



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 02:07 PM UTC

PDB ID : 8WAL / pdb_00008wal
EMDB ID : EMD-37396
Title : Structure of transcribing complex 3 (TC3), the initially transcribing complex with Pol II positioned 3nt downstream of TSS.
Authors : Chen, X.; Liu, W.; Wang, Q.; Wang, X.; Ren, Y.; Qu, X.; Li, W.; Xu, Y.
Deposited on : 2023-09-07
Resolution : 8.52 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:

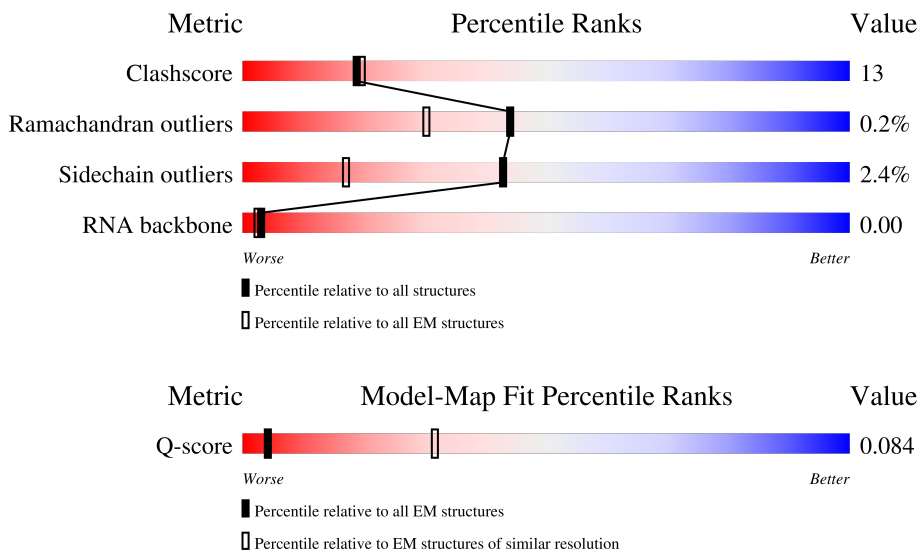
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 8.52 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	270 (8.04 - 9.02)

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	0	309	
2	1	548	
3	2	395	



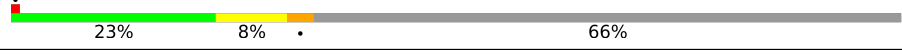



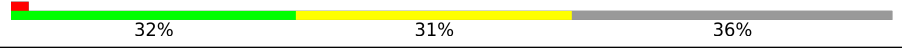
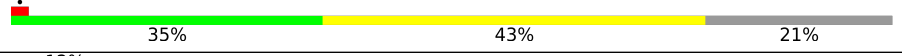



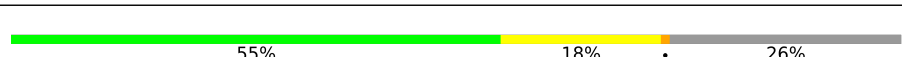
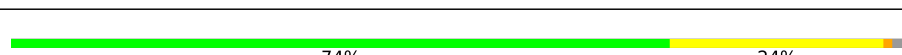
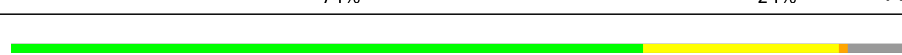
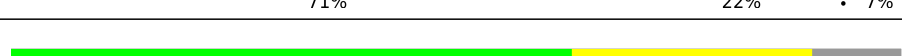
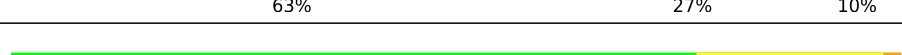
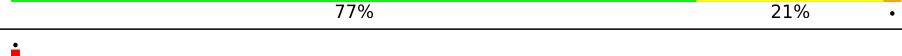




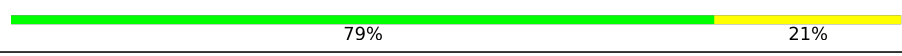
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Mol	Chain	Length	Quality of chain
4	3	308	65% 19% 15%
5	4	462	66% 18% 15%
6	5	71	10% 52% 20% 24%
7	6	782	7% 65% 12% 23%
8	7	760	73% 21% 6%
9	N	8	25% 25% 50%
10	Z	3	33% 67% 33%
11	A	1872	14% 24% 5% 70%
12	B	1199	6% 69% 11% 20%
13	D	1085	8% 12% 85%
13	d	1085	14% 13% 85%
14	E	800	18% 55% 12% 32%
14	e	800	54% 56% 10% 33%
15	F	677	28% 44% 15% 39%
15	f	677	29% 48% 11% 40%
16	G	349	30% 36% 59%
17	H	310	13% 52% 14% 33%
18	I	264	20% 39% 6% 55%
18	i	264	44% 42% 54%
19	J	218	11% 32% 8% 59%
19	j	218	40% 36% 7% 56%
20	L	161	38% 32% 12% 53%
20	l	161	66% 59% 7% 34%
21	O	109	76% 15% 9%
22	P	339	45% 8% 47%

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Mol	Chain	Length	Quality of chain
23	Q	376	
24	R	316	
25	S	517	
26	T	249	
27	U	439	
28	V	291	
29	X	99	
30	Y	99	
31	c	929	
32	k	211	
33	m	124	
34	o	1970	
35	p	1174	
36	q	275	
37	r	142	
38	s	210	
39	t	127	
40	u	172	
41	v	150	
42	w	125	
43	x	67	
44	y	117	
45	z	58	

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
48	W0F	Z	2500	-	-	X	-

2 Entry composition [i](#)

There are 49 unique types of molecules in this entry. The entry contains 108683 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 CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	171	1420	882	249	279	10	0	0

- Molecule 2 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	265	2167	1382	378	395	12	0	0

- Molecule 3 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	329	2567	1621	440	479	27	0	0

- Molecule 4 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	263	2066	1323	344	380	19	0	0

- Molecule 5 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	394	3189	2068	552	557	12	0	0

- Molecule 6 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	54	428	277	67	82	2	0	0

- Molecule 7 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	605	4890	3127	848	885	30	0	0

- Molecule 8 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	7	714	5751	3683	999	1040	29	0	0

- Molecule 9 is a protein called Alpha-amanitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	N	8	64	39	10	14	1	0	0

- Molecule 10 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	Z	3	75	30	12	28	5	0	0

- Molecule 11 is a protein called Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	A	559	4580	2924	795	834	27	0	0

- Molecule 12 is a protein called Transcription initiation factor TFIID subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	B	963	7796	5011	1315	1412	58	0	0

- Molecule 13 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	D	164	1366	851	256	255	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	d	158	Total	C	N	O	S	0	0
			1307	814	238	252	3		

- Molecule 14 is a protein called Transcription initiation factor TFIID subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	547	Total	C	N	O	S	0	0
			4376	2774	759	822	21		
14	e	539	Total	C	N	O	S	0	0
			4327	2746	748	814	19		

- Molecule 15 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	412	Total	C	N	O	S	0	0
			3143	1994	548	583	18		
15	f	403	Total	C	N	O	S	0	0
			3081	1954	533	576	18		

- Molecule 16 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	144	Total	C	N	O	S	0	0
			1171	742	215	210	4		

- Molecule 17 is a protein called Transcription initiation factor TFIID subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	209	Total	C	N	O	S	0	0
			1633	1034	283	311	5		

- Molecule 18 is a protein called Transcription initiation factor TFIID subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	120	Total	C	N	O	S	0	0
			959	610	166	177	6		
18	i	121	Total	C	N	O	S	0	0
			967	615	167	178	7		

- Molecule 19 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	90	Total	C	N	O	S	0	0
			720	466	115	135	4		
19	j	95	Total	C	N	O	S	0	0
			759	488	124	143	4		

- Molecule 20 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	76	Total	C	N	O	S	0	0
			622	388	109	122	3		
20	l	107	Total	C	N	O	S	0	0
			876	547	158	166	5		

- Molecule 21 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 22 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	179	Total	C	N	O	S	0	0
			1422	923	251	241	7		

- Molecule 23 is a protein called Transcription initiation factor IIA beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 24 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	282	Total	C	N	O	S	0	0
			2167	1353	384	412	18		

- Molecule 25 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	176	Total	C	N	O	S	0	0
			1461	921	268	268	4		

- Molecule 26 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	T	222	1788	1127	320	338	3	0	0

- Molecule 27 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	U	184	1520	957	272	280	11	0	0

- Molecule 28 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	V	165	1357	865	235	253	4	0	0

- Molecule 29 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
29	X	63	1301	616	245	377	63	0	0

- Molecule 30 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
30	Y	78	1592	757	293	464	78	0	0

- Molecule 31 is a protein called Transcription initiation factor TFIID subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	c	127	1011	638	174	193	6	0	0

- Molecule 32 is a protein called Transcription initiation factor TFIID subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	k	98	785	499	142	139	5	0	0

- Molecule 33 is a protein called Transcription initiation factor TFIID subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	m	87	Total	C	N	O	S	0	0
			724	456	131	131	6		

- Molecule 34 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	o	1452	Total	C	N	O	S	0	0
			11510	7235	2056	2146	73		

- Molecule 35 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	p	1149	Total	C	N	O	S	0	0
			9175	5796	1614	1701	64		

- Molecule 36 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	q	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 37 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	r	128	Total	C	N	O	S	0	0
			1050	656	178	212	4		

- Molecule 38 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	s	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

- Molecule 39 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	t	82	Total	C	N	O	S	0	0
			657	418	113	121	5		

- Molecule 40 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	u	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 41 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	v	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 42 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	w	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- Molecule 43 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	x	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 44 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	y	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 45 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	z	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 46 is ZINC ION (CCD ID: ZN) (formula: Zn).

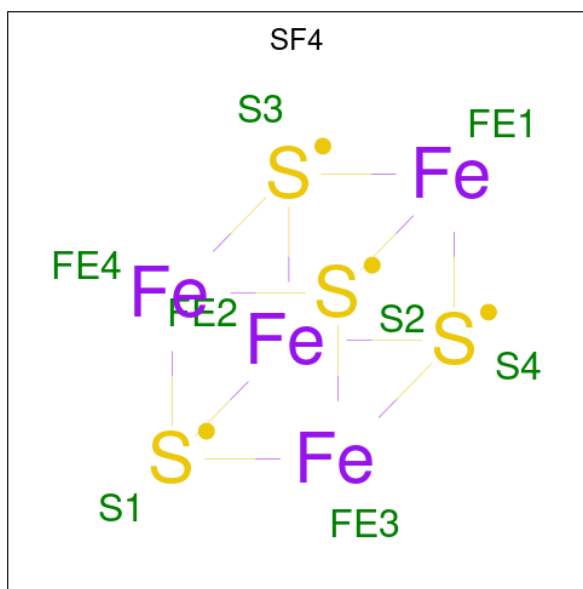
Mol	Chain	Residues	Atoms		AltConf
46	0	2	Total	Zn	0
			2	2	
46	2	3	Total	Zn	0
			3	3	
46	3	2	Total	Zn	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
46	R	1	Total	Zn	0
			1	1	
46	U	1	Total	Zn	0
			1	1	
46	o	2	Total	Zn	0
			2	2	
46	p	1	Total	Zn	0
			1	1	
46	q	1	Total	Zn	0
			1	1	
46	w	2	Total	Zn	0
			2	2	
46	x	1	Total	Zn	0
			1	1	
46	z	1	Total	Zn	0
			1	1	

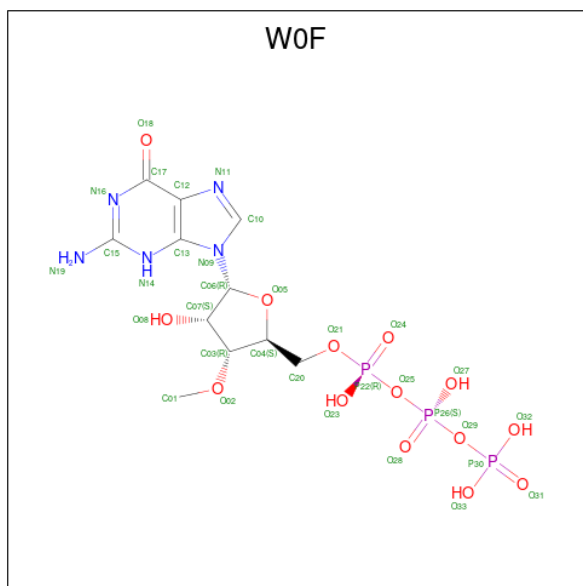
- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
47	7	1	Total	Fe	S	0
			8	4	4	

- Molecule 48 is [(2 {S},3 {R},4 {S},5 {R})-5-(2-azanyl-6-oxidanylidene-3 {H}-purin-9-yl)-3-methoxy-4-oxidanyl-oxolan-2-yl]methoxy-oxidanyl-phosphoryl phosphono hydrogen phosphate (CCD ID: W0F) (formula: C₁₁H₁₈N₅O₁₄P₃) (labeled as "Ligand of Interest" by

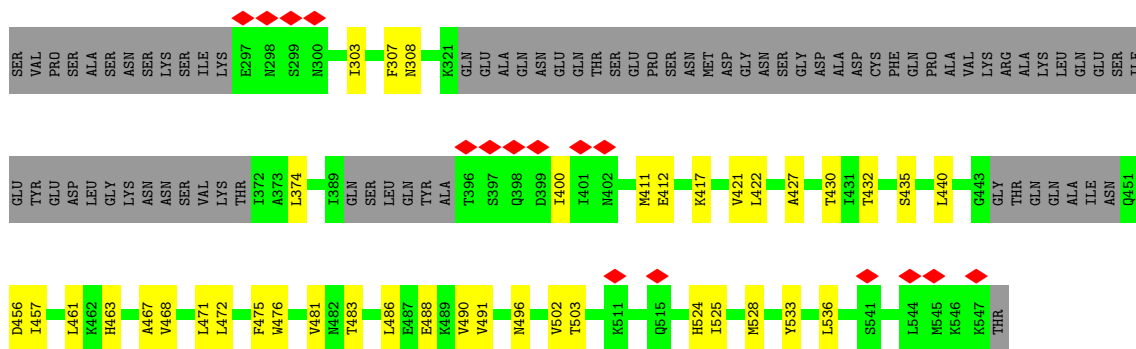
depositor).



