



wwPDB EM Validation Summary Report ⓘ

Feb 18, 2024 – 10:28 AM EST

PDB ID : 7SZK
EMDB ID : EMD-25571
Title : Cryo-EM structure of 27a bound to E. coli RNAP and rrnBP1 promoter complex
Authors : Shin, Y.; Murakami, K.S.
Deposited on : 2021-11-28
Resolution : 2.94 Å(reported)

This is a wwPDB EM Validation Summary 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:

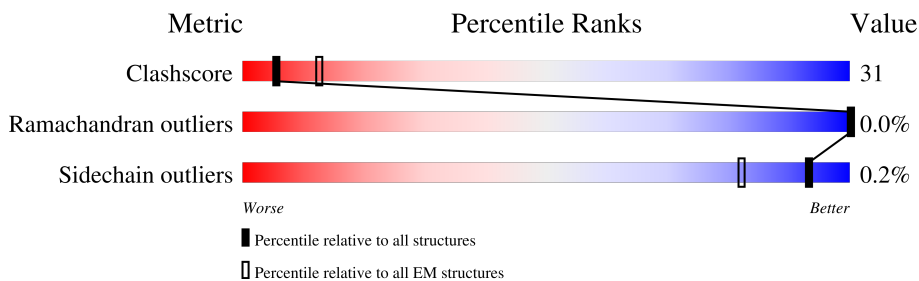
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 2.94 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	
1	B	329	
2	C	1342	
3	D	1407	
4	E	91	
5	F	613	
6	X	64	
7	Y	64	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	D9X	C	3001	X	-	-	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 29840 atoms, of which 81 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
			Total	C	N	O	S		
1	A	231	Total	C	N	O	S	0	0
			1794	1117	318	353	6		
1	B	230	Total	C	N	O	S	0	0
			1786	1112	317	351	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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
			Total	C	N	O	S		
3	D	1340	Total	C	N	O	S	0	0
			10382	6522	1849	1962	49		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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
			Total	C	N	O	S		
5	F	466	Total	C	N	O	S	0	0
			3799	2384	679	713	23		

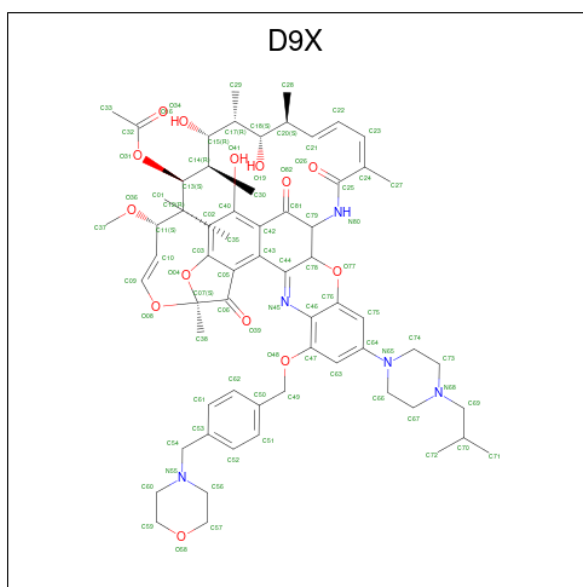
- Molecule 6 is a DNA chain called DNA (5'-D(P*CP*TP*CP*GP*TP*AP*GP*AP*GP*TP*CP*CP*GP*TP*GP*TP*CP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	X	18	370	175	71	106	18	0	0

- Molecule 7 is a DNA chain called DNA (5'-D(P*CP*TP*CP*GP*TP*AP*GP*AP*GP*TP*CP*CP*GP*TP*GP*TP*CP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	Y	18	368	175	65	110	18	0	0

- Molecule 8 is (2S,7R,7aR,13aP,16Z,18E,20S,21S,22R,23R,24R,25S,26R,27S,28E)-5,21,23-trihydroxy-27-methoxy-2,4,16,20,22,24,26-heptamethyl-10-[4-(2-methylpropyl)piperazin-1-yl]-12-({4-[(morpholin-4-yl)methyl]phenyl}methoxy)-1,6,15-trioxo-1,2,7,7a-tetrahydro-6H-2,7-(epoxypentadeca[1,11,13]trienoimino)[1]benzofuro[4,5-a]phenoxazin-25-yl acetate (three-letter code: D9X) (formula: C₆₃H₈₁N₅O₁₄).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
8	C	1	163	63	81	5	14	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

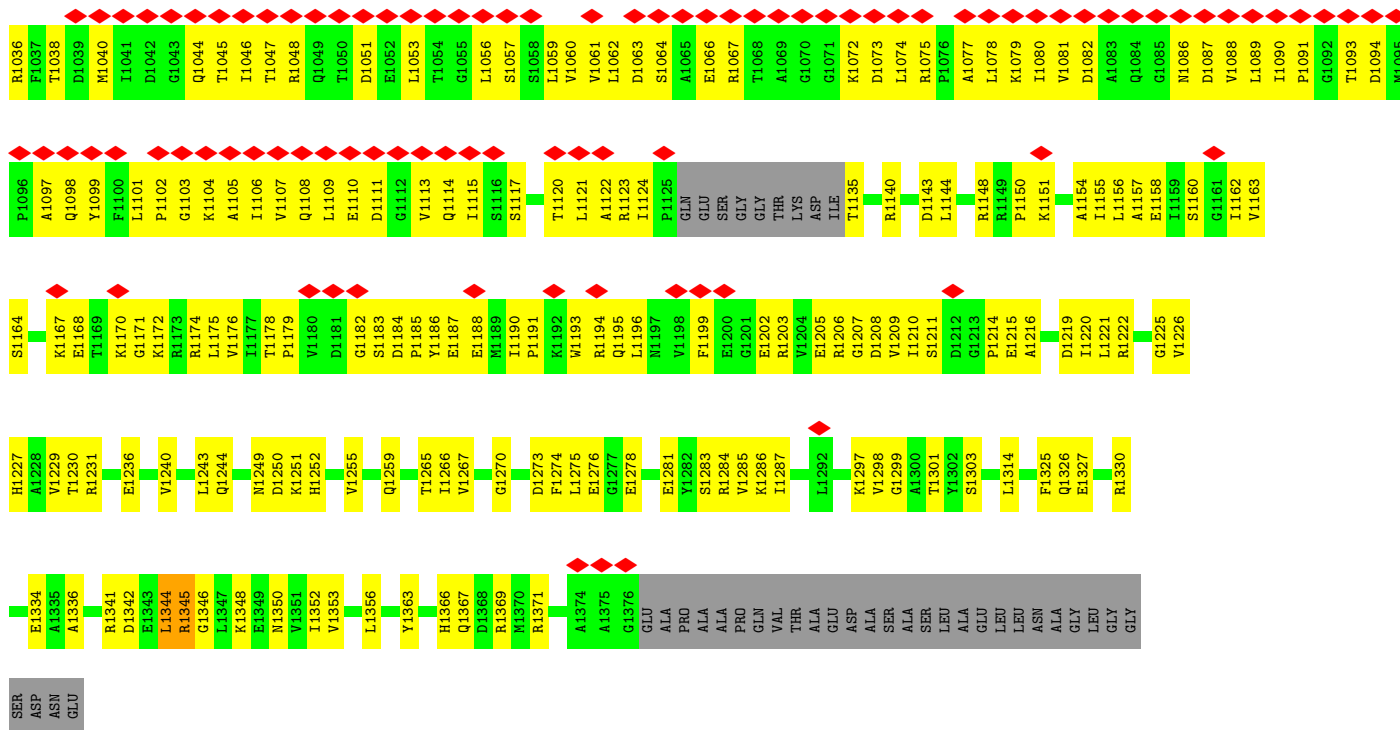
Mol	Chain	Residues	Atoms		AltConf
9	D	1	Total	Mg	0
			1	1	

