



## Full wwPDB EM Validation Report ⓘ

Jun 1, 2023 – 01:23 pm BST

PDB ID : 8C4V  
EMDB ID : EMD-16430  
Title : Hantaan virus polymerase in replication elongation state  
Authors : Durieux trouilleton, Q.; Arragain, B.; Malet, H.  
Deposited on : 2023-01-04  
Resolution : 3.14 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](mailto: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>.

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

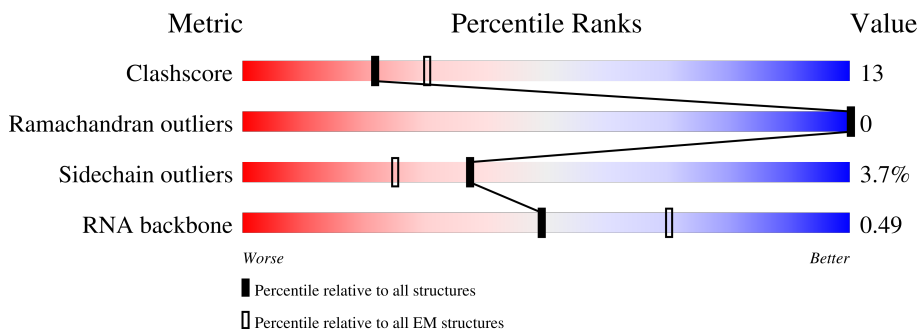
EMDB validation analysis : 0.0.1.dev50  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.33

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.14 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
RNA backbone	4643	859

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  $\geq 3$ , 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	2173	
2	H	20	
3	S	25	
3	T	25	
3	V	25	
4	P	25	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 11731 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1308	10536	6783	1768	1928	57	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP P23456
A	-20	GLY	-	expression tag	UNP P23456
A	-19	HIS	-	expression tag	UNP P23456
A	-18	HIS	-	expression tag	UNP P23456
A	-17	HIS	-	expression tag	UNP P23456
A	-16	HIS	-	expression tag	UNP P23456
A	-15	HIS	-	expression tag	UNP P23456
A	-14	HIS	-	expression tag	UNP P23456
A	-13	ASP	-	expression tag	UNP P23456
A	-12	TYR	-	expression tag	UNP P23456
A	-11	ASP	-	expression tag	UNP P23456
A	-10	ILE	-	expression tag	UNP P23456
A	-9	PRO	-	expression tag	UNP P23456
A	-8	THR	-	expression tag	UNP P23456
A	-7	THR	-	expression tag	UNP P23456
A	-6	GLU	-	expression tag	UNP P23456
A	-5	ASN	-	expression tag	UNP P23456
A	-4	LEU	-	expression tag	UNP P23456
A	-3	TYR	-	expression tag	UNP P23456
A	-2	PHE	-	expression tag	UNP P23456
A	-1	GLN	-	expression tag	UNP P23456
A	0	GLY	-	expression tag	UNP P23456
A	97	ALA	ASP	engineered mutation	UNP P23456

- Molecule 2 is a RNA chain called RNA (5'-R(P\*AP\*GP\*GP\*AP\*GP\*UP\*AP\*UP\*CP\*CP\*AP\*CP\*CP\*GP\*CP\*AP\*AP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	19	Total	C	N	O	P	0	0
			409	183	79	128	19		

- Molecule 3 is a RNA chain called RNA (5'-R(P\*AP\*CP\*UP\*AP\*CP\*UP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	V	9	Total	C	N	O	P	0	0
			191	85	31	66	9		
3	T	12	Total	C	N	O	P	0	0
			251	113	42	84	12		
3	S	7	Total	C	N	O	P	0	0
			146	66	25	48	7		

- Molecule 4 is a RNA chain called RNA (5'-R(P\*AP\*GP\*UP\*AP\*GP\*UP\*AP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	9	Total	C	N	O	P	0	0
			197	88	39	61	9		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

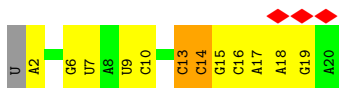
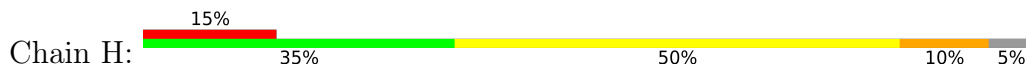
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	