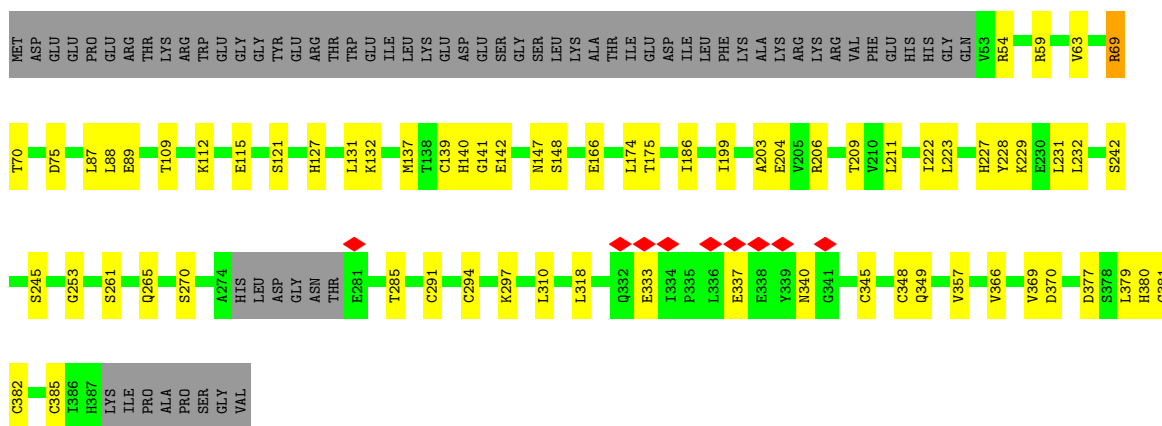
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
48	Z	1	33	11	5	14	3	0

- Molecule 49 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

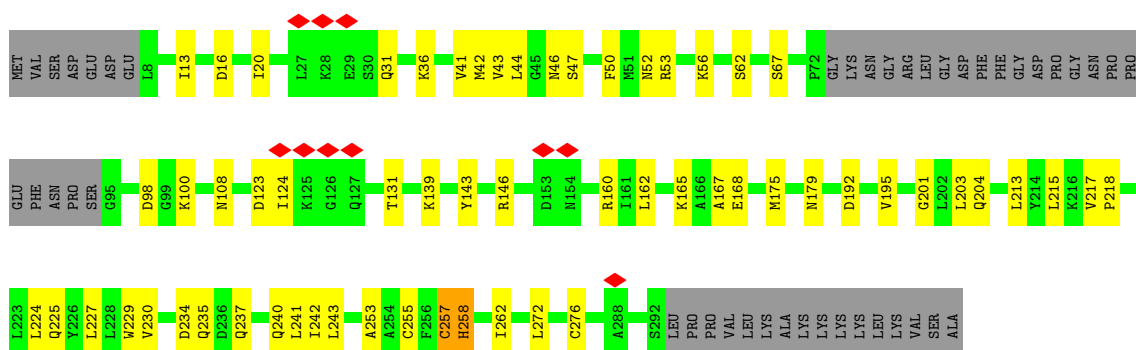
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
49	o	1	1	1	0



• Molecule 3: General transcription factor IIIH subunit 2

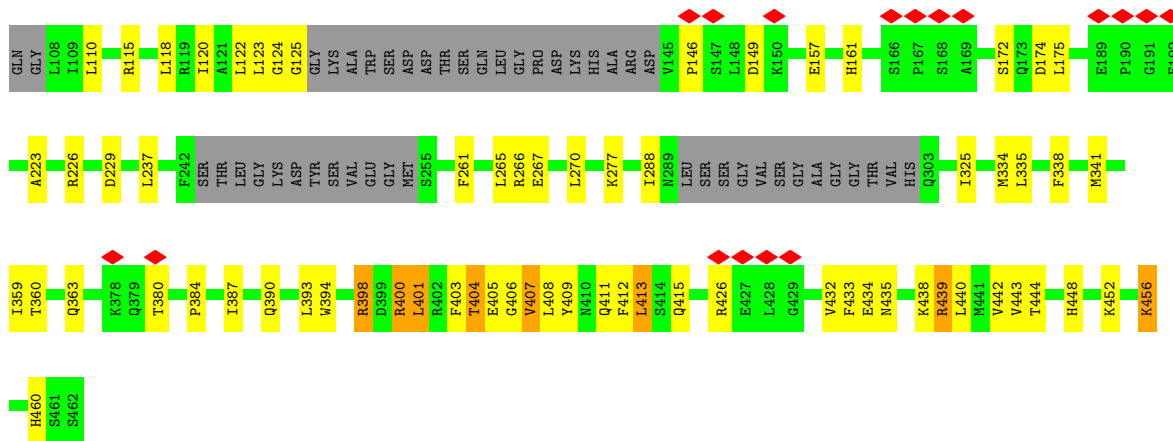


• Molecule 4: General transcription factor IIIH subunit 3

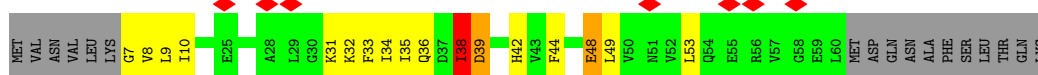


• Molecule 5: General transcription factor IIIH subunit 4

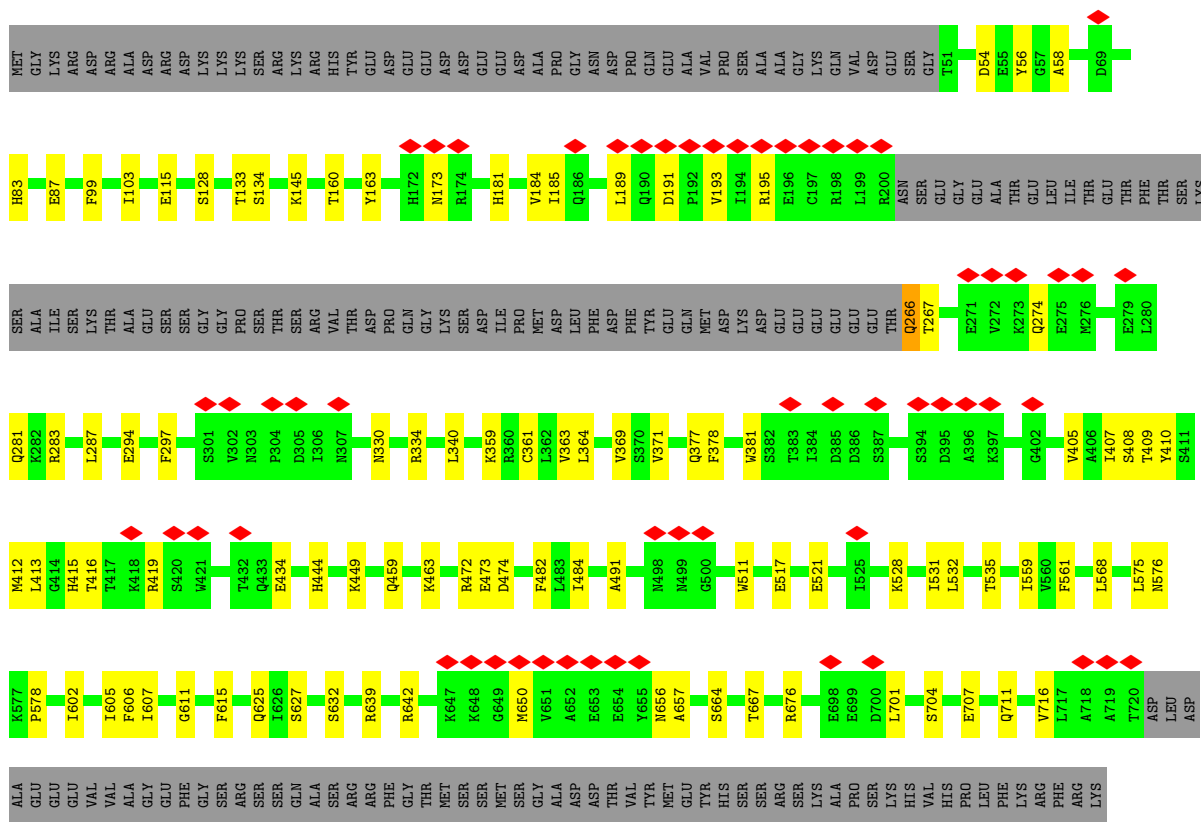




• Molecule 6: General transcription factor IIIH subunit 5

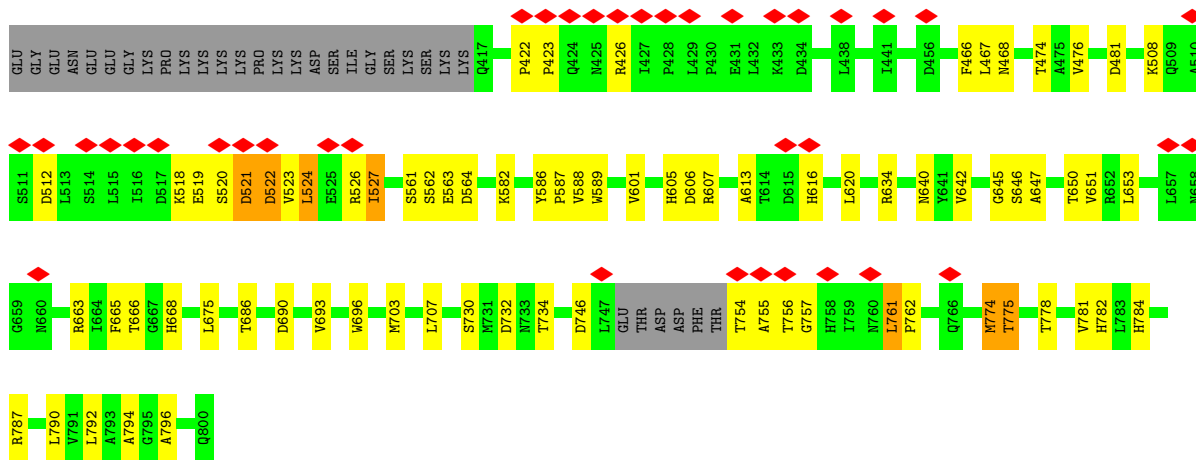


• Molecule 7: General transcription and DNA repair factor IIIH helicase subunit XPB