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

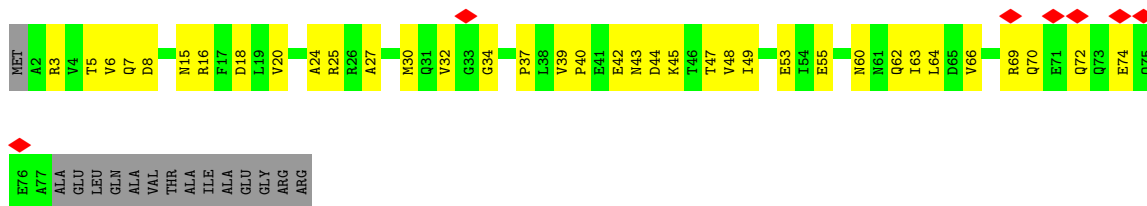
Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total 2	Zn 2	0



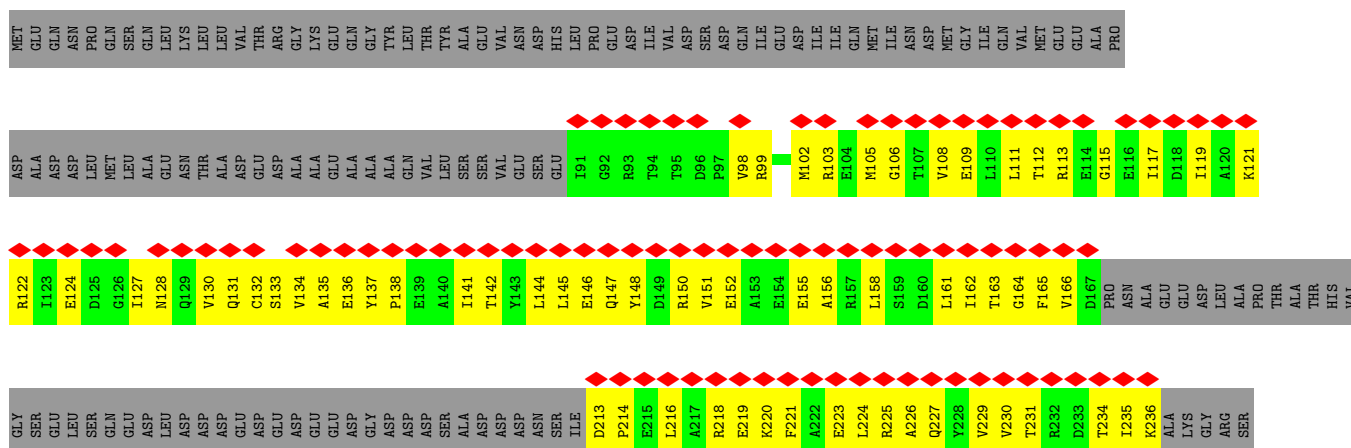
RES	VAL
T91	Y3
V98	S4
L102	Y5
V103	T6
L104	E7
Y105	K8
E106	K9
R107	R12
E108	K13
A109	D14
P110	K17
V114	L28
K115	S29
D116	L30
I117	Q31
E119	Q36
Q120	K37
F121	E40
V122	E45
Y123	Q46
M124	Y47
G125	Q46
E126	Y47
I127	A51
A52	A52
V56	V56
F57	F57
P58	P58
L59	L59
Q60	Q60
S61	S61
Y62	Y62
S63	S63
G64	G64
N65	N65
S66	S66
E67	E67
Y70	Y70
R74	R74
L75	L75
F80	F80
D81	D81
V82	V82
D83	D83
E84	E84
C85	C85
Q86	Q86
R88	R88
R200	R200
K203	K203
L204	L204
P205	P205
A206	A206
T207	T207
I208	I208
L209	L209
T210	T210
L211	L211
L213	L213
N214	N214
Y215	Y215
T216	T216
T217	T217
E218	E218
Q219	Q219
L220	L220
L221	L221
D222	D222
L223	L223
E226	E226
V228	V228
I229	I229
F230	F230
Q231	Q231
E231	E231
I232	I232
R233	R233
D234	D234
N235	N235
K236	K236
L237	L237
Q238	Q238
E240	E240
L241	L241
V242	V242
P243	P243
E244	E244
R245	R245
L246	L246
R247	R247
G248	G248
E249	E249
T250	T250
A251	A251
S252	S252
F253	F253
D254	D254
I255	I255
E256	E256
A257	A257
N258	N258
Q259	Q259
K260	K260
Y262	Y262
V263	V263
E264	E264
K265	K265
G266	G266
R268	R268
I269	I269
T270	T270
L210	L210
A271	A271
R272	R272
K273	K273
L274	L274
Q275	Q275
L277	L277
E278	E278
K279	K279
D280	D280
D281	D281
K283	K283
V282	V282
L284	L284
I285	I285
E286	E286
V287	V287
P288	P288
V289	V289
Y291	Y291
L292	L292
A293	A293
G294	G294
D300	D300
Y301	Y301
I302	I302
D303	D303
E304	E304
S305	S305
T306	T306
G307	G307
E308	E308
L309	L309
C311	C311
A312	A312
M315	M315
E316	E316
L317	L317
S318	S318
L319	L319
D320	D320
L321	L321
A322	A322
K324	K324
L325	L325
S326	S326
Q327	Q327
S328	S328
G329	G329
H330	H330
K331	K331
R332	R332
I333	I333
E334	E334
T335	T335
L336	L336
F337	F337
T338	T338
N339	N339
D340	D340
Y346	Y346
T350	T350
L351	L351
R352	R352
V353	V353
D358	D358
R359	R359
L360	L360
S361	S361
A362	A362
L363	L363
Y367	Y367
R368	R368
M369	M369
G373	G373
E379	E379
A380	A380
A381	A381
N387	N387
S391	S391
D396	D396
L397	L397
S398	S398
G401	G401
N406	N406
R411	R411
G418	G418
K422	K422
I425	I425
M429	M429
D434	D434
I435	I435
R436	R436
K439	K439
L448	L448
I453	I453
V456	V456
M459	M459
Q463	Q463
F464	F464
R465	R465
L468	L468
V471	V471
R472	R472
A473	A473
A474	A474
V475	V475
K476	K476
E477	E477
R478	R478
L479	L479
S480	S480
L481	L481
G482	G482
D483	D483
L484	L484
D485	D485
T486	T486
L487	L487
M488	M488
P489	P489
M492	M492
I493	I493
M494	M494
A495	A495
K496	K496
P497	P497
I498	I498
F505	F505
L511	L511
S512	S512
Q513	Q513
F514	F514
L521	L521
I524	I524
T525	T525
R528	R528
E529	E529
I530	I530
L533	L533
R540	R540
E541	E541
R542	R542
A543	A543
F545	F545
R548	R548
D549	D549
V550	V550
T553	T553
V558	V558
I561	I561
E562	E562
T563	T563
P564	P564
E565	E565
N568	N568
L571	L571
I572	I572
M573	M573
S574	S574
S576	S576
V577	V577
Q580	Q580
L581	L581
N582	N582
G585	G585
F586	F586
L587	L587
E588	E588
T589	T589
P590	P590
K593	K593
V594	V594
T595	T595
D596	D596
G597	G597
V598	V598
F599	F599
T600	T600
D601	D601
E602	E602
V615	V615
I616	I616
S621	S621
D624	D624
E625	E625
E626	E626
F629	F629
D632	D632
L633	L633
V634	V634
T635	T635
R636	R636
R637	R637
S638	S638
E641	E641
L644	L644
R647	R647
D648	D648
Q649	Q649
V650	V650
D651	D651
M653	M653
V660	V660
V661	V661
S662	S662
A665	A665
S666	S666
R678	R678
M685	M685
V690	V690
R694	R694
A695	A695
D696	D696
K697	K697
P698	P698
L699	L699
V714	V714
T715	T715
A716	A716
V717	V717
S718	S718
V724	V724
D727	D727
T728	T728
A729	A729
I734	I734
E738	E738
M741	M741
I748	I748
N760	N760
Q761	Q761
N762	N762
Q767	Q767
E778	E778
D781	D781
V782	V782
L783	L783
A784	A784
Q798	Q798
N799	N799
M800	M800
N808	N808
E813	E813
L817	L817
E820	E820
V823	V823
R827	R827
H832	H832
K844	K844
L845	L845
E849	E849
I850	I850
T851	T851
A852	A852
I854	I854
P855	P855
N856	N856
D866	D866
E867	E867
S868	S868
G869	G869
Y872	Y872
T878	T878
G879	G879
K886	K886
V887	V887
T888	T888
P889	P889
K890	K890
G891	G891
E892	E892
L895	L895
T896	T896
P897	P897
E898	E898
E899	E899
K900	K900
R903	R903
G907	G907
E908	E908
K909	K909
D912	D912
V913	V913
K914	K914
D915	D915
P921	P921
Q924	Q924
I929	I929
D937	D937
G938	G938
K943	K943
A956	A956
L960	L960
S961	S961
E962	E962
Q965	Q965
E968	E968
R974	R974
I975	I975
R976	R976
A977	A977
V978	V978
L979	L979
V980	V980
I981	I981
G982	G982
G983	G983
V984	V984
M1066	M1066
G1071	G1071
N1072	N1072
K1073	K1073
I1076	I1076
S1077	S1077
K1078	K1078
I1082	I1082
P1083	P1083
V1103	V1103
P1104	P1104
R1106	R1106
M1107	M1107
N1108	N1108
I1109	I1109
T1115	T1115
K1122	K1122
G1125	G1125
Q1134	Q1134
Q1135	Q1135
Q1136	Q1136
E1137	E1137
K1140	K1140
L1141	L1141
R1142	R1142
L1151	L1151
D1154	D1154
Y1018	Y1018
Q1157	Q1157
K1158	K1158
V1159	V1159
D1160	D1160
L1161	L1161
T1163	T1163
F1164	F1164
S1165	S1165
D1166	D1166
E1167	E1167
E1168	E1168
V1169	V1169
M1170	M1170
G1179	G1179
M1180	M1180
T1037	T1037
Q1038	Q1038
L1042	L1042
A1043	A1043
P1044	P1044
G1045	G1045
Y1046	Y1046
R1058	R1058
I1182	I1182
A1183	A1183
T1184	T1184
F1185	F1185
V1186	V1186
F1187	F1187
D1188	D1188
G1189	G1189
E1192	E1192
A1193	A1193
K1196	K1196
E1197	E1197
L1198	L1198
L1201	L1201
T1206	T1206
Y1213	Y1213
T1217	T1217
G1218	G1218
E1219	E1219
Q1220	Q1220
V1225	V1225
T1227	T1227
G1228	G1228
Y1229	Y1229
K1234	K1234
L1235	L1235
M1236	M1236
H1244	H1244
A1245	A1245
R1246	R1246
S1252	S1252
L1253	L1253
V1254	V1254
T1255	T1255
P1258	P1258
L1259	L1259
G1260	G1260
G1261	G1261
K1262	K1262
Q1264	Q1264
F1265	F1265
G1266	G1266
R1269	R1269
G1271	G1271



• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor RpoD



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	285262	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 K3 (6k x 4k)	Depositor
Maximum map value	4.617	Depositor
Minimum map value	-2.879	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	403.2, 403.2, 403.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	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, D9X, 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	0.24	0/1816	0.51	0/2461
1	B	0.24	0/1808	0.50	0/2450
2	C	0.25	0/10739	0.49	0/14489
3	D	0.24	0/10539	0.49	0/14234
4	E	0.23	0/607	0.49	0/817
5	F	0.24	0/3849	0.49	0/5171
6	X	0.43	0/415	0.81	0/638
7	Y	0.49	0/411	0.89	0/632
All	All	0.25	0/30184	0.51	0/40892

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
3	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	1344	LEU	Peptide

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	1794	0	1819	81	0
1	B	1786	0	1813	93	0
2	C	10570	0	10582	529	0
3	D	10382	0	10570	719	0
4	E	605	0	612	34	0
5	F	3799	0	3885	408	0
6	X	370	0	202	29	0
7	Y	368	0	204	27	0
8	C	82	81	0	1	0
9	D	1	0	0	0	0
10	D	2	0	0	0	0
All	All	29759	81	29687	1837	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 31.

The worst 5 of 1837 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)
5:F:344:LEU:HD12	5:F:347:ILE:HD11	1.30	1.13
5:F:151:VAL:HG22	5:F:156:ALA:HB3	1.30	1.12
5:F:383:ASN:HB3	5:F:412:LEU:HD11	1.33	1.09
3:D:201:LEU:HB2	3:D:221:ILE:HD11	1.35	1.09
6:X:63:DT:H2''	6:X:64:DG:H5'	1.32	1.08

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	229/329 (70%)	216 (94%)	13 (6%)	0	100	100
1	B	228/329 (69%)	216 (95%)	12 (5%)	0	100	100
2	C	1338/1342 (100%)	1235 (92%)	103 (8%)	0	100	100
3	D	1334/1407 (95%)	1253 (94%)	80 (6%)	1 (0%)	51	80
4	E	74/91 (81%)	71 (96%)	3 (4%)	0	100	100
5	F	458/613 (75%)	444 (97%)	14 (3%)	0	100	100
All	All	3661/4111 (89%)	3435 (94%)	225 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	1345	ARG

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	199/286 (70%)	199 (100%)	0	100	100
1	B	198/286 (69%)	198 (100%)	0	100	100
2	C	1155/1157 (100%)	1151 (100%)	4 (0%)	92	97
3	D	1113/1168 (95%)	1111 (100%)	2 (0%)	93	98
4	E	65/75 (87%)	65 (100%)	0	100	100
5	F	415/540 (77%)	415 (100%)	0	100	100
All	All	3145/3512 (90%)	3139 (100%)	6 (0%)	93	98