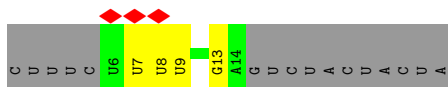
1936	4936	L1023	R1024	N1025	Y1026	I1027	D1034	I1037	R944	W945	E949	S955	N956	H957	K958	F959	N1960	R961	R962	K963	S1065	S1066	Y1969	S970	A971	K975	W976	S977	P978	N981	S982	A983	K984	F985	R986	S990	H991	L992	H993	N994	G995	L996	K1000	Y1005	I1006	D1007	A1008	L1009	K1014	T1015	D1016
V1134	M1135	M1138	W1139	K1140	S1141	M1142	L1145	H1146	E1147	K1156	I1157	T1162	T1163	Q1058	N1060	K1063	L1172	S1173	T1174	F1175	F1176	C1179	I1183	P1184	F1185	W1186	K1187	I1188	L1189	L1190	L1196	Y1201	F1202	A1206	A1207	A1208	L1218	Q1223	V1229	C1232	R1238	L1239	Y1240	G1241	T1242						
A1243	M1246	P1262	I1263	P1264	L1265	I1273	M1274	E1275	L1276	T1281	M1283	M1287	L1288	L1289	K1290	L1401	L1402	Q1403	L1404	E1405	F1406	R1407	M1408	Q1409	A1410	K1411	Q1412	H1413	M1414	K1302	K1415	M1304	L1314	L1317	E1320	T1321	F1322	Q1323	H1324	E1325	R1326	Q1329	F1330	S1331	F1332	I1333	F1341	K1344	E1346		
K1356	F1357	L1358	T1367	I1372	R1376	L1380	R1385	K1386	I1392	Q1398	S1400	P1401	L1402	Q1403	L1404	E1405	F1406	M1408	Q1409	A1410	K1411	Q1412	H1413	M1414	K1415	C1417	R1418	L1419	T1425	V1429	S1441	Q1445	D1448	L1449	F1450	T1454	SER	CYS	THR	PHE	SER	LYS	K1536	T1537							
GLU	TYR	ALA	K1465	D1466	L1468	M1469	G1470	S1551	I1471	H1472	C1473	V1475	I1476	P1477	T1478	K1479	Q1480	V1481	Q1482	R1483	A1484	F1490	T1491	V1492	R1493	E1494	LYS	ASP	GLN	ILE	ILE	ASN	S1502	I1503	V1506	I1507	K1510	T1514	E1517	M1518	V1521	L1522	A1525	D1529	S1530	K1536	T1537				
M1538	K1539	D1540	Y1543	G1547	L1548	D1549	I1550	S1551	D1554	V1555	M1556	K1557	I1558	A1560	P1561	M1562	L1563	Y1564	K1565	SER	SER	S1569	R1570	V1571	I1572	I1573	V1574	M1577	E1583	R1587	Y1588	W1589	S1592	M1593	S1594	L1595	V1596	K1597	T1598	R1600	VAL	PRO	LYS	HIS	GLY	LEU	GLN				
ALA	VAL	SER	ILE	ASN	ARG	LYS	GLU	ASP	GLN	LYS	ASP	ALA	ALA	LEU	LYS	LYS	GLY	TYR	VAL	TRP	TRP	S1569	R1570	V1571	I1572	I1573	V1574	M1577	E1583	R1587	Y1588	W1589	S1592	M1593	S1594	L1595	V1596	K1597	T1598	R1600	VAL	PRO	LYS	HIS	GLY	LEU	GLN				
VAL	GLY	VAL	PRO	ASN	PRO	ILE	ASP	PRO	ALA	ALA	ASP	ALA	ALA	LEU	LYS	LYS	GLY	TYR	VAL	TRP	TRP	S1569	R1570	V1571	I1572	I1573	V1574	M1577	E1583	R1587	Y1588	W1589	S1592	M1593	S1594	L1595	V1596	K1597	T1598	R1600	VAL	PRO	LYS	HIS	GLY	LEU	GLN				
ARG	VAL	THR	PHE	ASN	PRO	ASN	GLY	ASP	ALA	ALA	ASP	ALA	ALA	LEU	LYS	LYS	GLY	TYR	VAL	TRP	TRP	S1569	R1570	V1571	I1572	I1573	V1574	M1577	E1583	R1587	Y1588	W1589	S1592	M1593	S1594	L1595	V1596	K1597	T1598	R1600	VAL	PRO	LYS	HIS	GLY	LEU	GLN				
ARG	HIS	MET	VAL	LEU	PHE	LYS	THR	GLU	ASP	GLY	LYS	PRO	ASN	PRO	CYS	CYS	VAL	LEU	VAL	VAL	VAL	S1569	R1570	V1571	I1572	I1573	V1574	M1577	E1583	R1587	Y1588	W1589	S1592	M1593	S1594	L1595	V1596	K1597	T1598	R1600	VAL	PRO	LYS	HIS	GLY	LEU	GLN				
ASP	SER	PRO	ARG	LEU	PHE	LEU	ALA	HIS	THR	ILE	ASP	TYR	GLN	ASN	ALA	VAL	LEU	VAL	VAL	VAL	VAL	S1569	R1570	V1571	I1572	I1573	V1574	M1577	E1583	R1587	Y1588	W1589	S1592	M1593	S1594	L1595	V1596	K1597	T1598	R1600	VAL	PRO	LYS	HIS	GLY	LEU	GLN				
PRO	ALA	ALA	TYR	SER	LEU	ILE	MET	ASN	HIS	VAL	ASP	PHE	ASP	ASN	ALA	VAL	LEU	VAL	VAL	VAL	VAL	S1569	R1570	V1571	I1572	I1573	V1574	M1577	E1583	R1587	Y1588	W1589	S1592	M1593	S1594	L1595	V1596	K1597	T1598	R1600	VAL	PRO	LYS	HIS	GLY	LEU	GLN				
SER	LEU	VAL	ASP	ASP	GLY	ASP	ASP	ASP	ASP	ASP	ASP	PHE	ASP	ASP	ASN	VAL	LEU	VAL	VAL	VAL	VAL	S1569	R1570	V1571	I1572	I1573	V1574	M1577	E1583	R1587	Y1588	W1589	S1592	M1593	S1594	L1595	V1596	K1597	T1598	R1600	VAL	PRO	LYS	HIS	GLY	LEU	GLN				
VAL	LYS	ILE	LEU	GLU	ARG	ILE	ILE	ASP	GLY	THR	SER	VAL	GLU	GLU	ILE	VAL	VAL	VAL	VAL	VAL	VAL	S1569	R1570	V1571	I1572	I1573	V1574	M1577	E1583	R1587	Y1588	W1589	S1592	M1593	S1594	L1595	V1596	K1597	T1598	R1600	VAL	PRO	LYS	HIS	GLY	LEU	GLN				
ILE	VAL	ARG	GLY	TRP	GLY	PRO	CYS	VAL	VAL	VAL	SER	ASN	PRO	VAL	ASN	ASN	GLY	ASN	ASN	ASN	ASN	S1569	R1570	V1571	I1572	I1573	V1574	M1577	E1583	R1587	Y1588	W1589	S1592	M1593	S1594	L1595	V1596	K1597	T1598	R1600	VAL	PRO	LYS	HIS	GLY	LEU	GLN				