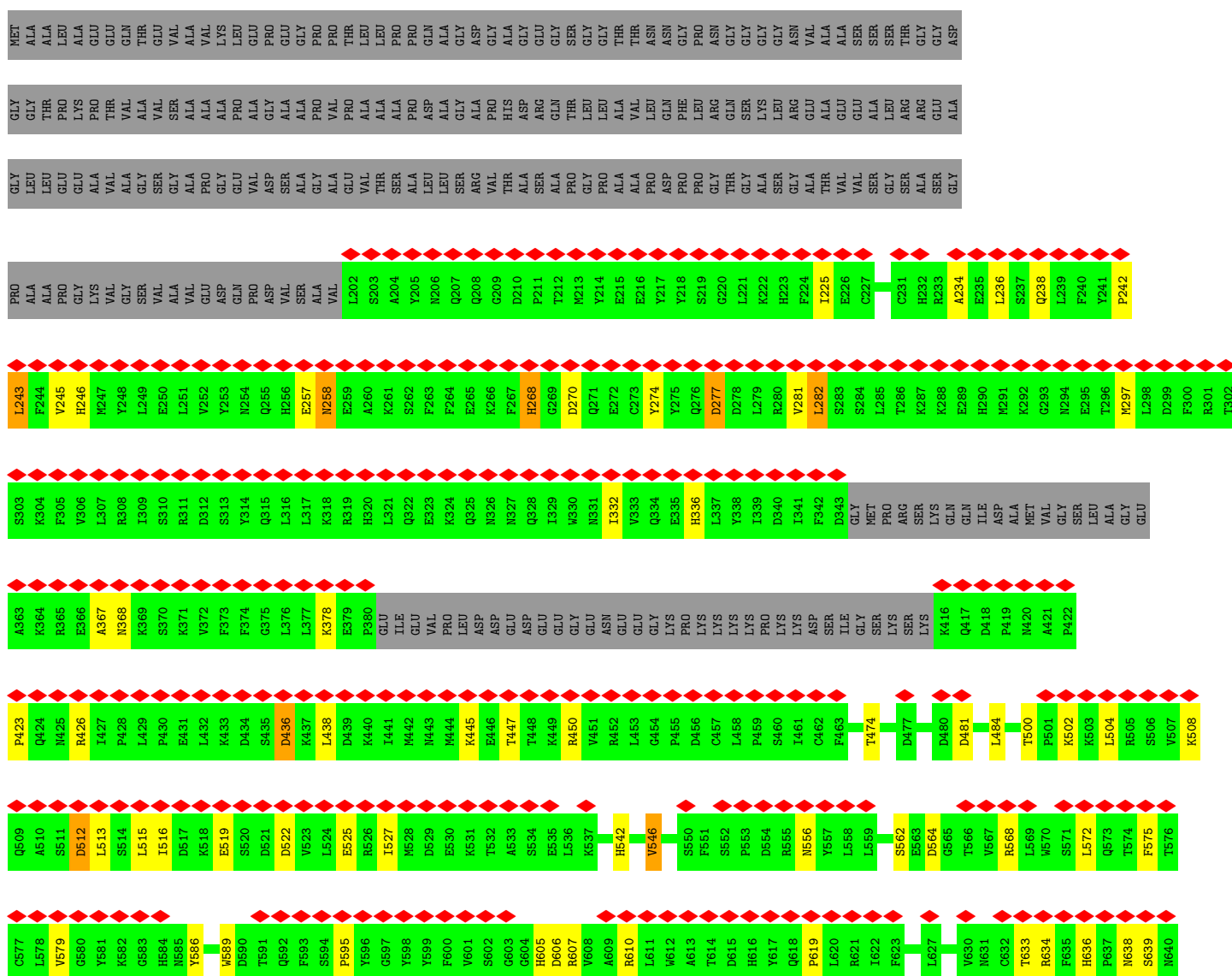


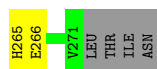
• Molecule 8: General transcription and DNA repair factor IIIH helicase subunit XPD

T1200	K1201	D1202	E1203	E1204	F1205	I1206	L1207	M1208	N1209	P1210	Q1211	R1212	S1213	T1214	V1215	W1216	X1217	Y1218	Z1219	AA1220	AB1221	AC1222	AD1223	AE1224	AF1225	AG1226	AH1227	AI1228	AJ1229	AK1230	AL1231	AM1232	AN1233	AO1234	AP1235	AQ1236	AR1237	AS1238	AT1239	AV1240	AW1241	AX1242	AY1243	AZ1244	BA1245	BB1246	BC1247	BD1248	BE1249	BF1250	BG1251	BH1252	BI1253	BJ1254	BK1255	BL1256	BM1257	BN1258	BO1259	BP1260	BQ1261	BR1262	BS1263	BT1264	BV1265	BW1266	BX1267	BY1268	BZ1269	CA1270	CB1271	CC1272	CD1273	CE1274	CF1275	CG1276	CH1277	CI1278	CJ1279	CK1280	CL1281	CM1282	CN1283	CO1284	CP1285	CQ1286	CR1287	CS1288	CT1289	CU1290	CV1291	CG1292	CH1293	CI1294	CJ1295	CK1296	CL1297	CM1298	CN1299	CO1300	CP1301	CQ1302	CR1303	CS1304	CT1305	CU1306	CV1307	CG1308	CH1309	CI1310	CJ1311	CK1312	CL1313	CM1314	CN1315	CO1316	CP1317	CQ1318	CR1319	CS1320	CT1321	CU1322	CV1323	CG1324	CH1325	CI1326	CJ1327	CK1328	CL1329	CM1330	CN1331	CO1332	CP1333	CQ1334	CR1335	CS1336	CT1337	CU1338	CV1339	CG1340	CH1341	CI1342	CJ1343	CK1344	CL1345	CM1346	CN1347	CO1348	CP1349	CQ1350	CR1351	CS1352	CT1353	CU1354	CV1355	CG1356	CH1357	CI1358	CJ1359	CK1360	CL1361	CM1362	CN1363	CO1364	CP1365	CQ1366	CR1367	CS1368	CT1369	CU1370	CV1371	CG1372	CH1373	CI1374	CJ1375	CK1376	CL1377	CM1378	CN1379	CO1380	CP1381	CQ1382	CR1383	CS1384	CT1385	CU1386	CV1387	CG1388	CH1389	CI1390	CJ1391	CK1392	CL1393	CM1394	CN1395	CO1396	CP1397	CQ1398	CR1399	CS1400	CT1401	CU1402	CV1403	CG1404	CH1405	CI1406	CJ1407	CK1408	CL1409	CM1410	CN1411	CO1412	CP1413	CQ1414	CR1415	CS1416	CT1417	CU1418	CV1419	CG1420	CH1421	CI1422	CJ1423	CK1424	CL1425	CM1426	CN1427	CO1428	CP1429	CQ1430	CR1431	CS1432	CT1433	CU1434	CV1435	CG1436	CH1437	CI1438	CJ1439	CK1440	CL1441	CM1442	CN1443	CO1444	CP1445	CQ1446	CR1447	CS1448	CT1449	CU1450	CV1451	CG1452	CH1453	CI1454	CJ1455	CK1456	CL1457	CM1458	CN1459	CO1460	CP1461	CQ1462	CR1463	CS1464	CT1465	CU1466	CV1467	CG1468	CH1469	CI1470	CJ1471	CK1472	CL1473	CM1474	CN1475	CO1476	CP1477	CQ1478	CR1479	CS1480	CT1481	CU1482	CV1483	CG1484	CH1485	CI1486	CJ1487	CK1488	CL1489	CM1490	CN1491	CO1492	CP1493	CQ1494	CR1495	CS1496	CT1497	CU1498	CV1499	CG1500	CH1501	CI1502	CJ1503	CK1504	CL1505	CM1506	CN1507	CO1508	CP1509	CQ1510	CR1511	CS1512	CT1513	CU1514	CV1515	CG1516	CH1517	CI1518	CJ1519	CK1520	CL1521	CM1522	CN1523	CO1524	CP1525	CQ1526	CR1527	CS1528	CT1529	CU1530	CV1531	CG1532	CH1533	CI1534	CJ1535	CK1536	CL1537	CM1538	CN1539	CO1540	CP1541	CQ1542	CR1543	CS1544	CT1545	CU1546	CV1547	CG1548	CH1549	CI1550	CJ1551	CK1552	CL1553	CM1554	CN1555	CO1556	CP1557	CQ1558	CR1559	CS1560	CT1561	CU1562	CV1563	CG1564	CH1565	CI1566	CJ1567	CK1568	CL1569	CM1570	CN1571	CO1572	CP1573	CQ1574	CR1575	CS1576	CT1577	CU1578	CV1579	CG1580	CH1581	CI1582	CJ1583	CK1584	CL1585	CM1586	CN1587	CO1588	CP1589	CQ1590	CR1591	CS1592	CT1593	CU1594	CV1595	CG1596	CH1597	CI1598	CJ1599	CK1600	CL1601	CM1602	CN1603	CO1604	CP1605	CQ1606	CR1607	CS1608	CT1609	CU1610	CV1611	CG1612	CH1613	CI1614	CJ1615	CK1616	CL1617	CM1618	CN1619	CO1620	CP1621	CQ1622	CR1623	CS1624	CT1625	CU1626	CV1627	CG1628	CH1629	CI1630	CJ1631	CK1632	CL1633	CM1634	CN1635	CO1636	CP1637	CQ1638	CR1639	CS1640	CT1641	CU1642	CV1643	CG1644	CH1645	CI1646	CJ1647	CK1648	CL1649	CM1650	CN1651	CO1652	CP1653	CQ1654	CR1655	CS1656	CT1657	CU1658	CV1659	CG1660	CH1661	CI1662	CJ1663	CK1664	CL1665	CM1666	CN1667	CO1668	CP1669	CQ1670	CR1671	CS1672	CT1673	CU1674	CV1675	CG1676	CH1677	CI1678	CJ1679	CK1680	CL1681	CM1682	CN1683	CO1684	CP1685	CQ1686	CR1687	CS1688	CT1689	CU1690	CV1691	CG1692	CH1693	CI1694	CJ1695	CK1696	CL1697	CM1698	CN1699	CO1700	CP1701	CQ1702	CR1703	CS1704	CT1705	CU1706	CV1707	CG1708	CH1709	CI1710	CJ1711	CK1712	CL1713	CM1714	CN1715	CO1716	CP1717	CQ1718	CR1719	CS1720	CT1721	CU1722	CV1723	CG1724	CH1725	CI1726	CJ1727	CK1728	CL1729	CM1730	CN1731	CO1732	CP1733	CQ1734	CR1735	CS1736	CT1737	CU1738	CV1739	CG1740	CH1741	CI1742	CJ1743	CK1744	CL1745	CM1746	CN1747	CO1748	CP1749	CQ1750	CR1751	CS1752	CT1753	CU1754	CV1755	CG1756	CH1757	CI1758	CJ1759	CK1760	CL1761	CM1762	CN1763	CO1764	CP1765	CQ1766	CR1767	CS1768	CT1769	CU1770	CV1771	CG1772	CH1773	CI1774	CJ1775	CK1776	CL1777	CM1778	CN1779	CO1780	CP1781	CQ1782	CR1783	CS1784	CT1785	CU1786	CV1787	CG1788	CH1789	CI1790	CJ1791	CK1792	CL1793	CM1794	CN1795	CO1796	CP1797	CQ1798	CR1799	CS1800	CT1801	CU1802	CV1803	CG1804	CH1805	CI1806	CJ1807	CK1808	CL1809	CM1810	CN1811	CO1812	CP1813	CQ1814	CR1815	CS1816	CT1817	CU1818	CV1819	CG1820	CH1821	CI1822	CJ1823	CK1824	CL1825	CM1826	CN1827	CO1828	CP1829	CQ1830	CR1831	CS1832	CT1833	CU1834	CV1835	CG1836	CH1837	CI1838	CJ1839	CK1840	CL1841	CM1842	CN1843	CO1844	CP1845	CQ1846	CR1847	CS1848	CT1849	CU1850	CV1851	CG1852	CH1853	CI1854	CJ1855	CK1856	CL1857	CM1858	CN1859	CO1860	CP1861	CQ1862	CR1863	CS1864	CT1865	CU1866	CV1867	CG1868	CH1869	CI1870	CJ1871	CK1872	CL1873	CM1874	CN1875	CO1876	CP1877	CQ1878	CR1879	CS1880	CT1881	CU1882	CV1883	CG1884	CH1885	CI1886	CJ1887	CK1888	CL1889	CM1890	CN1891	CO1892	CP1893	CQ1894	CR1895	CS1896	CT1897	CU1898	CV1899	CG1900	CH1901	CI1902	CJ1903	CK1904	CL1905	CM1906	CN1907	CO1908	CP1909	CQ1910	CR1911	CS1912	CT1913	CU1914	CV1915	CG1916	C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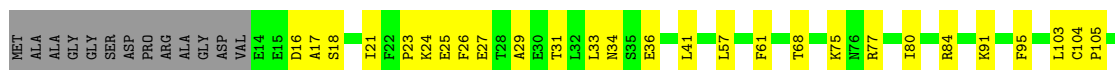


● Molecule 14: Transcription initiation factor TFIID subunit 5

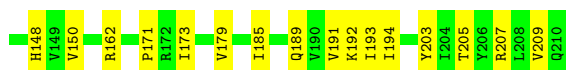
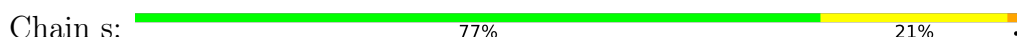




• Molecule 37: DNA-directed RNA polymerase II subunit RPB4



• Molecule 38: DNA-directed RNA polymerase II subunit E



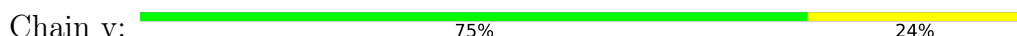
• Molecule 39: DNA-directed RNA polymerase II subunit F

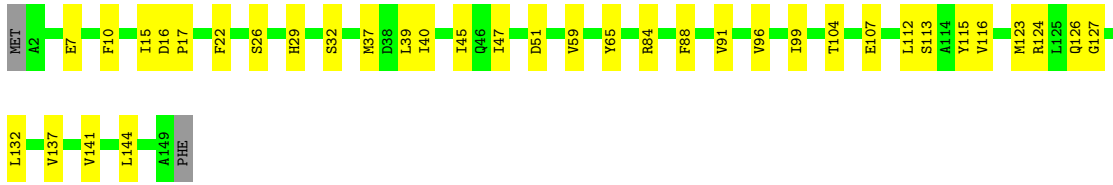


• Molecule 40: DNA-directed RNA polymerase II subunit RPB7



• Molecule 41: DNA-directed RNA polymerases I, II, and III subunit RPABC3

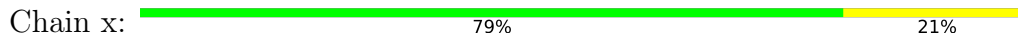




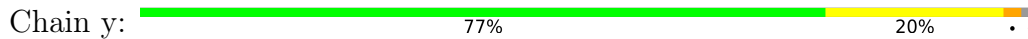
- Molecule 42: DNA-directed RNA polymerase II subunit RPB9