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	478	ARG
3	D	709	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	972	LYS
2	C	283	LYS
2	C	272	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	158	GLN
3	D	792	ASN
3	D	1098	GLN
3	D	962	ASN
3	D	157	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 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	D9X	C	3001	-	86,90,90	4.46	39 (45%)	114,133,133	1.53	17 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	D9X	C	3001	-	2/2/27/27	15/72/133/133	0/7/9/9

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	3001	D9X	C47-C46	12.28	1.59	1.40
8	C	3001	D9X	C03-C02	11.88	1.60	1.39
8	C	3001	D9X	C63-C64	9.84	1.57	1.39
8	C	3001	D9X	C75-C76	9.64	1.56	1.38
8	C	3001	D9X	C75-C64	9.54	1.56	1.39

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	3001	D9X	O04-C03-C05	-6.07	110.21	114.36
8	C	3001	D9X	O31-C32-C33	4.85	120.01	111.09
8	C	3001	D9X	C05-C03-C02	-4.02	122.17	125.33
8	C	3001	D9X	O04-C03-C02	3.76	127.61	121.14
8	C	3001	D9X	C74-N65-C66	-3.75	103.23	111.52

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	C	3001	D9X	C78
8	C	3001	D9X	C79

5 of 15 torsion outliers are listed below:

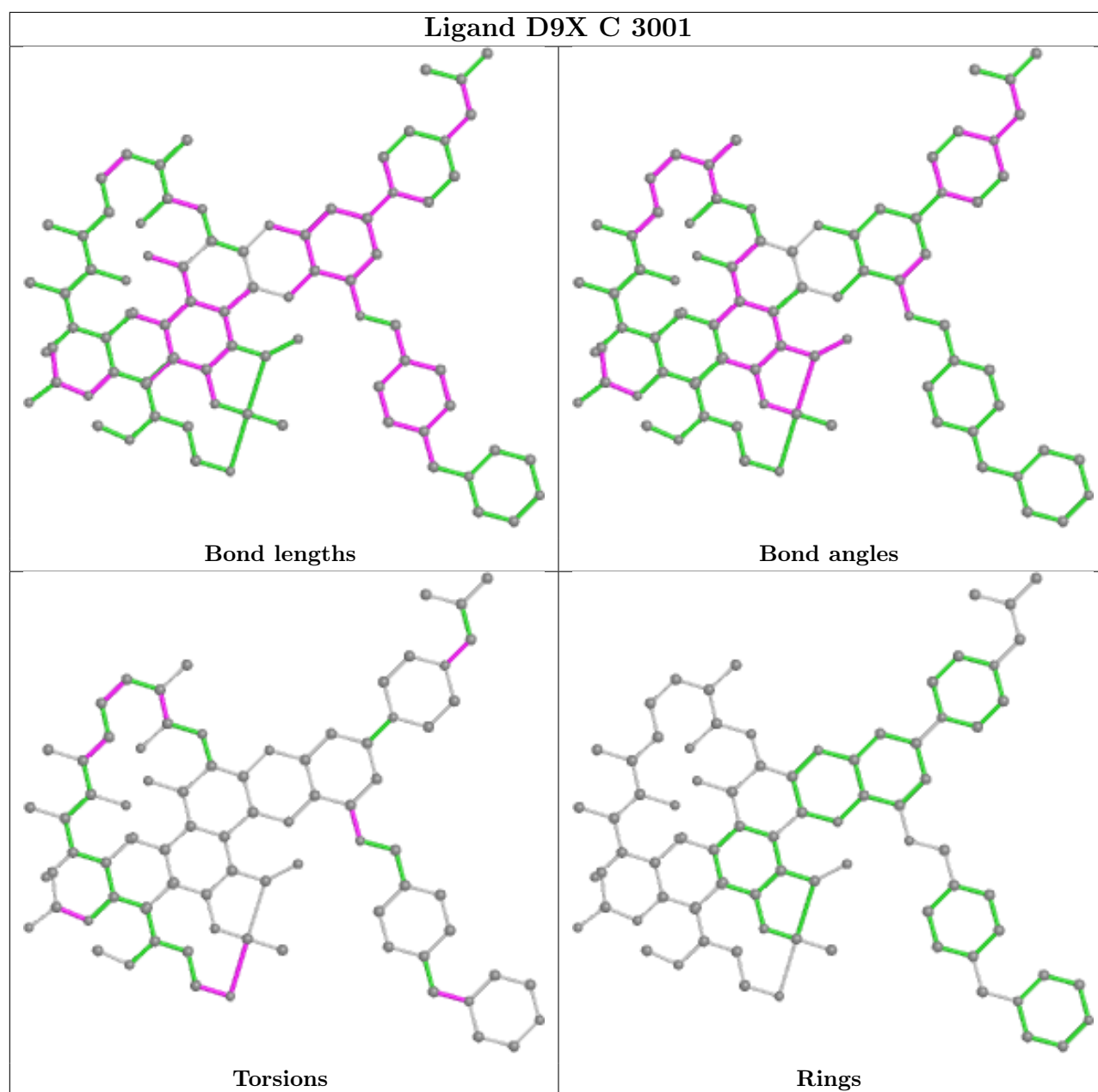
Mol	Chain	Res	Type	Atoms
8	C	3001	D9X	C38-C07-O08-C09
8	C	3001	D9X	O04-C07-O08-C09
8	C	3001	D9X	C33-C32-O31-C13
8	C	3001	D9X	C53-C54-N55-C56
8	C	3001	D9X	C53-C54-N55-C60

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	3001	D9X	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

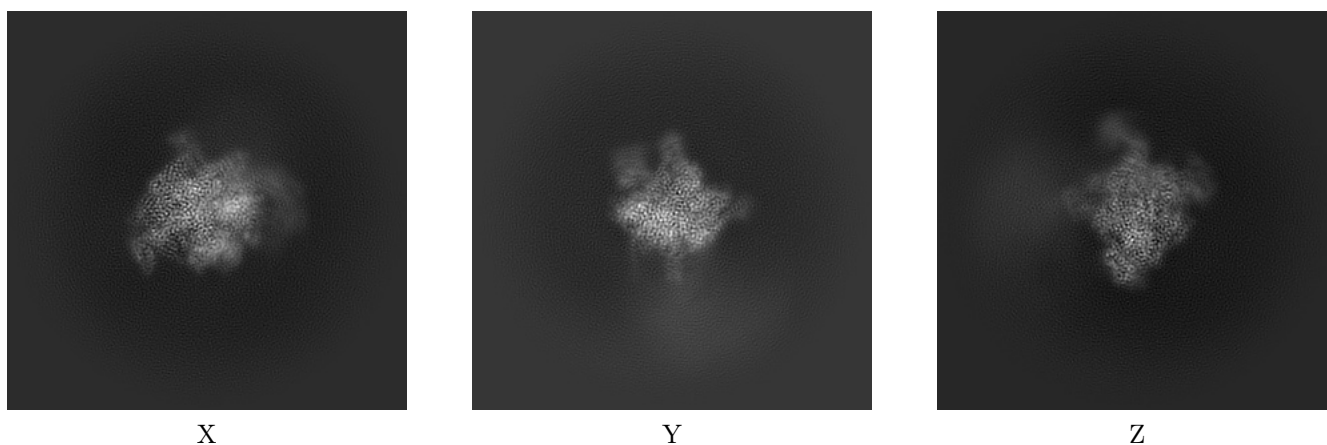
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25571. 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](#)

