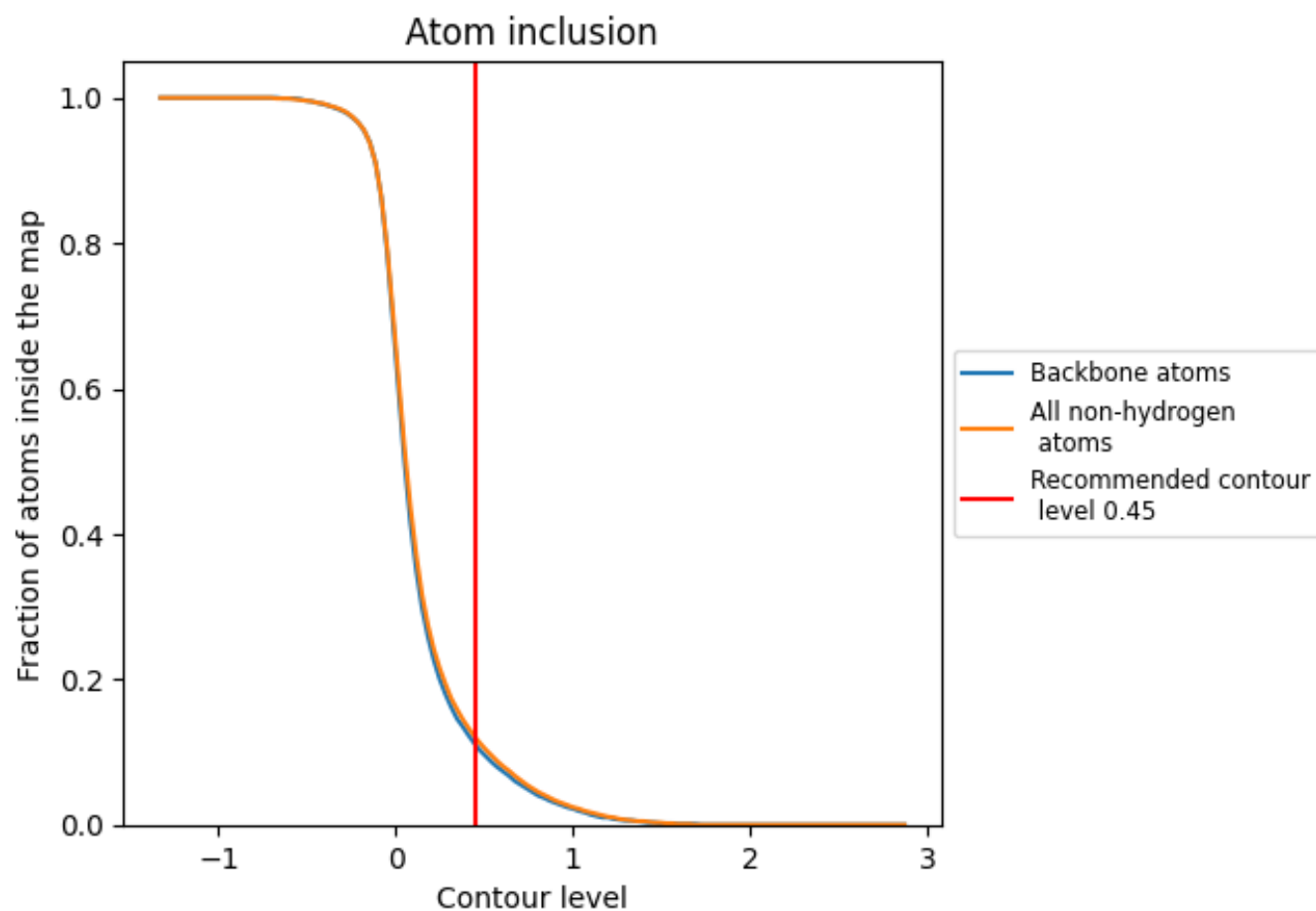
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 11% of all backbone atoms, 12% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.1200	-0.0110
A	0.0840	-0.0070
B	0.0490	-0.0030
C	0.1390	-0.0150
D	0.1490	-0.0060
E	0.0680	-0.0180
F	0.0010	-0.0220
N	0.1130	-0.0070
R	0.2280	-0.0290
T	0.1530	-0.0050

1.0

0.0

<0.0