PHE  
TYR

- Molecule 2: RNA (5'-R(P\*AP\*GP\*GP\*AP\*GP\*UP\*AP\*UP\*CP\*CP\*AP\*CP\*CP\*GP\*CP\*A P\*AP\*GP\*A)-3')



- Molecule 3: RNA (5'-R(P\*AP\*CP\*UP\*AP\*CP\*UP\*A)-3')



- Molecule 3: RNA (5'-R(P\*AP\*CP\*UP\*AP\*CP\*UP\*A)-3')



- Molecule 3: RNA (5'-R(P\*AP\*CP\*UP\*AP\*CP\*UP\*A)-3')



- Molecule 4: RNA (5'-R(P\*AP\*GP\*UP\*AP\*GP\*UP\*AP\*GP\*A)-3')



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	159681	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	2200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	45454	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.281	Depositor
Minimum map value	-0.186	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0271	Depositor
Map size (Å)	286.0, 286.0, 286.0	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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

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	0.39	0/10771	0.58	0/14552
2	H	0.45	0/458	0.78	0/712
3	S	0.60	0/162	0.91	0/249
3	T	0.53	0/279	0.79	0/431
3	V	0.21	0/212	0.68	0/328
4	P	0.29	0/221	0.75	0/343
All	All	0.40	0/12103	0.61	0/16615

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10536	0	10561	280	0
2	H	409	0	208	13	0
3	S	146	0	76	8	0
3	T	251	0	129	4	0
3	V	191	0	96	4	0
4	P	197	0	98	8	0
5	A	1	0	0	0	0
All	All	11731	0	11168	296	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.