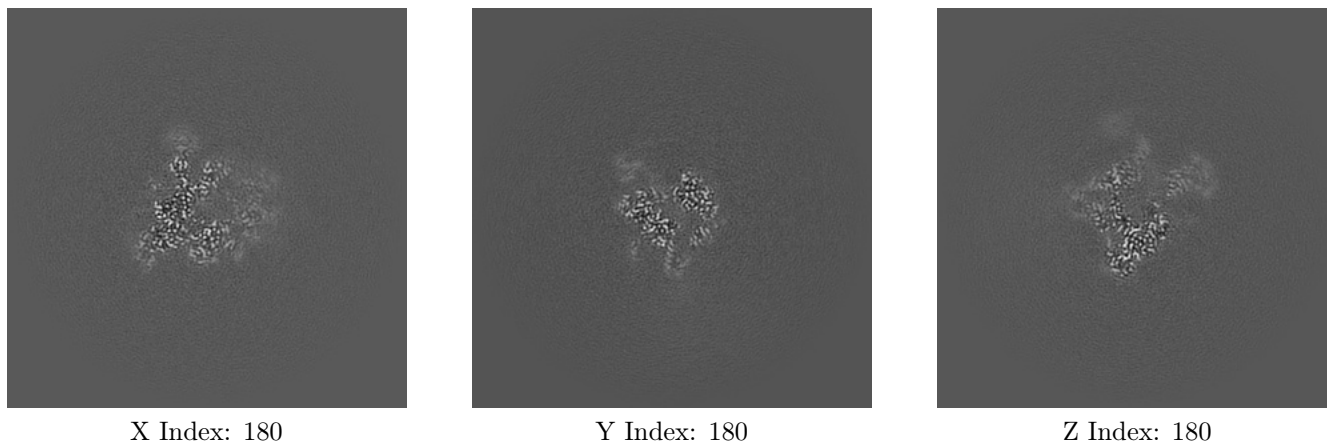
6.1.1 Primary map



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

6.2 Central slices [i](#)

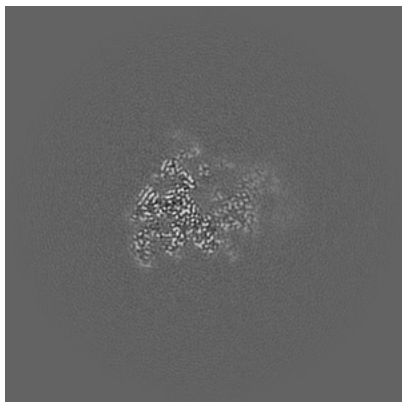
6.2.1 Primary map



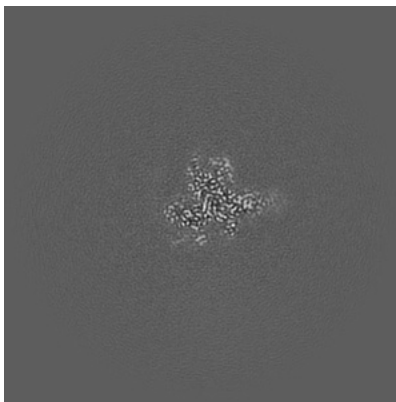
The images above show central slices of the map in three orthogonal directions.

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

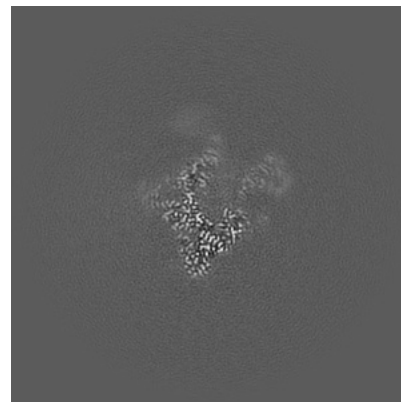
6.3.1 Primary map



X Index: 172



Y Index: 160

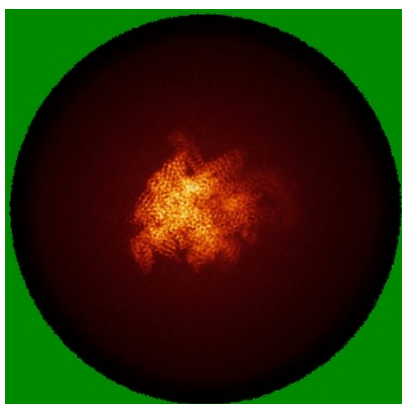


Z Index: 178

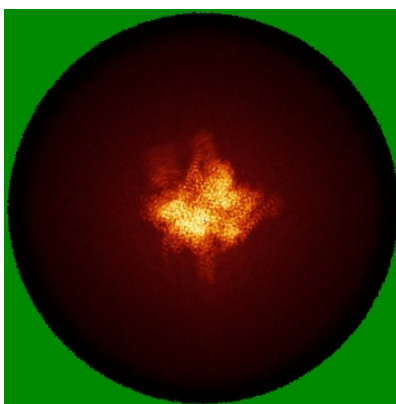
The images above show the largest variance slices of the map in three orthogonal directions.