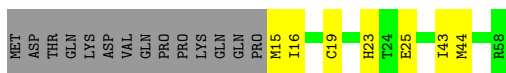
- Molecule 43: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 44: DNA-directed RNA polymerase II subunit RPB11-a



- Molecule 45: RPB12



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7488	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.220	Depositor
Minimum map value	-1.775	Depositor
Average map value	0.043	Depositor
Map value standard deviation	0.191	Depositor
Recommended contour level	0.517	Depositor
Map size (\AA)	426.88, 426.88, 426.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.334, 1.334, 1.334	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, G2L, CSX, ZN, W0F, HYP, TRX, ILX, SF4, ATP

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	0	0.41	0/1437	0.70	3/1926 (0.2%)
2	1	0.20	0/2210	0.34	0/2975
3	2	0.19	0/2624	0.33	1/3555 (0.0%)
4	3	0.24	0/2103	0.36	0/2846
5	4	0.31	0/3262	0.45	1/4418 (0.0%)
6	5	0.41	0/433	0.79	1/585 (0.2%)
7	6	0.19	0/4994	0.33	0/6745
8	7	0.17	0/5875	0.30	0/7955
9	N	0.41	0/22	0.99	0/26
10	Z	0.50	0/21	0.56	0/30
11	A	0.63	0/4698	0.95	5/6345 (0.1%)
12	B	0.46	1/7993 (0.0%)	0.69	6/10836 (0.1%)
13	D	0.56	0/1379	0.88	3/1843 (0.2%)
13	d	0.48	0/1321	0.71	0/1772
14	E	0.45	1/4482 (0.0%)	0.72	3/6069 (0.0%)
14	e	0.55	1/4433 (0.0%)	0.77	0/6004
15	F	0.63	1/3201 (0.0%)	1.00	7/4347 (0.2%)
15	f	0.47	0/3140	0.79	6/4268 (0.1%)
16	G	0.68	0/1190	0.94	1/1601 (0.1%)
17	H	0.63	3/1673 (0.2%)	0.86	5/2285 (0.2%)
18	I	0.20	0/981	0.41	0/1332
18	i	0.21	0/989	0.40	0/1343
19	J	0.83	0/736	1.15	2/998 (0.2%)
19	j	0.73	0/775	0.96	0/1049
20	L	0.69	0/630	1.14	1/852 (0.1%)
20	l	0.59	0/888	0.88	0/1194
21	O	0.26	0/816	0.36	0/1105
22	P	0.12	0/1448	0.26	0/1948
23	Q	0.19	0/945	0.35	0/1274
24	R	0.38	1/2199 (0.0%)	0.63	5/2967 (0.2%)
25	S	0.57	0/1496	0.95	7/2013 (0.3%)
26	T	0.43	0/1817	0.63	2/2445 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	U	0.35	0/1545	0.69	1/2075 (0.0%)
28	V	0.24	0/1380	0.58	0/1854
29	X	0.31	0/1460	0.61	0/2251
30	Y	0.40	0/1785	0.59	0/2750
31	c	0.48	0/1035	0.67	0/1406
32	k	0.28	0/799	0.53	1/1070 (0.1%)
33	m	0.85	0/733	1.18	1/977 (0.1%)
34	o	0.32	0/11723	0.47	4/15830 (0.0%)
35	p	0.34	1/9358 (0.0%)	0.47	5/12633 (0.0%)
36	q	0.32	1/2102 (0.0%)	0.41	0/2857
37	r	0.12	0/1064	0.23	0/1428
38	s	0.28	0/1751	0.43	1/2366 (0.0%)
39	t	0.24	0/667	0.29	0/901
40	u	0.23	0/1382	0.39	1/1874 (0.1%)
41	v	0.26	0/1207	0.38	0/1628
42	w	0.21	0/948	0.31	0/1284
43	x	0.36	0/542	0.48	0/730
44	y	0.27	0/939	0.34	0/1271
45	z	0.33	0/377	0.51	0/500
All	All	0.41	10/111008 (0.0%)	0.62	73/150636 (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
6	5	0	1
24	R	0	2
35	p	0	2
All	All	0	5

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	28	ASN	C-O	-7.47	1.15	1.24
24	R	105	ARG	C-O	7.47	1.33	1.24
17	H	27	ASP	C-O	-7.05	1.15	1.24
17	H	31	LEU	C-O	-6.16	1.16	1.24
12	B	61	ASN	C-O	-6.02	1.18	1.24

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	55	LYS	CB-CA-C	-11.44	95.03	111.85
12	B	491	HIS	N-CA-C	-9.47	100.96	111.28
25	S	60	GLU	N-CA-C	-9.25	100.31	111.69
24	R	106	THR	N-CA-C	9.18	125.27	111.04
15	f	149	PRO	O-C-N	8.90	125.40	121.31

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	5	36	GLN	Mainchain
24	R	105	ARG	Mainchain
24	R	106	THR	Peptide
35	p	391	LYS	Mainchain
35	p	426	GLY	Mainchain

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	0	1420	0	1420	122	0
2	1	2167	0	2175	39	0
3	2	2567	0	2539	94	0
4	3	2066	0	2097	103	0
5	4	3189	0	3243	141	0
6	5	428	0	434	42	0
7	6	4890	0	4949	94	0
8	7	5751	0	5794	141	0
9	N	64	0	51	7	0
10	Z	75	0	31	10	0
11	A	4580	0	4502	98	0
12	B	7796	0	7751	116	0
13	D	1366	0	1390	76	0
13	d	1307	0	1318	14	0
14	E	4376	0	4256	75	0
14	e	4327	0	4197	58	0
15	F	3143	0	3093	101	0
15	f	3081	0	3012	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	G	1171	0	1222	16	0
17	H	1633	0	1621	33	0
18	I	959	0	969	13	0
18	i	967	0	977	10	0
19	J	720	0	719	13	0
19	j	759	0	759	14	0
20	L	622	0	620	19	0
20	l	876	0	893	10	0
21	O	806	0	818	17	0
22	P	1422	0	1514	21	0
23	Q	930	0	888	12	0
24	R	2167	0	2193	61	0
25	S	1461	0	1429	71	0
26	T	1788	0	1819	69	0
27	U	1520	0	1520	215	0
28	V	1357	0	1381	90	0
29	X	1301	0	709	40	0
30	Y	1592	0	875	51	0
31	c	1011	0	975	18	0
32	k	785	0	818	8	0
33	m	724	0	744	24	0
34	o	11510	0	11615	441	0
35	p	9175	0	9196	367	0
36	q	2059	0	2007	59	0
37	r	1050	0	1033	34	0
38	s	1720	0	1737	65	0
39	t	657	0	684	12	0
40	u	1351	0	1358	166	0
41	v	1186	0	1147	31	0
42	w	927	0	860	26	0
43	x	533	0	553	9	0
44	y	920	0	942	30	0
45	z	372	0	378	7	0
46	0	2	0	0	0	0
46	2	3	0	0	0	0
46	3	2	0	0	0	0
46	R	1	0	0	0	0
46	U	1	0	0	0	0
46	o	2	0	0	0	0
46	p	1	0	0	0	0
46	q	1	0	0	0	0
46	w	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	x	1	0	0	0	0
46	z	1	0	0	0	0
47	7	8	0	0	0	0
48	Z	33	0	0	10	0
49	o	1	0	0	0	0
All	All	108683	0	107225	2782	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 13.

The worst 5 of 2782 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)
34:o:189:PRO:HD3	34:o:202:TRP:CZ2	1.24	1.67
27:U:152:PHE:CE1	40:u:95:VAL:HB	1.30	1.65
34:o:189:PRO:HD3	34:o:202:TRP:CH2	1.23	1.65
27:U:139:LEU:HB2	40:u:160:ILE:CG1	1.25	1.61
36:q:44:ILE:CD1	36:q:178:PRO:HB3	1.32	1.57

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	0	169/309 (55%)	156 (92%)	13 (8%)	0	100	100
2	1	253/548 (46%)	243 (96%)	10 (4%)	0	100	100
3	2	325/395 (82%)	313 (96%)	12 (4%)	0	100	100
4	3	259/308 (84%)	253 (98%)	6 (2%)	0	100	100
5	4	384/462 (83%)	365 (95%)	19 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	5	52/71 (73%)	48 (92%)	2 (4%)	2 (4%)	2	19
7	6	601/782 (77%)	573 (95%)	27 (4%)	1 (0%)	43	78
8	7	710/760 (93%)	683 (96%)	27 (4%)	0	100	100
9	N	4/8 (50%)	3 (75%)	1 (25%)	0	100	100
11	A	543/1872 (29%)	519 (96%)	23 (4%)	1 (0%)	43	78
12	B	959/1199 (80%)	911 (95%)	48 (5%)	0	100	100
13	D	158/1085 (15%)	153 (97%)	5 (3%)	0	100	100
13	d	154/1085 (14%)	150 (97%)	4 (3%)	0	100	100
14	E	541/800 (68%)	518 (96%)	22 (4%)	1 (0%)	43	78
14	e	531/800 (66%)	482 (91%)	48 (9%)	1 (0%)	43	78
15	F	408/677 (60%)	391 (96%)	16 (4%)	1 (0%)	43	78
15	f	399/677 (59%)	380 (95%)	19 (5%)	0	100	100
16	G	138/349 (40%)	135 (98%)	3 (2%)	0	100	100
17	H	207/310 (67%)	189 (91%)	13 (6%)	5 (2%)	4	27
18	I	118/264 (45%)	115 (98%)	3 (2%)	0	100	100
18	i	119/264 (45%)	115 (97%)	4 (3%)	0	100	100
19	J	86/218 (39%)	82 (95%)	4 (5%)	0	100	100
19	j	91/218 (42%)	85 (93%)	4 (4%)	2 (2%)	5	29
20	L	74/161 (46%)	72 (97%)	2 (3%)	0	100	100
20	l	105/161 (65%)	100 (95%)	5 (5%)	0	100	100
21	O	97/109 (89%)	95 (98%)	2 (2%)	0	100	100
22	P	177/339 (52%)	175 (99%)	2 (1%)	0	100	100
23	Q	109/376 (29%)	102 (94%)	7 (6%)	0	100	100
24	R	278/316 (88%)	258 (93%)	17 (6%)	3 (1%)	11	46
25	S	174/517 (34%)	159 (91%)	13 (8%)	2 (1%)	11	46
26	T	218/249 (88%)	213 (98%)	4 (2%)	1 (0%)	24	63
27	U	180/439 (41%)	153 (85%)	27 (15%)	0	100	100
28	V	163/291 (56%)	139 (85%)	24 (15%)	0	100	100
31	c	125/929 (14%)	116 (93%)	9 (7%)	0	100	100
32	k	96/211 (46%)	91 (95%)	5 (5%)	0	100	100
33	m	85/124 (68%)	82 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	o	1448/1970 (74%)	1400 (97%)	43 (3%)	5 (0%)	36	72
35	p	1145/1174 (98%)	1111 (97%)	33 (3%)	1 (0%)	48	83
36	q	253/275 (92%)	248 (98%)	5 (2%)	0	100	100
37	r	126/142 (89%)	126 (100%)	0	0	100	100
38	s	207/210 (99%)	202 (98%)	5 (2%)	0	100	100
39	t	80/127 (63%)	78 (98%)	2 (2%)	0	100	100
40	u	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
41	v	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
42	w	112/125 (90%)	109 (97%)	3 (3%)	0	100	100
43	x	65/67 (97%)	64 (98%)	0	1 (2%)	8	40
44	y	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
45	z	42/58 (72%)	40 (95%)	2 (5%)	0	100	100
All	All	12996/22270 (58%)	12413 (96%)	556 (4%)	27 (0%)	44	78

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	5	48	GLU
14	E	523	VAL
17	H	156	PRO
24	R	95	GLU
25	S	87	VAL