All (296) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1325:GLU:HG3	1:A:1448:ASP:HB3	1.41	0.99
1:A:389:LEU:HD21	1:A:559:VAL:HG11	1.60	0.82
1:A:431:ILE:HG13	1:A:471:THR:HG22	1.62	0.81
1:A:583:THR:HG21	1:A:1186:VAL:HG22	1.63	0.80
1:A:1238:ARG:HE	3:S:22:A:H61	1.30	0.79
1:A:1295:GLY:HA3	1:A:1304:MET:HG2	1.68	0.76
1:A:971:ALA:HA	1:A:1162:THR:HG23	1.67	0.74
1:A:1184:PRO:HG2	1:A:1187:LYS:HE3	1.69	0.74
1:A:748:TRP:HE1	1:A:975:LYS:HD3	1.55	0.71
1:A:1120:VAL:HG11	1:A:1135:ASN:HB3	1.72	0.71
1:A:487:ILE:HG23	1:A:1402:LEU:HD11	1.72	0.69
1:A:1356:LYS:H	1:A:1356:LYS:HD2	1.58	0.69
1:A:849:ILE:HD12	1:A:1386:LYS:HE2	1.73	0.69
1:A:317:ALA:HB1	1:A:509:ILE:HG12	1.74	0.68
1:A:983:ALA:HA	1:A:986:ARG:HD3	1.75	0.68
1:A:916:ALA:HB1	1:A:922:GLU:HG2	1.75	0.67
1:A:922:GLU:OE1	1:A:924:ILE:HG22	1.95	0.67
1:A:589:THR:HG21	1:A:1595:LEU:HB3	1.75	0.67
1:A:569:ALA:HB2	1:A:728:GLU:HG3	1.76	0.66
1:A:1331:SER:H	1:A:1558:ARG:HG2	1.61	0.66
1:A:796:GLU:HG3	1:A:1075:LEU:HA	1.77	0.65
1:A:1292:ALA:HA	1:A:1304:MET:HG3	1.79	0.65
1:A:939:LEU:O	1:A:943:LEU:HD12	1.97	0.64
1:A:1034:ASP:HB2	1:A:1037:ILE:HD12	1.80	0.64
1:A:328:THR:HG1	1:A:545:THR:HG1	1.42	0.63
1:A:855:TYR:HE1	1:A:863:PRO:HG3	1.64	0.63
1:A:460:GLN:HE22	3:S:25:A:H61	1.47	0.62
1:A:792:LEU:O	1:A:796:GLU:HG2	1.99	0.62
1:A:748:TRP:NE1	1:A:975:LYS:HD3	2.16	0.61
1:A:1518:MET:O	1:A:1522:LEU:HG	2.01	0.60
1:A:586:GLN:O	1:A:590:GLU:HG3	2.02	0.60
1:A:524:PHE:HB3	1:A:561:SER:HB3	1.84	0.59
1:A:1404:LEU:O	1:A:1408:MET:HG3	2.03	0.59
1:A:913:ASP:HB2	1:A:1063:LYS:HZ3	1.68	0.59
1:A:288:PRO:HA	1:A:405:LEU:HD21	1.82	0.59
1:A:935:ILE:HD11	1:A:1101:LEU:HD23	1.83	0.59
1:A:467:LEU:HD21	1:A:601:ILE:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:LEU:HA	1:A:573:ALA:HB2	1.85	0.58
1:A:782:GLN:HG3	1:A:1156:LYS:HB2	1.85	0.58
1:A:1096:HIS:CG	1:A:1172:LEU:HD21	2.38	0.58
3:V:8:U:H2'	3:V:9:U:C6	2.38	0.58
1:A:490:SER:HB2	1:A:518:LEU:HB2	1.85	0.58
1:A:1358:LEU:HD12	1:A:1385:ARG:HB2	1.86	0.58
1:A:1238:ARG:HE	3:S:22:A:N6	2.00	0.58
1:A:1372:ILE:HD12	1:A:1372:ILE:H	1.69	0.58
1:A:1300:ARG:NH1	1:A:1300:ARG:HB2	2.19	0.57
1:A:1208:ALA:HB1	1:A:1232:CYS:HB3	1.86	0.57
1:A:1238:ARG:NE	3:S:22:A:H61	2.01	0.57
1:A:962:MET:HE3	1:A:1107:LEU:HB2	1.86	0.57
1:A:1367:THR:HG21	1:A:1517:GLU:HB3	1.86	0.57
1:A:306:THR:HA	3:S:21:U:H2'	1.87	0.56
2:H:16:C:H2'	2:H:17:A:C8	2.40	0.56
1:A:1188:ILE:HG13	1:A:1218:LEU:HD12	1.88	0.56
1:A:674:ASN:HD22	1:A:700:VAL:HG12	1.71	0.56
1:A:559:VAL:HB	2:H:2:A:H1'	1.88	0.56
2:H:13:C:H5	3:V:13:G:H1	1.52	0.56
1:A:464:ILE:HG23	1:A:473:TRP:CH2	2.41	0.56
1:A:1241:GLY:O	1:A:1243:ALA:N	2.39	0.56
1:A:617:MET:HB2	1:A:731:LEU:O	2.05	0.56
1:A:923:TYR:HA	1:A:926:TYR:HD2	1.69	0.56
1:A:1539:LYS:HD2	1:A:1550:ILE:HG12	1.88	0.56
1:A:830:LEU:HD11	1:A:1392:ILE:HG23	1.88	0.54
1:A:1320:GLU:HB3	1:A:1330:PHE:HB2	1.89	0.54
1:A:492:LEU:HD23	1:A:517:SER:OG	2.07	0.54
1:A:763:LEU:HG	1:A:768:TYR:HB3	1.90	0.54
1:A:588:TYR:HE2	1:A:708:ILE:HG21	1.73	0.54
1:A:976:TRP:HE1	1:A:1065:SER:HG	1.55	0.54
1:A:1174:THR:HG22	1:A:1183:ILE:HG23	1.89	0.54
1:A:930:LYS:HA	1:A:933:LEU:HD13	1.89	0.54
1:A:1076:PHE:CE2	1:A:1091:PHE:HE2	2.26	0.54
1:A:1202:PHE:CE2	3:T:23:C:H5''	2.43	0.54
1:A:1543:TYR:HA	1:A:1547:GLY:HA2	1.88	0.53
2:H:19:G:H22	3:V:7:U:H3	1.56	0.53
1:A:581:THR:HG23	1:A:604:VAL:HG13	1.89	0.53