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

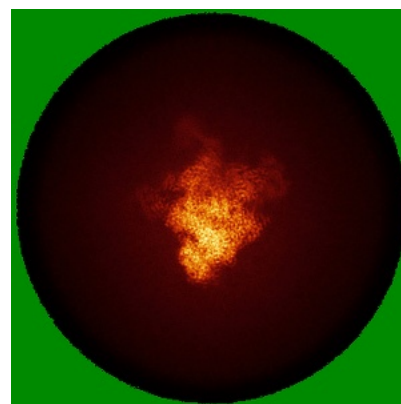
6.4.1 Primary map



X



Y

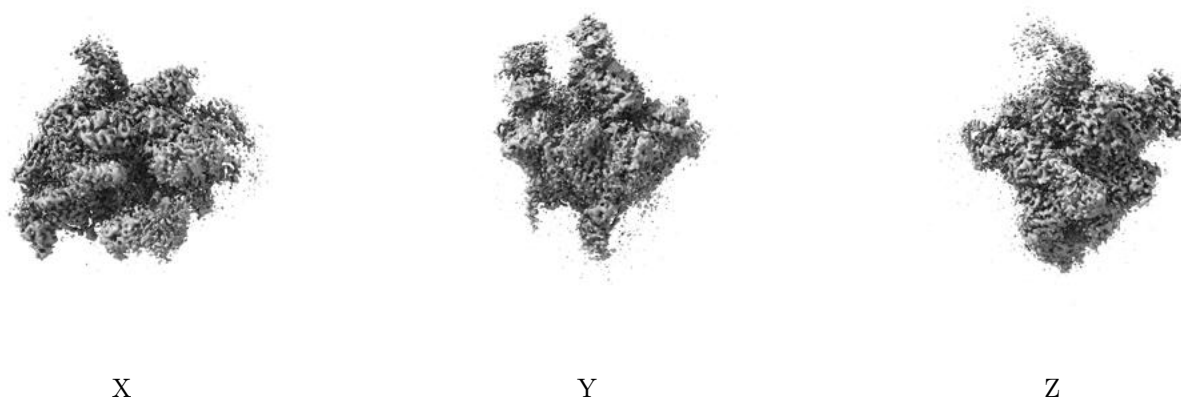


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

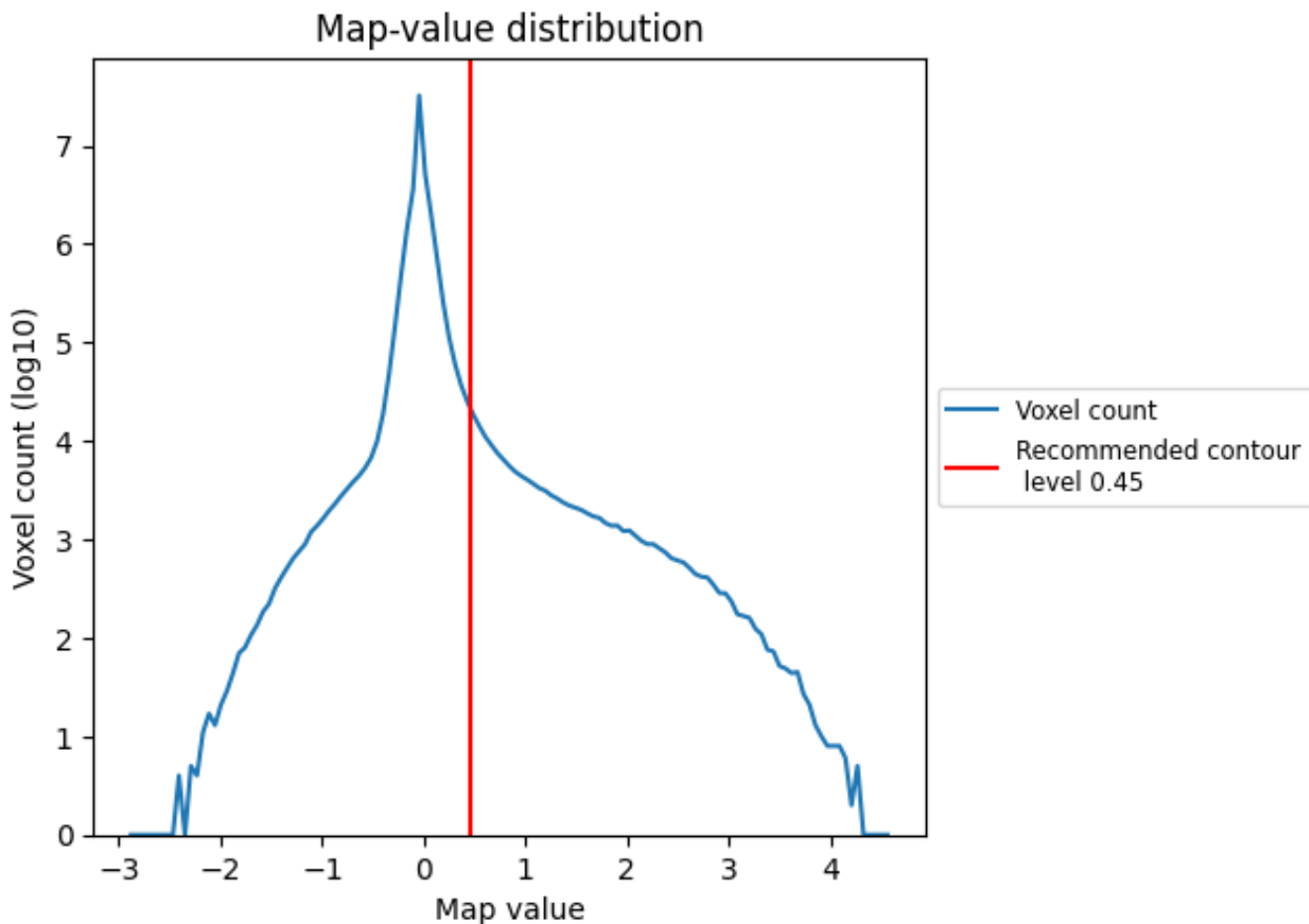
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

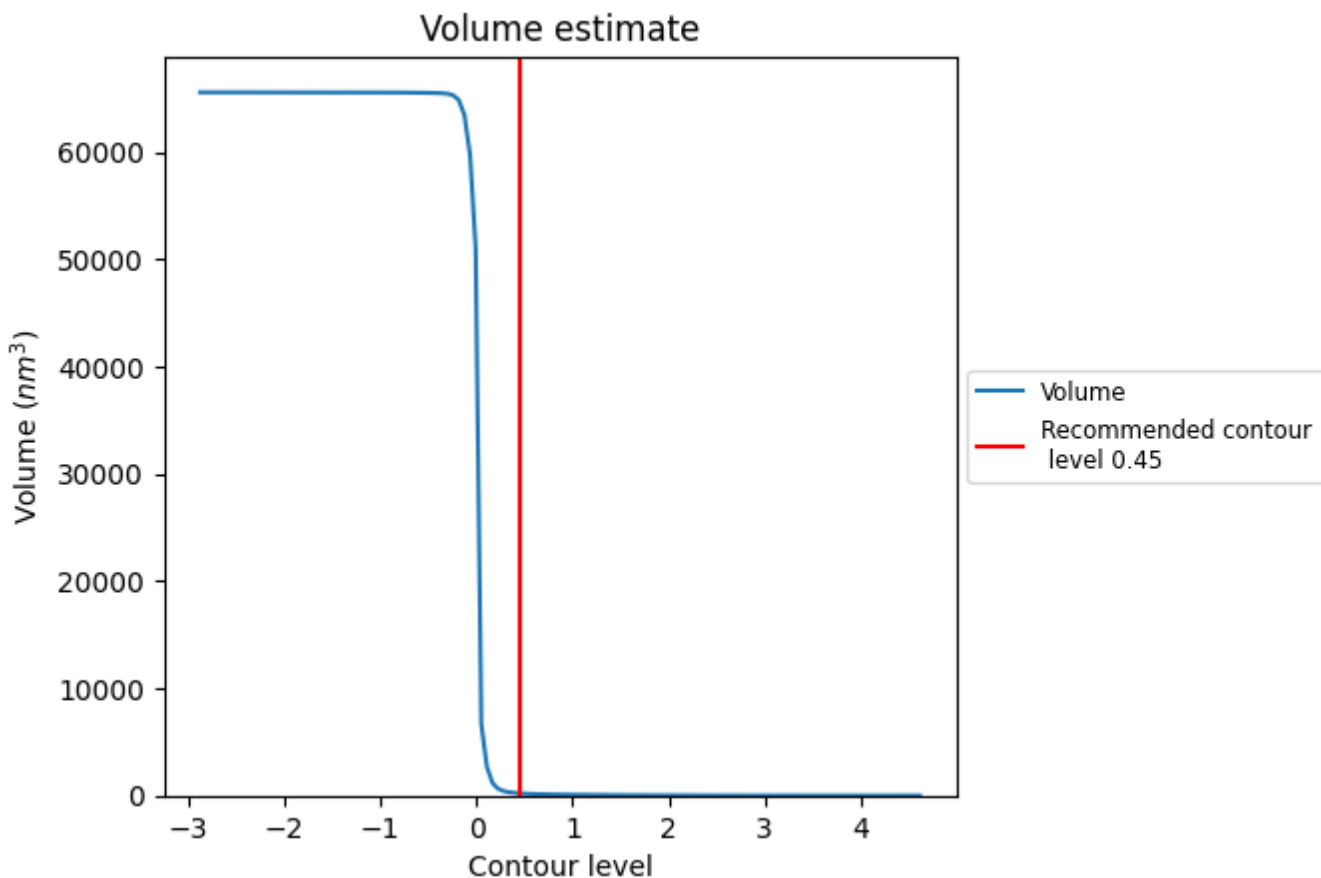
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