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	0	164/283 (58%)	158 (96%)	6 (4%)	30	51
2	1	241/484 (50%)	241 (100%)	0	100	100
3	2	295/352 (84%)	294 (100%)	1 (0%)	86	86
4	3	234/272 (86%)	232 (99%)	2 (1%)	70	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	4	346/399 (87%)	339 (98%)	7 (2%)	48	66
6	5	48/64 (75%)	47 (98%)	1 (2%)	47	65
7	6	536/688 (78%)	535 (100%)	1 (0%)	87	87
8	7	624/664 (94%)	624 (100%)	0	100	100
9	N	2/2 (100%)	2 (100%)	0	100	100
11	A	496/1665 (30%)	452 (91%)	44 (9%)	9	28
12	B	876/1083 (81%)	862 (98%)	14 (2%)	55	70
13	D	147/815 (18%)	136 (92%)	11 (8%)	12	33
13	d	146/815 (18%)	144 (99%)	2 (1%)	59	72
14	E	480/657 (73%)	467 (97%)	13 (3%)	39	61
14	e	475/657 (72%)	462 (97%)	13 (3%)	39	61
15	F	328/574 (57%)	307 (94%)	21 (6%)	16	37
15	f	322/574 (56%)	312 (97%)	10 (3%)	35	56
16	G	132/322 (41%)	124 (94%)	8 (6%)	17	38
17	H	181/270 (67%)	175 (97%)	6 (3%)	33	55
18	I	106/235 (45%)	106 (100%)	0	100	100
18	i	107/235 (46%)	107 (100%)	0	100	100
19	J	79/154 (51%)	72 (91%)	7 (9%)	9	28
19	j	83/154 (54%)	82 (99%)	1 (1%)	63	75
20	L	71/141 (50%)	66 (93%)	5 (7%)	14	35
20	l	98/141 (70%)	97 (99%)	1 (1%)	68	78
21	O	90/98 (92%)	90 (100%)	0	100	100
22	P	154/293 (53%)	154 (100%)	0	100	100
23	Q	105/324 (32%)	105 (100%)	0	100	100
24	R	238/268 (89%)	233 (98%)	5 (2%)	47	65
25	S	154/448 (34%)	132 (86%)	22 (14%)	3	13
26	T	196/218 (90%)	193 (98%)	3 (2%)	57	72
27	U	167/373 (45%)	166 (99%)	1 (1%)	78	83
28	V	150/261 (58%)	149 (99%)	1 (1%)	76	81
31	c	113/833 (14%)	111 (98%)	2 (2%)	51	68
32	k	87/182 (48%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	m	80/106 (76%)	71 (89%)	9 (11%)	5	19
34	o	1280/1749 (73%)	1257 (98%)	23 (2%)	51	68
35	p	1004/1027 (98%)	986 (98%)	18 (2%)	51	68
36	q	234/252 (93%)	227 (97%)	7 (3%)	36	57
37	r	118/126 (94%)	118 (100%)	0	100	100
38	s	191/192 (100%)	187 (98%)	4 (2%)	47	65
39	t	71/111 (64%)	71 (100%)	0	100	100
40	u	152/153 (99%)	150 (99%)	2 (1%)	61	74
41	v	129/131 (98%)	126 (98%)	3 (2%)	44	64
42	w	103/112 (92%)	100 (97%)	3 (3%)	37	58
43	x	56/56 (100%)	54 (96%)	2 (4%)	31	52
44	y	104/106 (98%)	101 (97%)	3 (3%)	37	58
45	z	41/55 (74%)	40 (98%)	1 (2%)	43	64
All	All	11634/19174 (61%)	11351 (98%)	283 (2%)	43	64

5 of 283 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	q	58	VAL
38	s	7	THR
14	e	268	HIS
14	E	761	LEU
14	E	521	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 218 such sidechains are listed below:

Mol	Chain	Res	Type
26	T	229	HIS
34	o	703	GLN
13	d	912	ASN
27	U	183	GLN
32	k	205	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	Z	1/3 (33%)	1 (100%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	Z	3	G2L

There are no RNA pucker outliers to report.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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
9	ILX	N	1	9	8,9,10	0.63	0	8,11,13	1.42	1 (12%)
9	TRX	N	2	9	15,16,17	1.06	1 (6%)	17,22,24	1.00	1 (5%)
10	G2L	Z	3	30,10,49	23,26,30	1.19	2 (8%)	31,38,44	2.12	7 (22%)
9	CSX	N	6	9	3,6,7	1.12	0	1,6,8	2.15	1 (100%)
9	HYP	N	8	9	7,8,9	0.84	0	5,10,12	2.36	2 (40%)

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
9	ILX	N	1	9	-	7/11/12/14	-
9	TRX	N	2	9	-	2/5/6/8	0/2/2/2
10	G2L	Z	3	30,10,49	-	2/9/27/31	0/3/3/3
9	CSX	N	6	9	-	2/2/5/7	-
9	HYP	N	8	9	-	0/0/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Z	3	G2L	C5-C4	3.19	1.47	1.38
10	Z	3	G2L	C6-N1	-2.40	1.34	1.38
9	N	2	TRX	CD2-CE2	2.17	1.44	1.41

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Z	3	G2L	C5-C4-N3	-6.24	118.45	128.39
10	Z	3	G2L	C2-N3-C4	5.13	121.14	112.30
10	Z	3	G2L	N9-C4-N3	4.65	135.25	125.95
9	N	8	HYP	CB-CG-CD	3.47	107.02	103.16
9	N	8	HYP	O-C-CA	-3.33	116.20	124.77

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	N	1	ILX	C-CA-CB-CG2
9	N	1	ILX	OD1-CD1-CG1-CB
9	N	1	ILX	OD1-CD1-CG1-OG1
9	N	6	CSX	N-CA-CB-SG
9	N	6	CSX	C-CA-CB-SG

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	N	1	ILX	2	0
9	N	2	TRX	1	0
10	Z	3	G2L	7	0
9	N	6	CSX	1	0
9	N	8	HYP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 18 are monoatomic - leaving 2 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
48	W0F	Z	2500	-	34,35,35	4.04	14 (41%)	43,55,55	3.45	17 (39%)
47	SF4	7	1000	8	0,12,12	-	-	-		

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
48	W0F	Z	2500	-	-	3/24/40/40	0/3/3/3
47	SF4	7	1000	8	-	-	0/6/5/5

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	Z	2500	W0F	P26-O29	13.67	1.74	1.59
48	Z	2500	W0F	C03-C04	-9.79	1.27	1.52
48	Z	2500	W0F	P22-O25	8.35	1.68	1.59
48	Z	2500	W0F	O05-C04	6.91	1.60	1.45
48	Z	2500	W0F	O05-C06	-5.98	1.28	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	Z	2500	W0F	O05-C06-N09	-14.55	75.38	108.36
48	Z	2500	W0F	C07-C06-N09	8.29	136.31	113.25
48	Z	2500	W0F	O05-C04-C03	-5.78	92.71	104.92
48	Z	2500	W0F	O27-P26-O25	-5.27	93.02	107.27
48	Z	2500	W0F	O05-C04-C20	4.93	125.14	109.33

There are no chirality outliers.

All (3) torsion outliers are listed below:

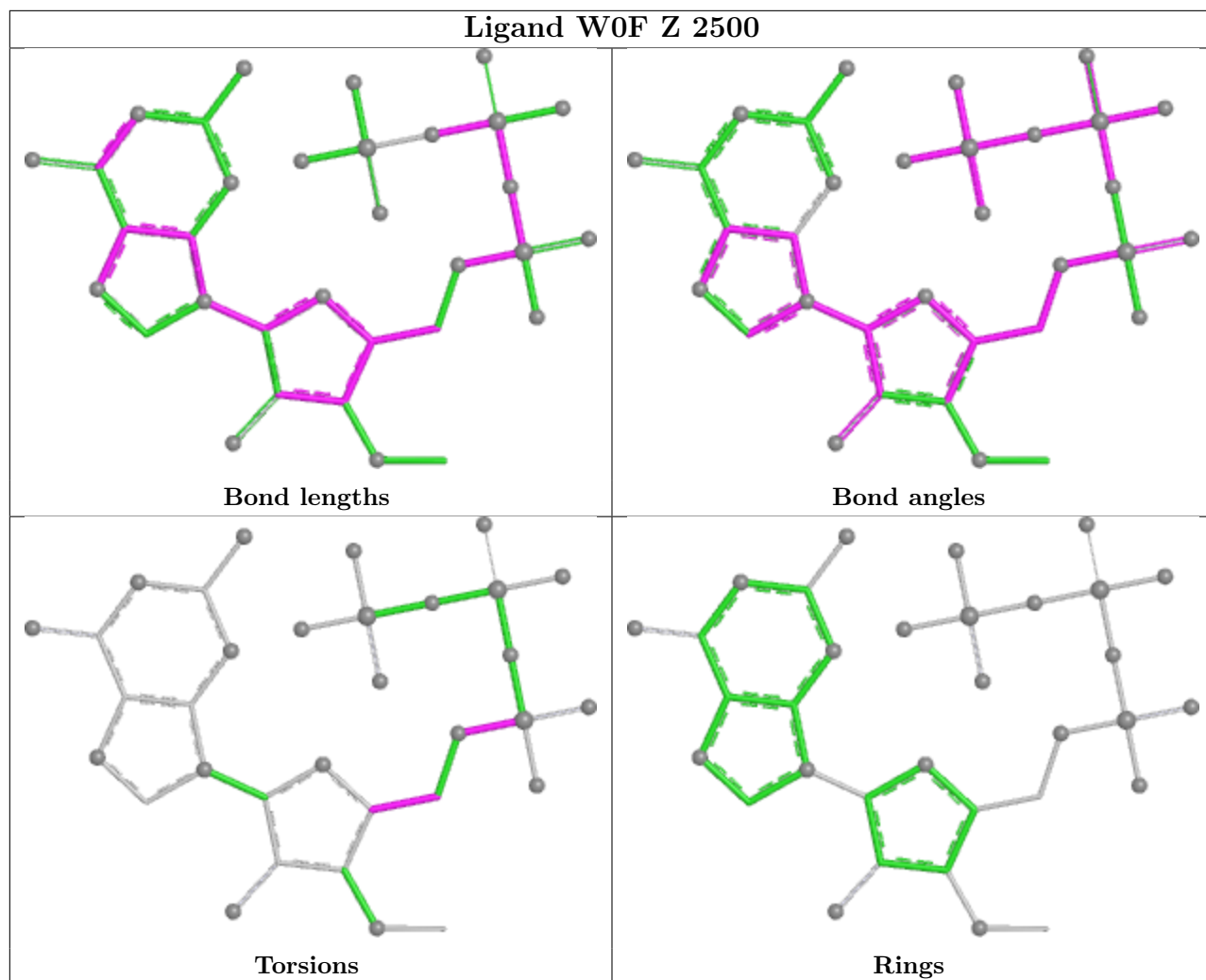
Mol	Chain	Res	Type	Atoms
48	Z	2500	W0F	C20-O21-P22-O24
48	Z	2500	W0F	C20-O21-P22-O25
48	Z	2500	W0F	C03-C04-C20-O21

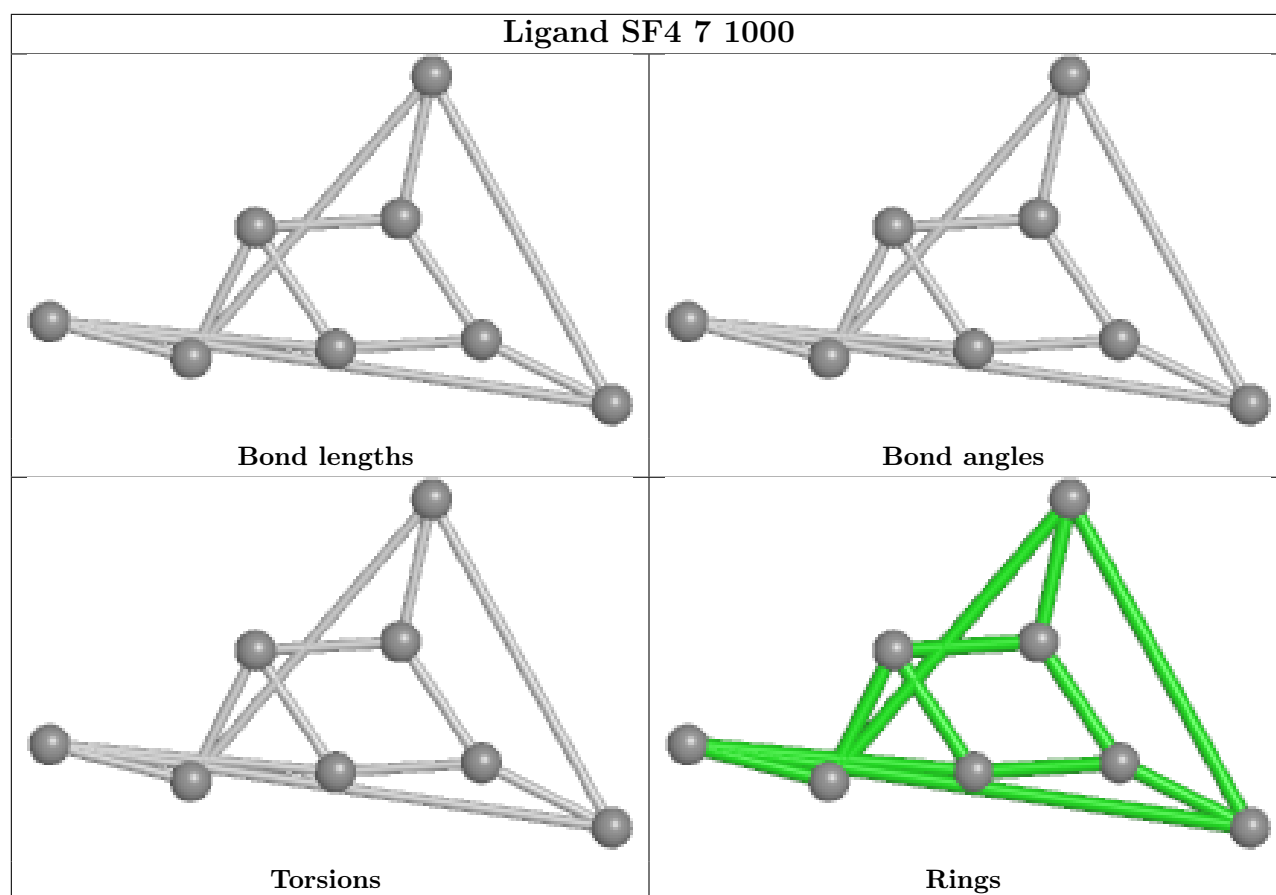
There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	Z	2500	W0F	10	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.