1:A:975:LYS:HB3	1:A:978:PRO:O	2.08	0.53
1:A:236:ILE:HD13	1:A:787:GLN:HB3	1.90	0.53
1:A:732:HIS:CD2	1:A:737:GLU:HG2	2.44	0.53
1:A:825:THR:HG21	4:P:13:A:H5'	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:ILE:HG13	1:A:576:LYS:HD3	1.89	0.53
1:A:911:TYR:CG	1:A:1005:VAL:HG21	2.44	0.53
1:A:337:MET:SD	1:A:511:PHE:HD2	2.32	0.53
1:A:622:ILE:HG12	1:A:650:ARG:HD3	1.90	0.53
1:A:1229:VAL:HG21	1:A:1273:ILE:HD13	1.90	0.53
1:A:389:LEU:HD23	1:A:526:ARG:HD2	1.89	0.52
1:A:873:ARG:HG3	1:A:873:ARG:HH11	1.74	0.52
1:A:1475:VAL:HA	1:A:1599:ILE:HD13	1.91	0.52
1:A:1322:PHE:HB2	1:A:1332:PHE:CZ	2.45	0.52
1:A:292:LEU:HD22	1:A:537:LEU:HB3	1.92	0.52
1:A:351:ASN:HB3	1:A:359:PHE:CE1	2.45	0.52
1:A:981:ASN:HB3	1:A:984:LYS:HG3	1.92	0.52
1:A:892:ARG:HH11	1:A:1058:GLN:HE22	1.58	0.51
1:A:1202:PHE:HD1	1:A:1263:ILE:CG2	2.23	0.51
1:A:1412:GLN:HB3	1:A:1413:HIS:HD2	1.73	0.51
1:A:898:THR:HG23	1:A:900:PRO:HD2	1.92	0.51
1:A:1322:PHE:HB2	1:A:1332:PHE:HZ	1.75	0.51
1:A:367:GLU:HB3	1:A:494:ARG:HG2	1.93	0.51
1:A:337:MET:SD	1:A:511:PHE:HB3	2.51	0.51
1:A:451:LEU:HD13	1:A:1593:MET:SD	2.51	0.51
1:A:738:GLU:HA	1:A:883:ARG:HD2	1.93	0.51
1:A:498:TRP:CD2	1:A:514:PRO:HD3	2.46	0.51
1:A:253:ARG:HH11	1:A:255:ARG:NH2	2.09	0.50
1:A:334:ILE:HG23	1:A:511:PHE:CZ	2.47	0.50
1:A:878:MET:HA	1:A:1016:ASP:HB2	1.94	0.50
1:A:924:ILE:HG23	1:A:1063:LYS:HD3	1.93	0.50
1:A:949:GLU:HG2	1:A:961:ARG:HH11	1.76	0.50
1:A:354:ALA:O	1:A:368:PRO:HB3	2.11	0.50
1:A:822:PHE:HA	1:A:827:ASN:HB2	1.94	0.50
1:A:735:MET:HG2	1:A:1026:TYR:CG	2.47	0.49
1:A:1091:PHE:HD2	1:A:1093:PHE:HZ	1.60	0.49
1:A:496:LYS:HA	2:H:13:C:H42	1.77	0.49
1:A:1415:LYS:HD3	1:A:1425:THR:HG23	1.94	0.49
1:A:1465:LYS:HD2	1:A:1468:LEU:HD12	1.94	0.49
1:A:1550:ILE:HD12	1:A:1556:MET:HE2	1.94	0.49
1:A:1023:LEU:O	1:A:1027:ILE:HG13	2.12	0.49
1:A:1572:VAL:HG23	1:A:1574:VAL:HG13	1.94	0.49
1:A:924:ILE:HB	1:A:1096:HIS:O	2.13	0.49
1:A:1024:ARG:HH22	1:A:1041:LEU:HD11	1.78	0.49
1:A:1241:GLY:C	1:A:1243:ALA:H	2.16	0.49
1:A:285:SER:HB3	1:A:405:LEU:HD22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1570:ARG:HH21	1:A:1589:TRP:HH2	1.60	0.49
1:A:926:TYR:HB2	1:A:931:LYS:HG2	1.93	0.49
1:A:1239:LEU:O	1:A:1409:GLN:HA	2.13	0.49
4:P:19:A:H2'	4:P:20:G:H8	1.78	0.49
1:A:897:THR:HB	1:A:901:THR:HB	1.94	0.48
1:A:971:ALA:HB1	1:A:1157:ILE:HD12	1.95	0.48
1:A:1283:MET:O	1:A:1287:ASN:HB2	2.13	0.48
2:H:18:A:H2'	2:H:19:G:C8	2.48	0.48
1:A:488:ALA:HA	3:S:19:A:N7	2.28	0.48
1:A:637:TYR:HB2	1:A:1164:VAL:HG22	1.93	0.48
1:A:1202:PHE:HD1	1:A:1263:ILE:HG21	1.78	0.48
1:A:454:PHE:HZ	1:A:1599:ILE:HD11	1.77	0.48
1:A:518:LEU:HD13	1:A:564:LEU:HA	1.96	0.48
1:A:1290:LYS:HB2	1:A:1454:THR:HG23	1.94	0.48
1:A:1330:PHE:HD1	1:A:1558:ARG:HB2	1.78	0.48
1:A:248:LYS:HG2	1:A:1130:HIS:CD2	2.49	0.48
1:A:464:ILE:O	1:A:468:LYS:HB2	2.13	0.48
1:A:1206:ALA:HB1	1:A:1281:ILE:HG21	1.96	0.48
1:A:1356:LYS:HD2	1:A:1356:LYS:N	2.28	0.48
1:A:1558:ARG:O	1:A:1561:PRO:HD2	2.14	0.48
1:A:429:LEU:O	1:A:471:THR:HG23	2.13	0.47
1:A:1106:TYR:HB2	1:A:1138:MET:HG2	1.96	0.47
1:A:1402:LEU:HG	1:A:1406:PHE:CZ	2.49	0.47
1:A:1503:ILE:HD11	1:A:1563:LEU:O	2.14	0.47
1:A:1507:ILE:HD12	1:A:1507:ILE:H	1.79	0.47
1:A:248:LYS:HA	1:A:1130:HIS:HB3	1.96	0.47
1:A:321:ILE:HA	1:A:324:LEU:HG	1.96	0.47
1:A:531:PHE:HZ	1:A:543:LEU:HD21	1.80	0.47
1:A:785:TYR:CG	1:A:984:LYS:HG2	2.49	0.47