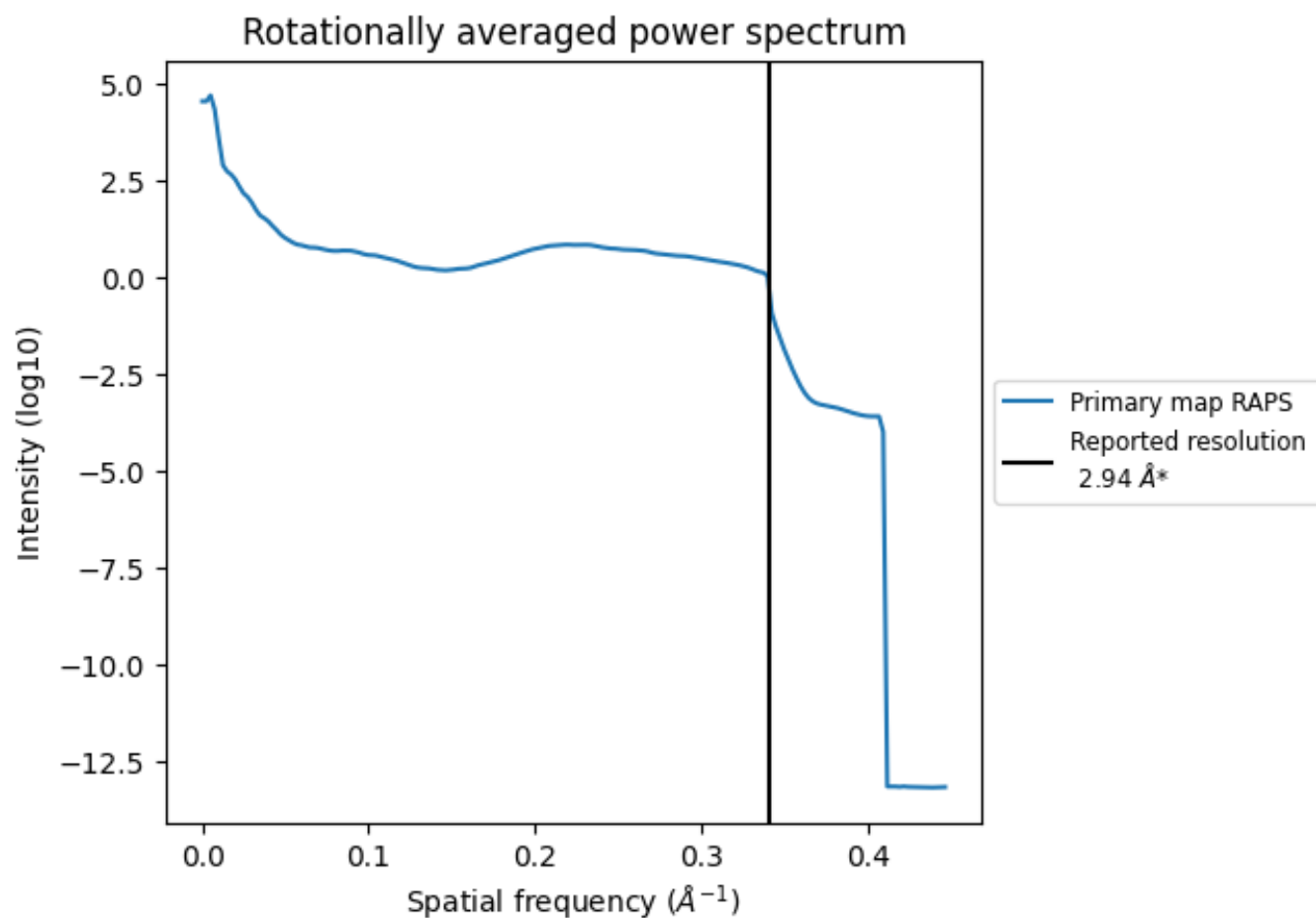
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 208 nm³; this corresponds to an approximate mass of 188 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.340\AA^{-1}

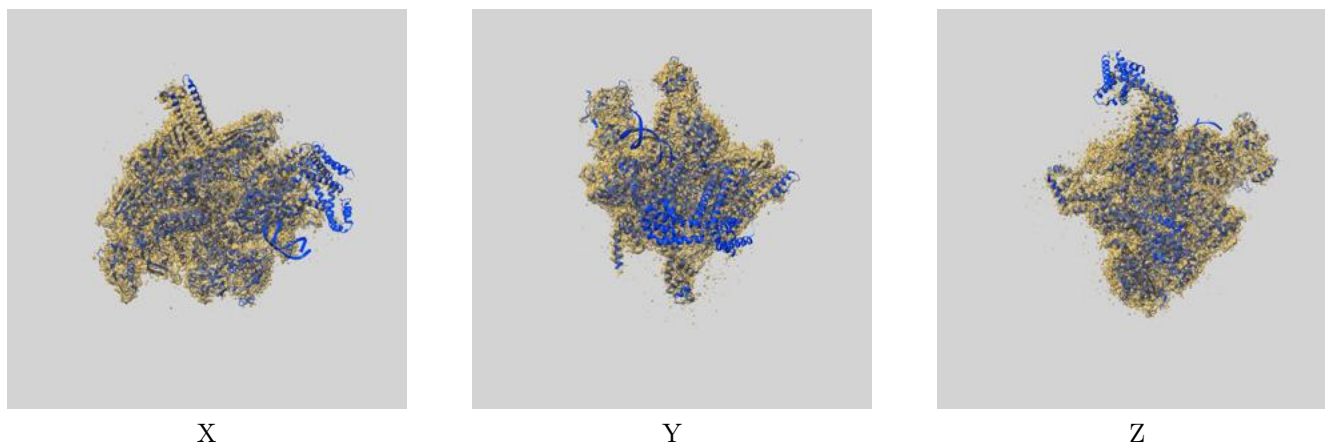
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