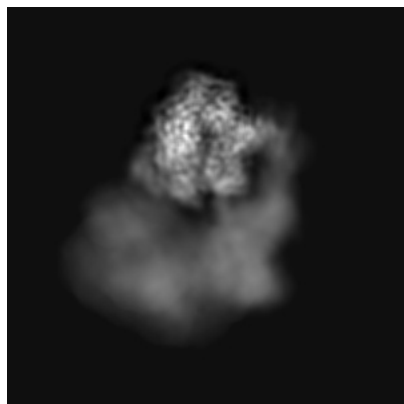
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37396. These allow visual inspection of the internal detail of the map and identification of artifacts.

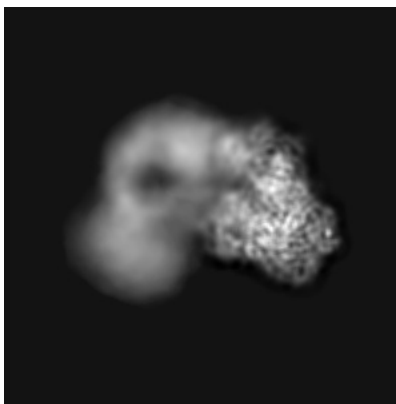
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

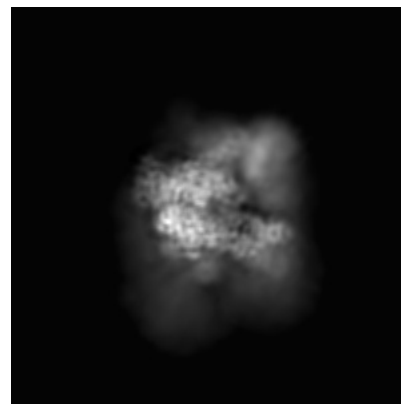
6.1.1 Primary map



X

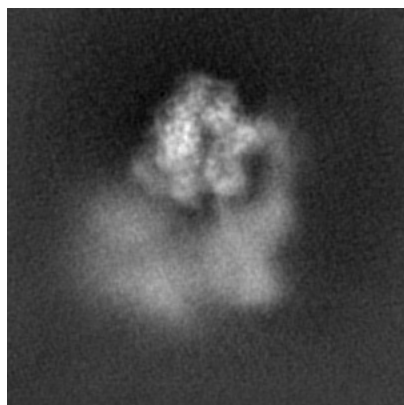


Y

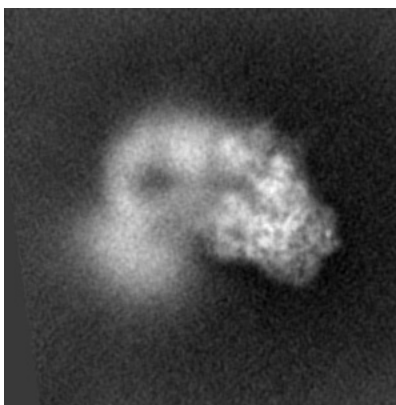


Z

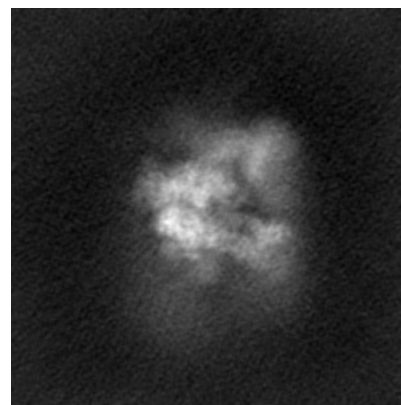
6.1.2 Raw map



X



Y

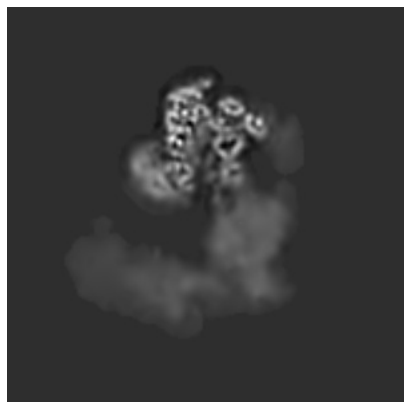


Z

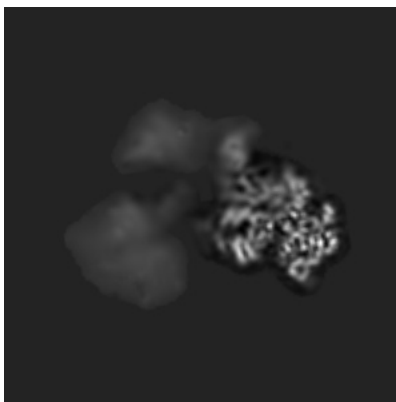
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

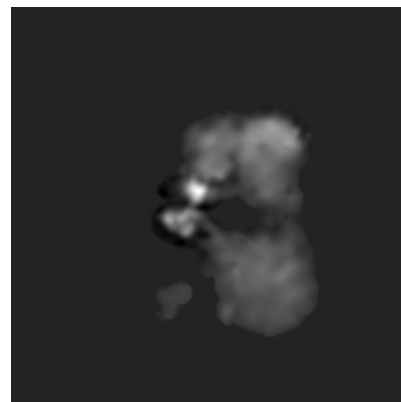
6.2.1 Primary map



X Index: 160

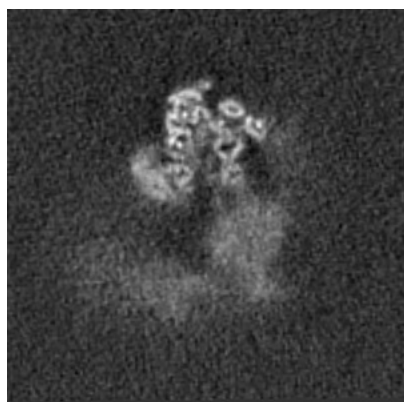


Y Index: 160

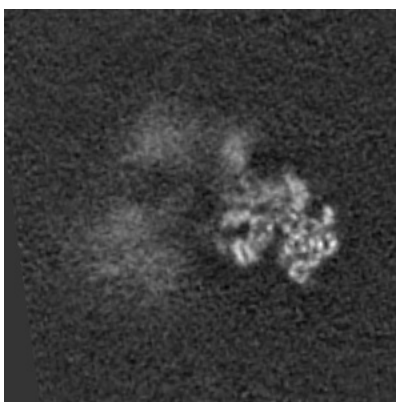


Z Index: 160

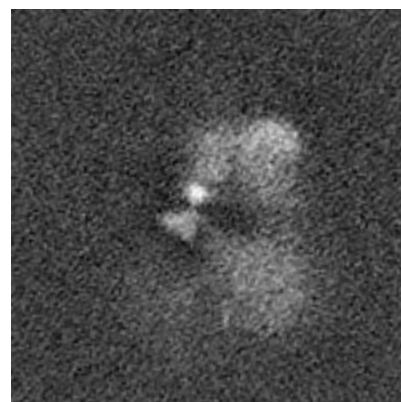
6.2.2 Raw map



X Index: 160



Y Index: 160

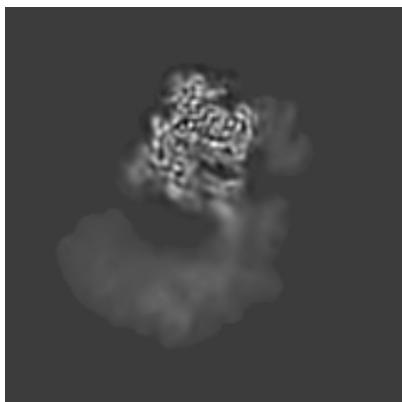


Z Index: 160

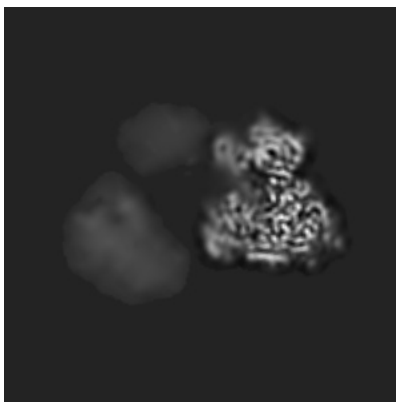
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 146

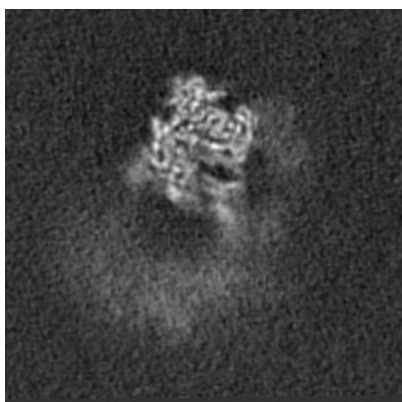


Y Index: 142

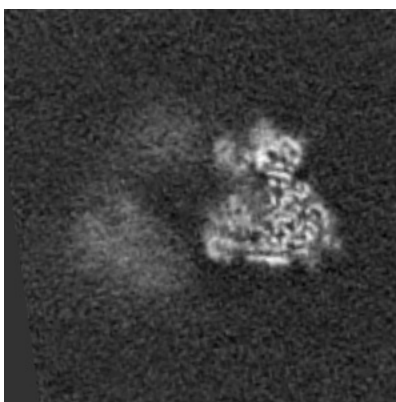


Z Index: 222

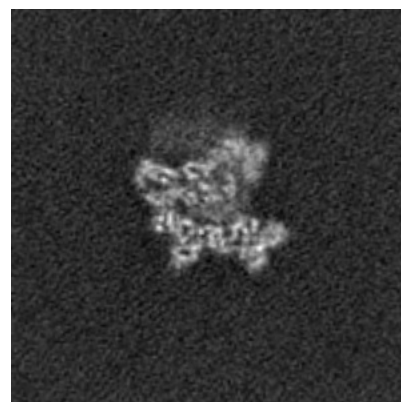
6.3.2 Raw map



X Index: 146



Y Index: 143

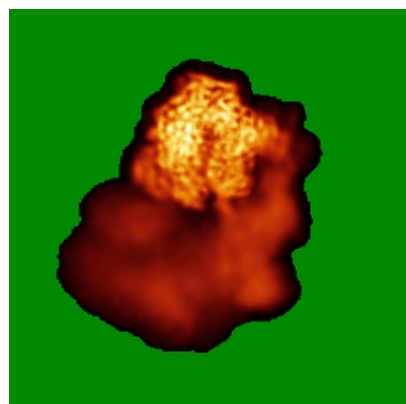


Z Index: 222

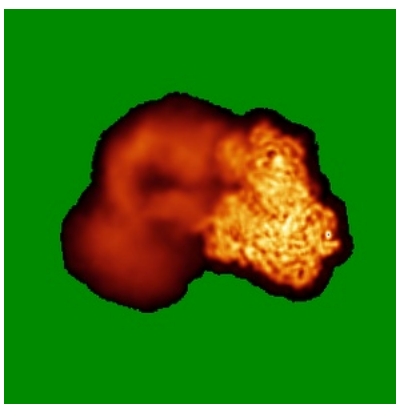
The images above show the largest variance slices of the map in three orthogonal directions.

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

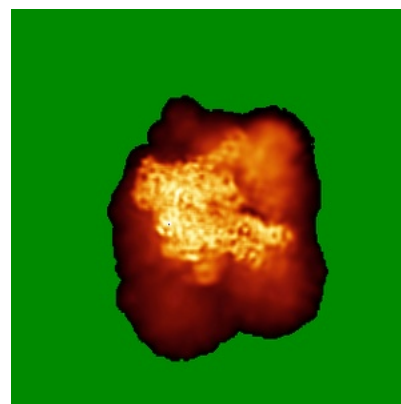
6.4.1 Primary map



X

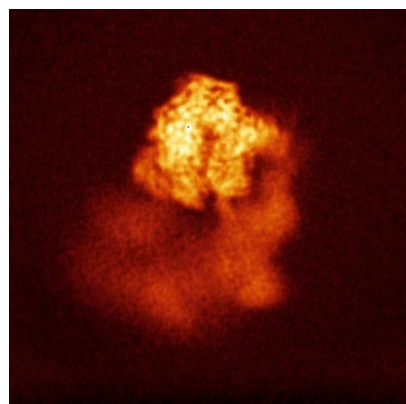


Y

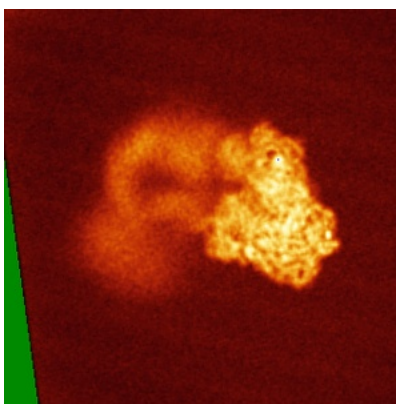


Z

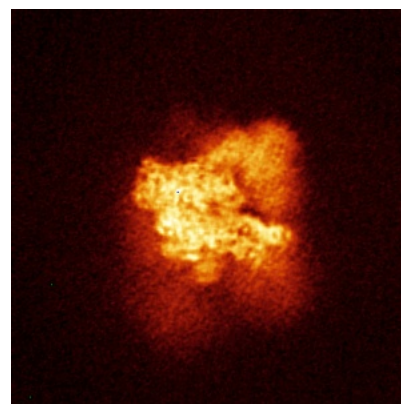
6.4.2 Raw map



X



Y



Z

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

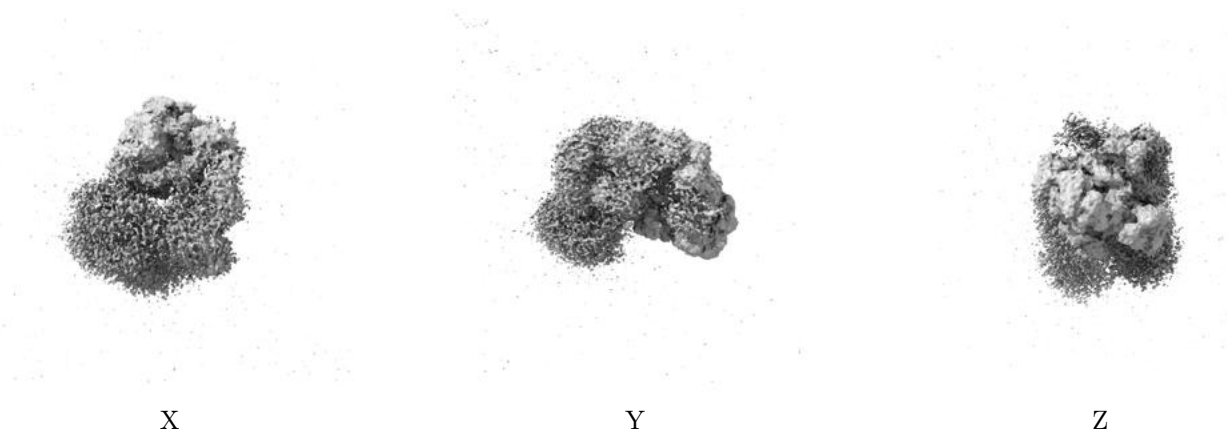
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.517. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