1:A:1066:SER:O	1:A:1070:VAL:HG23	2.14	0.47
1:A:877:ALA:HA	1:A:901:THR:OG1	2.15	0.47
1:A:994:ASN:HD22	1:A:996:LEU:HB2	1.80	0.47
1:A:617:MET:HG3	2:H:6:G:OP1	2.15	0.46
1:A:595:PHE:CE2	1:A:1596:VAL:HB	2.50	0.46
1:A:797:LEU:HD23	1:A:992:LEU:HD11	1.97	0.46
4:P:18:U:H2'	4:P:19:A:H8	1.80	0.46
1:A:624:ASP:O	1:A:627:ARG:HD3	2.15	0.46
4:P:14:G:H2'	4:P:15:U:C6	2.49	0.46
1:A:623:PHE:O	1:A:627:ARG:HG3	2.15	0.46
1:A:756:GLU:HA	1:A:764:VAL:HG21	1.97	0.46
3:T:19:A:H2'	3:T:20:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ILE:HD12	1:A:511:PHE:CG	2.50	0.46
1:A:645:GLU:O	1:A:649:GLU:HG3	2.15	0.46
1:A:304:PRO:HB2	3:S:24:U:C4	2.50	0.46
1:A:321:ILE:HD11	1:A:338:ALA:HB2	1.97	0.46
1:A:583:THR:HG23	1:A:1185:PHE:CE2	2.50	0.46
1:A:905:LEU:HD22	1:A:1060:ASN:HB3	1.98	0.46
1:A:1240:TYR:CE1	1:A:1411:LYS:HD2	2.50	0.46
1:A:1274:MET:CE	1:A:1589:TRP:HB3	2.46	0.46
1:A:491:GLY:HA3	3:S:19:A:N6	2.31	0.46
1:A:1201:TYR:CZ	1:A:1242:THR:HG21	2.51	0.46
1:A:936:GLN:O	1:A:940:GLU:HG2	2.16	0.45
1:A:1027:ILE:HG21	1:A:1041:LEU:HD12	1.97	0.45
1:A:1473:CYS:HB2	1:A:1599:ILE:HG23	1.97	0.45
1:A:741:ILE:HD13	1:A:883:ARG:HG2	1.97	0.45
1:A:877:ALA:HB1	1:A:901:THR:HG23	1.98	0.45
1:A:1555:VAL:HG12	1:A:1559:ILE:HD11	1.98	0.45
1:A:525:ILE:HG21	1:A:567:LEU:HD22	1.97	0.45
1:A:539:ASP:CG	1:A:542:ASN:HB2	2.37	0.45
4:P:13:A:O2'	4:P:14:G:OP1	2.28	0.45
1:A:584:TRP:CE3	1:A:604:VAL:HG11	2.52	0.45
1:A:1265:LEU:HG	1:A:1314:LEU:HD21	1.98	0.45
1:A:1510:LYS:HE2	1:A:1551:SER:HA	1.96	0.45
1:A:994:ASN:ND2	1:A:996:LEU:HB2	2.31	0.45
1:A:1293:LEU:HD11	1:A:1450:PHE:HB3	1.98	0.45
1:A:1539:LYS:HB3	1:A:1539:LYS:HE2	1.69	0.45
1:A:350:ILE:O	1:A:354:ALA:HB2	2.16	0.45
1:A:1262:PRO:HG2	1:A:1265:LEU:HB2	1.98	0.45
1:A:271:PHE:HZ	1:A:668:LEU:HD12	1.81	0.45
1:A:669:VAL:O	1:A:673:GLN:HG2	2.17	0.44
1:A:283:PRO:HG2	1:A:403:GLU:HG2	1.99	0.44
1:A:630:ILE:HD12	1:A:720:VAL:HG11	1.99	0.44
1:A:755:LYS:HG2	1:A:784:LEU:HD21	2.00	0.44
1:A:786:CYS:HB3	1:A:789:ALA:HB3	1.99	0.44
1:A:490:SER:OG	1:A:1402:LEU:HD21	2.17	0.44
1:A:650:ARG:CZ	1:A:650:ARG:HB3	2.47	0.44
1:A:701:TYR:HB2	1:A:710:TYR:HB2	1.98	0.44
1:A:873:ARG:HH21	1:A:1007:ASP:CG	2.21	0.44
1:A:1196:LEU:HD21	1:A:1208:ALA:HB2	1.99	0.44
1:A:1502:SER:O	1:A:1506:VAL:HG23	2.17	0.44
1:A:1561:PRO:HG3	3:T:25:A:N7	2.33	0.44
1:A:618:LYS:O	1:A:622:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:THR:HG23	1:A:1186:VAL:HG11	1.99	0.44
1:A:227:ILE:HB	1:A:1000:LYS:HD3	1.99	0.44
1:A:307:THR:HG23	1:A:353:TYR:HB3	2.00	0.44
1:A:633:VAL:HG21	1:A:668:LEU:HD22	1.98	0.44
1:A:833:MET:HA	1:A:896:ILE:HG23	2.00	0.44
1:A:1091:PHE:HD2	1:A:1093:PHE:CZ	2.36	0.44
1:A:1129:LEU:HD22	1:A:1129:LEU:H	1.82	0.44
1:A:460:GLN:O	1:A:465:ASP:HB2	2.17	0.44
1:A:516:LYS:HE3	1:A:520:VAL:HG13	2.00	0.44
1:A:876:LYS:HG3	1:A:877:ALA:N	2.33	0.44
1:A:626:LEU:HD13	1:A:664:ILE:HG12	2.00	0.44
2:H:19:G:H1	3:V:7:U:H3	1.66	0.44
1:A:1317:LEU:HD21	1:A:1419:LEU:HD12	2.00	0.44
1:A:822:PHE:HE2	1:A:855:TYR:HD1	1.66	0.43
1:A:251:LEU:HD11	1:A:1145:LEU:HD22	2.00	0.43
1:A:1241:GLY:HA2	1:A:1246:MET:SD	2.59	0.43
1:A:701:TYR:CZ	1:A:713:TYR:HB2	2.54	0.43
1:A:1412:GLN:HB3	1:A:1413:HIS:CD2	2.51	0.43
1:A:330:ALA:O	1:A:334:ILE:HG12	2.19	0.43
1:A:1196:LEU:O	1:A:1404:LEU:HD21	2.19	0.43
1:A:1514:THR:HB	1:A:1517:GLU:HG3	2.00	0.43
1:A:389:LEU:HA	2:H:2:A:C6	2.54	0.43
1:A:627:ARG:HD2	1:A:724:PHE:CD2	2.53	0.43