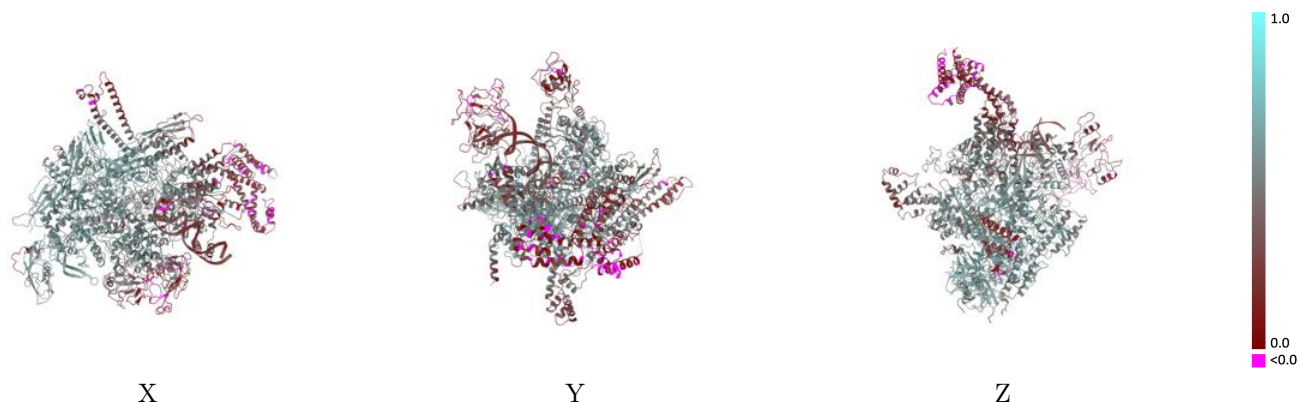
This section contains information regarding the fit between EMDB map EMD-25571 and PDB model 7SZK. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



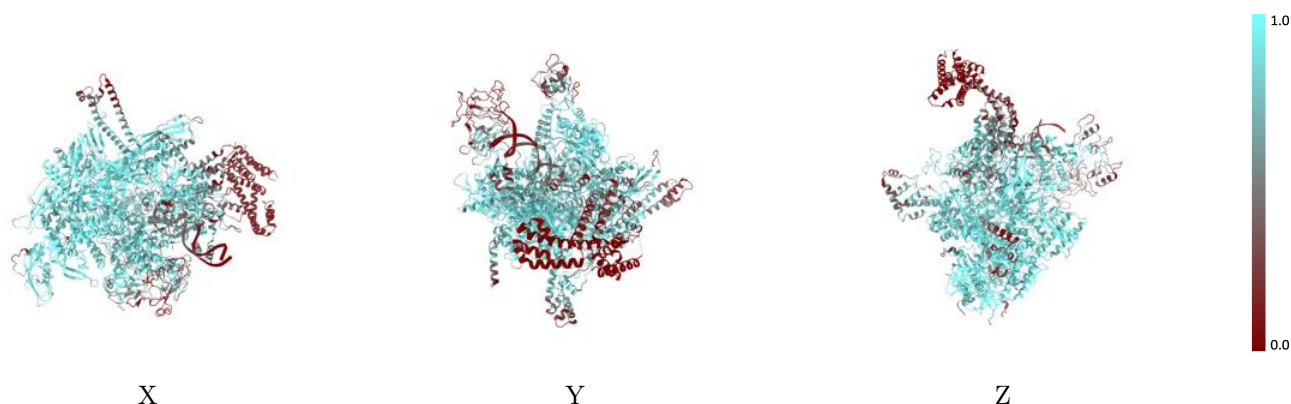
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



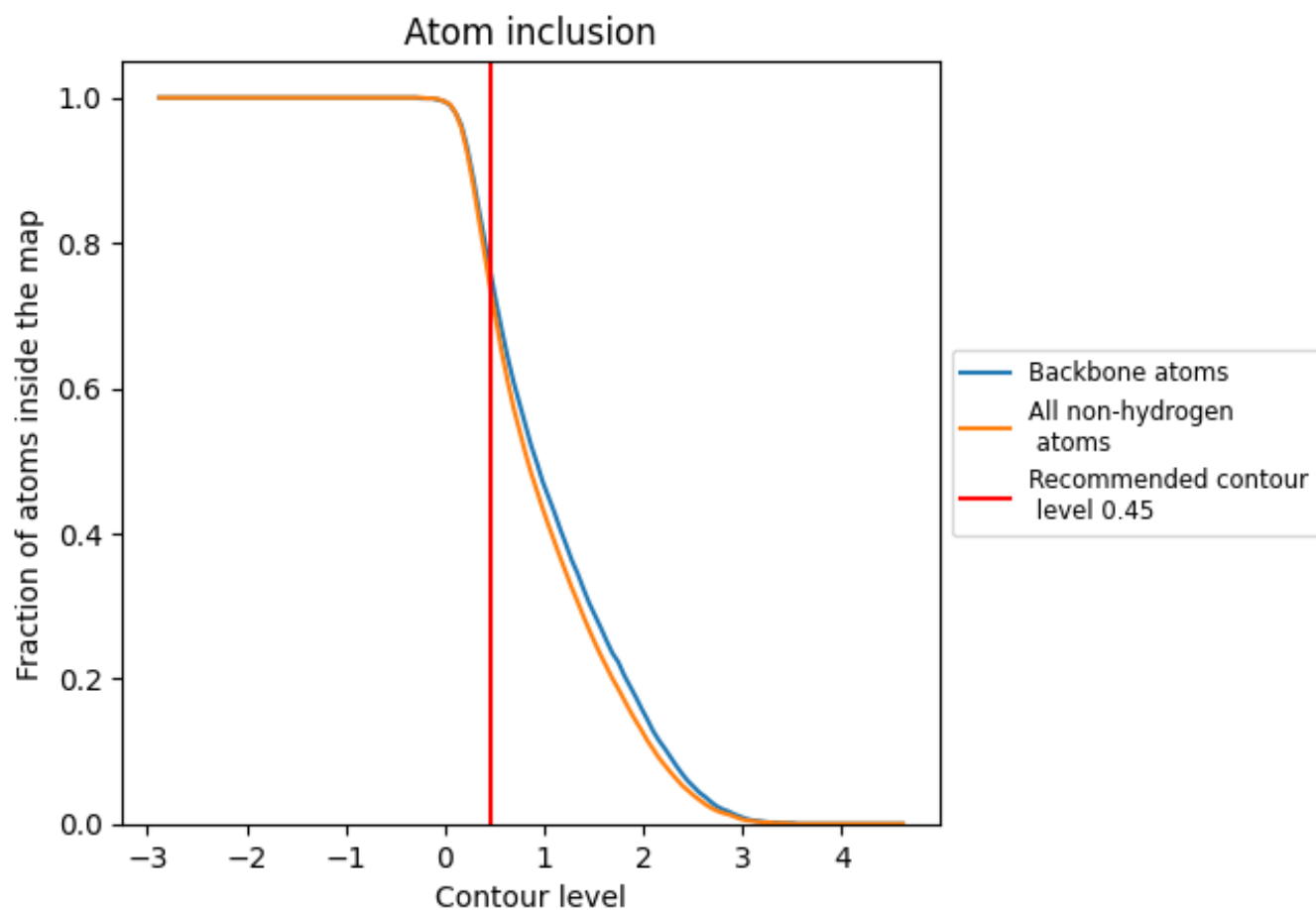
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 77% of all backbone atoms, 74% 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	 0.7430	 0.4620
A	 0.8940	 0.5550
B	 0.8630	 0.5260
C	 0.8400	 0.5060
D	 0.7900	 0.4750
E	 0.7720	 0.4880
F	 0.3080	 0.2590
X	 0.3110	 0.2910
Y	 0.3640	 0.3070