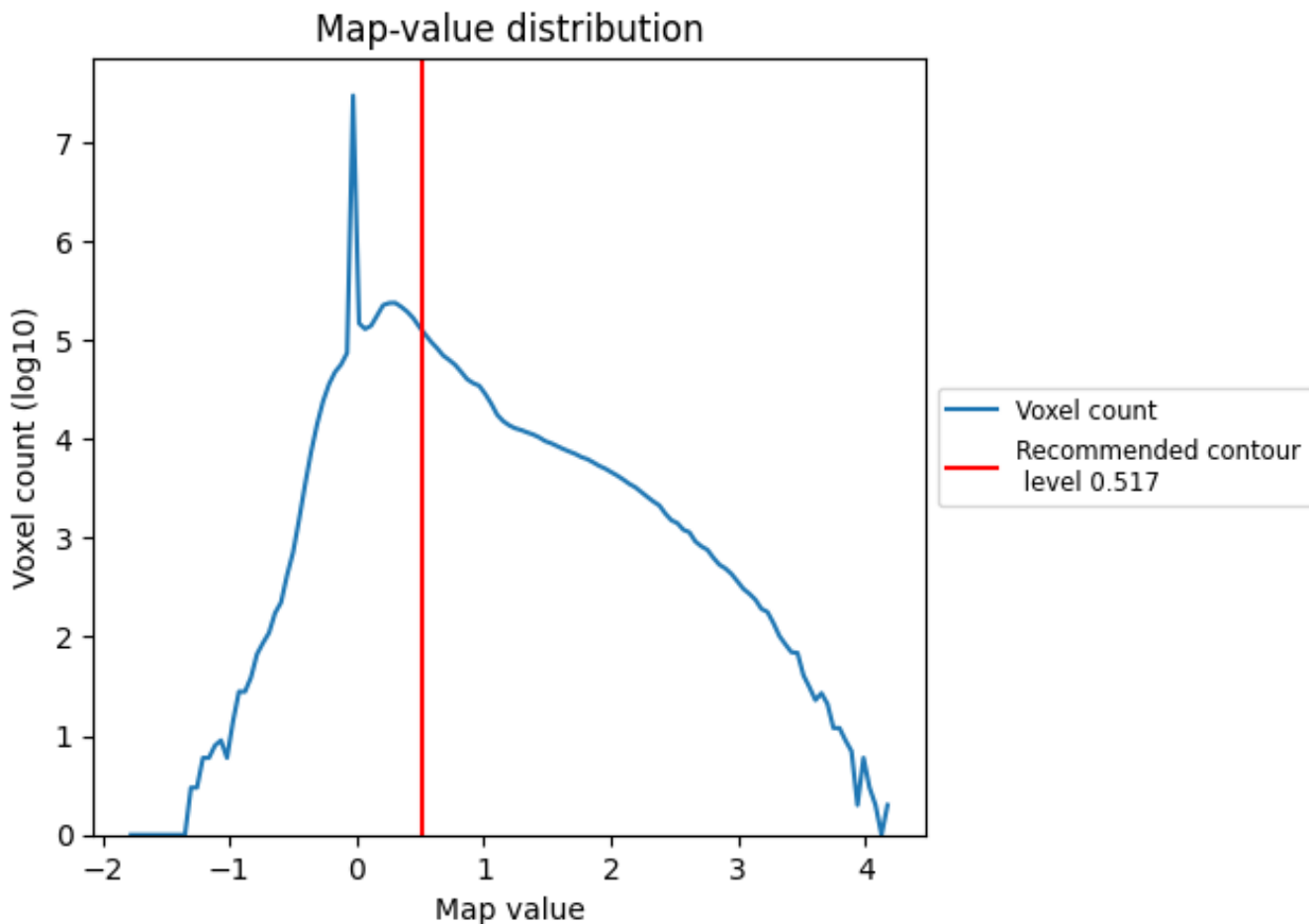
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

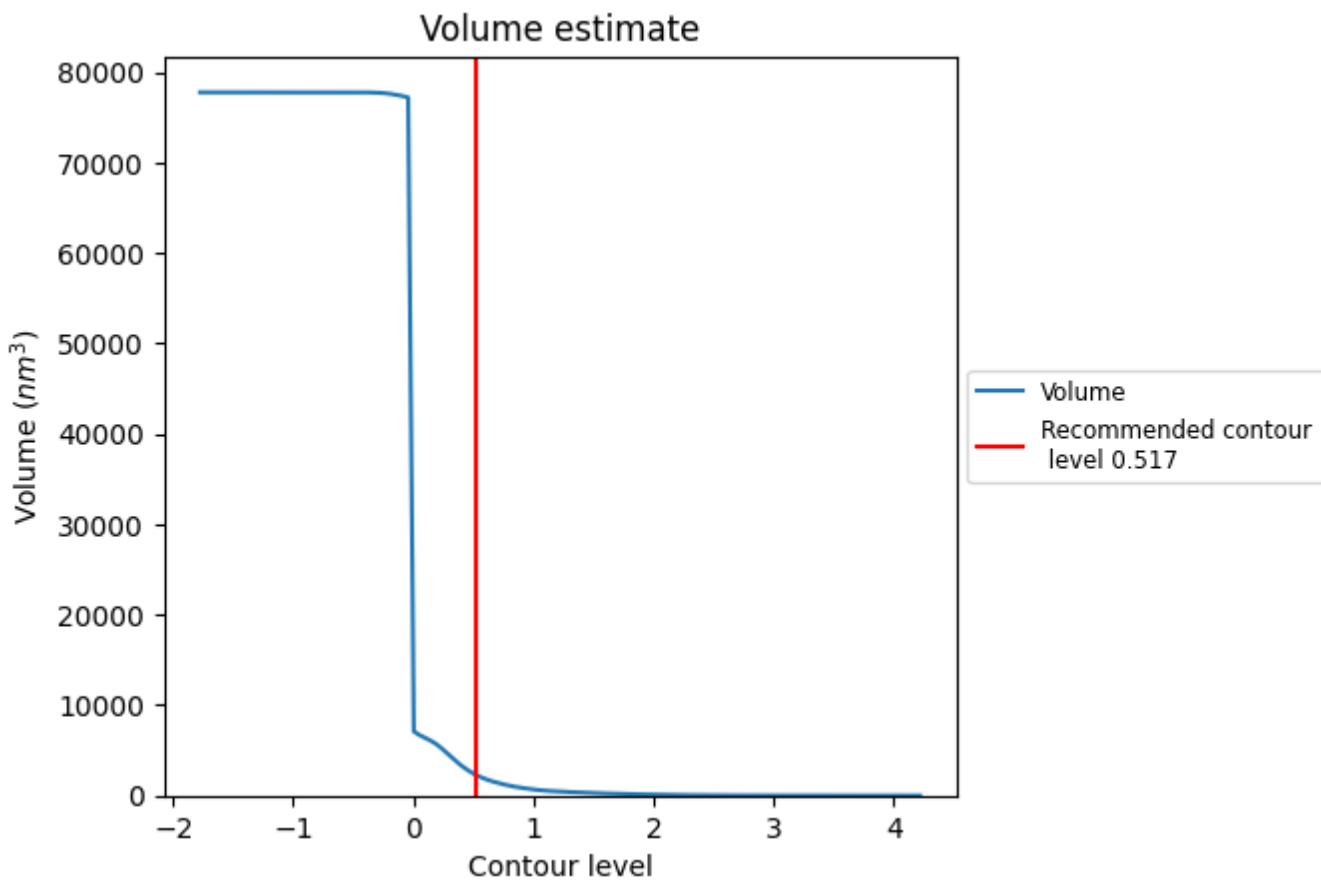
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

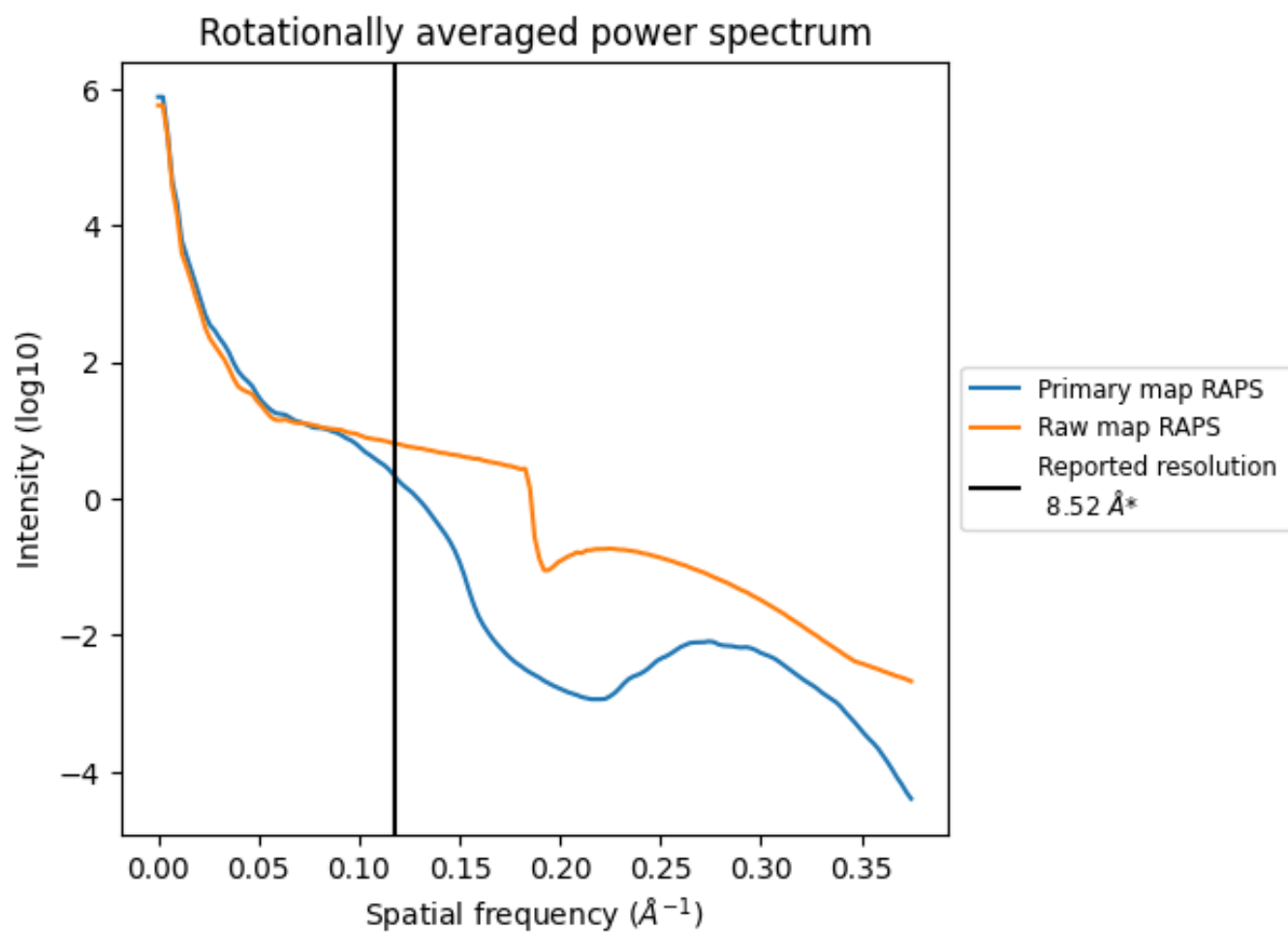
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 2319 nm³; this corresponds to an approximate mass of 2095 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