1:A:496:LYS:HG2	2:H:13:C:H41	1.83	0.43
1:A:834:SER:HB2	1:A:843:LEU:HG	1.99	0.43
1:A:1090:PHE:CZ	1:A:1092:GLU:HB2	2.54	0.43
1:A:1490:PHE:HB3	1:A:1570:ARG:HG3	2.01	0.43
1:A:241:GLU:HA	1:A:244:VAL:HG22	2.00	0.43
1:A:1171:PHE:HB3	1:A:1176:PHE:HE1	1.84	0.43
1:A:604:VAL:HG22	1:A:608:HIS:CD2	2.54	0.43
1:A:346:ARG:O	1:A:350:ILE:HG12	2.18	0.42
1:A:467:LEU:HD11	1:A:581:THR:HG21	2.01	0.42
1:A:618:LYS:HE2	1:A:651:PRO:HG2	2.01	0.42
1:A:857:SER:HA	1:A:1376:ARG:HH21	1.84	0.42
1:A:618:LYS:HD3	1:A:618:LYS:HA	1.73	0.42
1:A:640:PHE:N	1:A:641:PRO:HD2	2.34	0.42
1:A:942:ALA:HB1	1:A:1103:ILE:HG21	2.01	0.42
2:H:14:C:H2'	2:H:15:G:H8	1.84	0.42
4:P:19:A:H2'	4:P:20:G:C8	2.54	0.42
1:A:464:ILE:HD13	1:A:578:LEU:HD21	2.02	0.42
1:A:945:TRP:CZ3	1:A:964:ARG:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1015:THR:HG21	1:A:1057:LEU:HD21	2.00	0.42
1:A:1293:LEU:HD23	1:A:1293:LEU:HA	1.82	0.42
1:A:461:LYS:HE3	1:A:461:LYS:HB3	1.85	0.42
1:A:1346:GLU:HG3	1:A:1346:GLU:O	2.19	0.42
1:A:233:MET:HB2	1:A:990:SER:CB	2.49	0.42
1:A:451:LEU:HD11	1:A:1223:GLN:CG	2.50	0.42
1:A:389:LEU:HD23	1:A:526:ARG:HH11	1.84	0.42
1:A:558:LYS:HD2	2:H:2:A:O3'	2.20	0.42
1:A:849:ILE:O	1:A:853:ILE:HG13	2.19	0.42
1:A:911:TYR:CD1	1:A:1005:VAL:HG21	2.55	0.42
1:A:927:GLY:HA2	3:T:18:U:O3'	2.20	0.42
1:A:585:PHE:CE2	1:A:596:PRO:HD2	2.55	0.42
1:A:479:ILE:HD12	1:A:613:ILE:HD12	2.01	0.41
1:A:1138:MET:O	1:A:1142:MET:HG3	2.20	0.41
1:A:1183:ILE:CD1	1:A:1573:ILE:HG13	2.50	0.41
1:A:1289:LEU:HD12	1:A:1289:LEU:HA	1.90	0.41
1:A:739:ALA:HA	1:A:1023:LEU:HD22	2.03	0.41
1:A:969:VAL:HG22	1:A:1164:VAL:HG12	2.02	0.41
1:A:1241:GLY:C	1:A:1243:ALA:N	2.73	0.41
1:A:1275:GLU:HG2	1:A:1465:LYS:HD3	2.01	0.41
1:A:1417:CYS:HB3	1:A:1429:VAL:HG21	2.01	0.41
1:A:293:LEU:HD11	1:A:615:GLN:HB2	2.02	0.41
1:A:518:LEU:HD22	1:A:564:LEU:HB2	2.03	0.41
1:A:540:LYS:HB3	1:A:546:ILE:HD11	2.01	0.41
1:A:969:VAL:HG13	1:A:1164:VAL:HG12	2.01	0.41
1:A:1106:TYR:CD1	1:A:1139:TRP:HB3	2.56	0.41
1:A:1073:SER:HA	1:A:1146:HIS:HE2	1.86	0.41
1:A:282:TYR:HB2	1:A:404:SER:HB3	2.03	0.41
1:A:528:ILE:HD11	1:A:559:VAL:HG22	2.01	0.41
1:A:740:LYS:HA	1:A:743:LEU:HD13	2.03	0.41
1:A:985:PHE:HB2	1:A:1009:LEU:HD22	2.03	0.41
1:A:1014:LYS:HG2	1:A:1053:LYS:HG3	2.02	0.41
1:A:1076:PHE:CZ	1:A:1091:PHE:HE2	2.37	0.41
1:A:1331:SER:N	1:A:1558:ARG:HG2	2.31	0.41
1:A:1403:GLN:H	1:A:1403:GLN:HG3	1.61	0.41
1:A:337:MET:CE	1:A:498:TRP:HE3	2.33	0.41
1:A:576:LYS:HG2	1:A:1190:LEU:HD22	2.03	0.41
1:A:790:ILE:HD12	1:A:1068:PHE:CE1	2.56	0.41
1:A:1110:VAL:HG13	1:A:1111:ASP:OD2	2.21	0.41
4:P:13:A:H2'	4:P:14:G:C8	2.56	0.41
1:A:1057:LEU:HB2	1:A:1060:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1147:GLU:HG3	1:A:1157:ILE:HB	2.02	0.41
1:A:303:LYS:HE3	1:A:303:LYS:HB3	1.88	0.40
1:A:334:ILE:HD11	1:A:528:ILE:HB	2.03	0.40
1:A:357:ILE:HG23	1:A:358:GLN:HG3	2.02	0.40
1:A:454:PHE:CE1	1:A:1594:SER:HB2	2.56	0.40
1:A:463:LEU:HD11	1:A:581:THR:HG22	2.04	0.40
1:A:1063:LYS:HZ3	1:A:1063:LYS:HG3	1.74	0.40
1:A:1518:MET:O	1:A:1521:VAL:HG12	2.21	0.40
1:A:630:ILE:CD1	1:A:720:VAL:HG11	2.51	0.40
4:P:15:U:H2'	4:P:16:A:H8	1.86	0.40
1:A:334:ILE:HG21	1:A:530:VAL:HG21	2.03	0.40
1:A:617:MET:HG2	1:A:732:HIS:HA	2.02	0.40
2:H:17:A:H2'	2:H:18:A:C8	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1294/2173 (60%)	1239 (96%)	55 (4%)	0	100   100