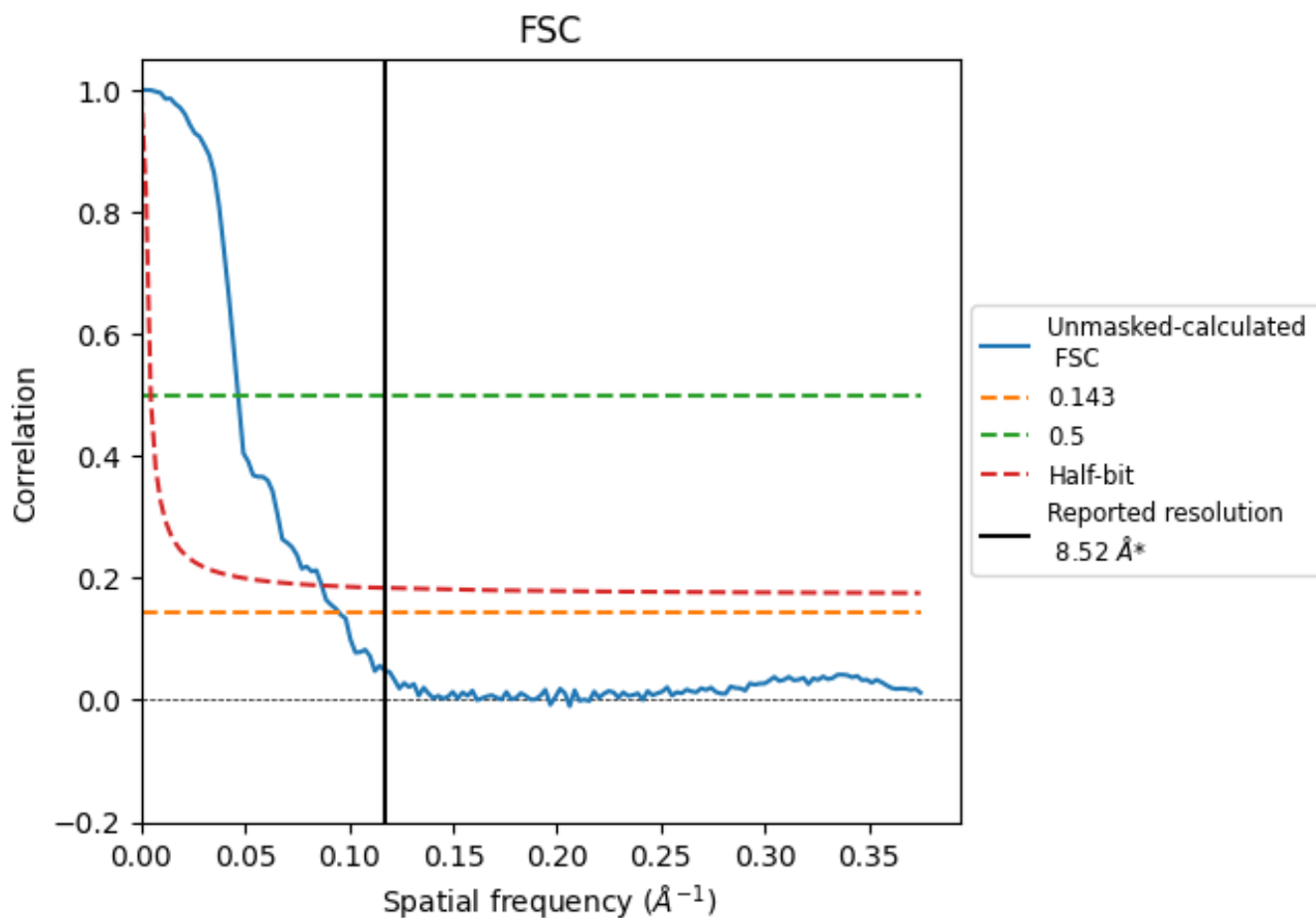


*Reported resolution corresponds to spatial frequency of 0.117 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.117 Å⁻¹

8.2 Resolution estimates [i](#)

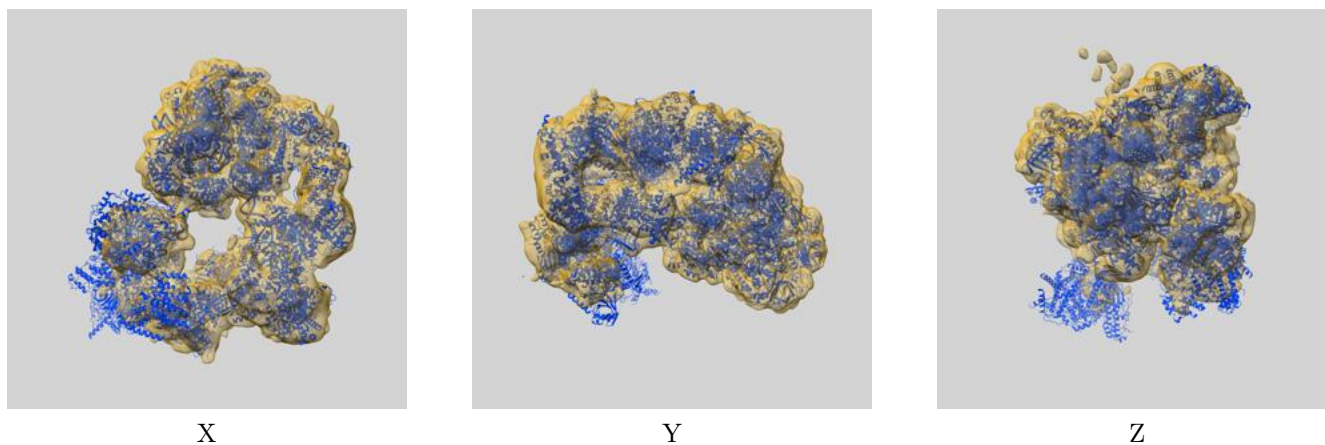
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.52	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.50	21.51	11.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 10.50 differs from the reported value 8.52 by more than 10 %

9 Map-model fit [i](#)

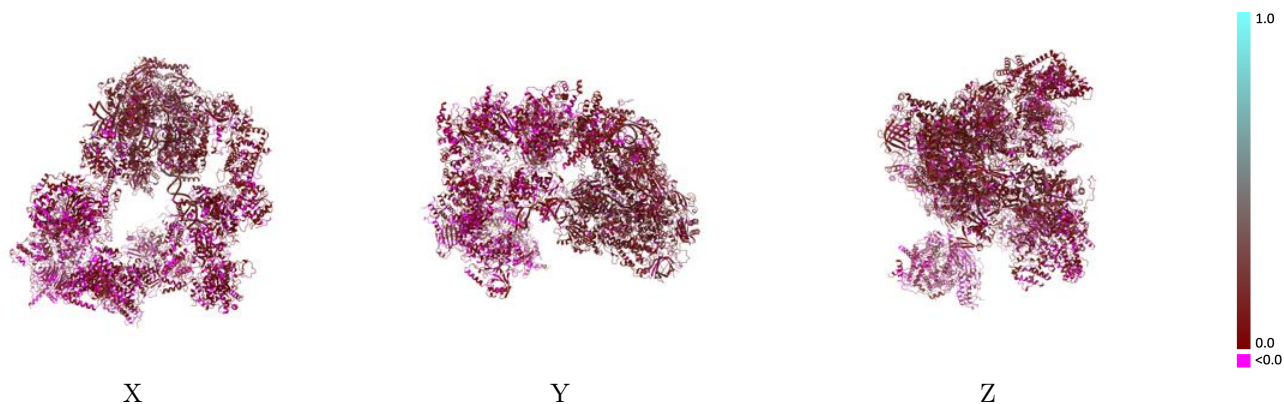
This section contains information regarding the fit between EMDB map EMD-37396 and PDB model 8WAL. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.517 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](#)

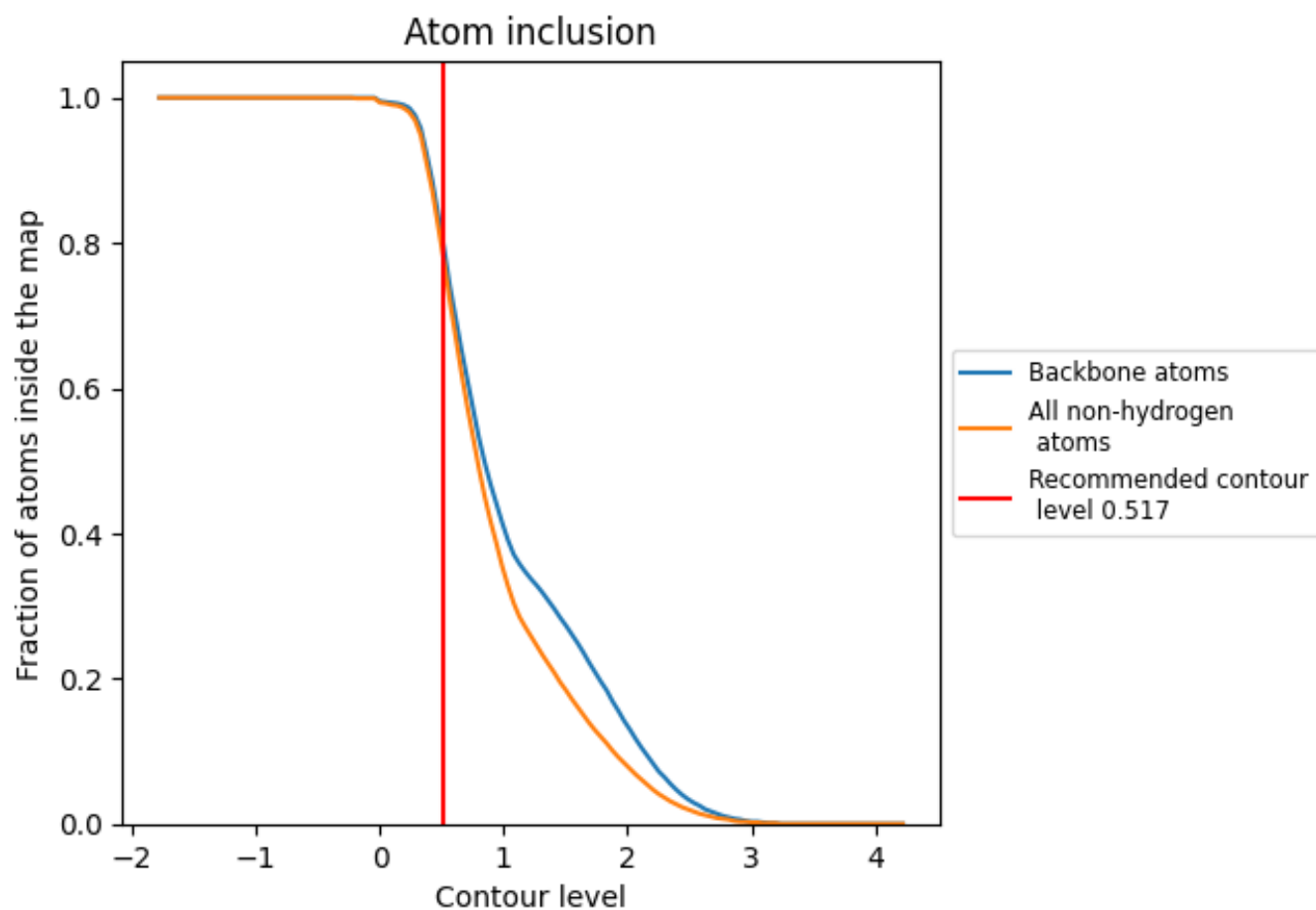


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 78% 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 (0.517) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7770	 0.0840
0	 0.7520	 0.0600
1	 0.8530	 0.0420
2	 0.9640	 0.0520
3	 0.9560	 0.0430
4	 0.9460	 0.0720
5	 0.8420	 0.0550
6	 0.8800	 0.0520
7	 0.9440	 0.0650
A	 0.5170	 0.0360
B	 0.9130	 0.0430
D	 0.4600	 0.0540
E	 0.7110	 0.0480
F	 0.5370	 0.0340
G	 0.2520	 0.0410
H	 0.7720	 0.0500
I	 0.5360	 0.0400
J	 0.6850	 0.0250
L	 0.1860	 0.0650
N	 0.9520	 0.1530
O	 0.9450	 0.0950
P	 0.9870	 0.1400
Q	 0.9420	 0.1000
R	 0.9600	 0.1530
S	 0.9610	 0.1000
T	 0.9600	 0.1340
U	 0.9660	 0.0980
V	 0.9680	 0.1190
X	 0.9590	 0.1820
Y	 0.9380	 0.1530
Z	 0.4720	 -0.0350
c	 0.1060	 0.0160
d	 0.0060	 0.0220
e	 0.1740	 0.0250
f	 0.5170	 0.0370



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.0390	 0.0210
j	 0.0710	 0.0320
k	 0.0000	 0.0090
l	 0.0000	 0.0340
m	 0.0000	 0.0130
o	 0.9460	 0.1440
p	 0.9380	 0.1400
q	 0.9660	 0.1530
r	 0.9790	 0.1350
s	 0.9600	 0.1560
t	 0.9400	 0.1500
u	 0.9830	 0.1210
v	 0.9700	 0.1590
w	 0.9650	 0.1400
x	 0.9390	 0.1300
y	 0.9450	 0.1550
z	 0.9920	 0.1730