There are no Ramachandran outliers to report.

### 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	1157/1940 (60%)	1114 (96%)	43 (4%)	34 65

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	ILE
1	A	279	CYS
1	A	286	ARG
1	A	309	SER
1	A	346	ARG
1	A	352	TYR
1	A	373	LEU
1	A	377	MET
1	A	390	ASN
1	A	454	PHE
1	A	479	ILE
1	A	503	TYR
1	A	549	ASP
1	A	599	TYR
1	A	627	ARG
1	A	744	GLU
1	A	814	SER
1	A	874	GLU
1	A	876	LYS
1	A	902	ARG
1	A	982	SER
1	A	1049	HIS
1	A	1134	VAL
1	A	1135	ASN
1	A	1141	SER
1	A	1173	SER
1	A	1276	LEU
1	A	1283	MET
1	A	1287	ASN
1	A	1322	PHE
1	A	1332	PHE
1	A	1344	LYS
1	A	1376	ARG
1	A	1380	LEU
1	A	1398	MET
1	A	1400	SER
1	A	1403	GLN
1	A	1414	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1417	CYS
1	A	1466	ASP
1	A	1475	VAL
1	A	1543	TYR
1	A	1556	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	GLN
1	A	460	GLN
1	A	1323	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	H	18/20 (90%)	5 (27%)	1 (5%)
3	S	6/25 (24%)	1 (16%)	0
3	T	11/25 (44%)	1 (9%)	0
3	V	8/25 (32%)	0	0
4	P	9/25 (36%)	1 (11%)	1 (11%)
All	All	52/120 (43%)	8 (15%)	2 (3%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	H	7	U
2	H	9	U
2	H	10	C
2	H	13	C
2	H	14	C
3	T	22	A
4	P	14	G
3	S	22	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	H	13	C
4	P	13	A

## 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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

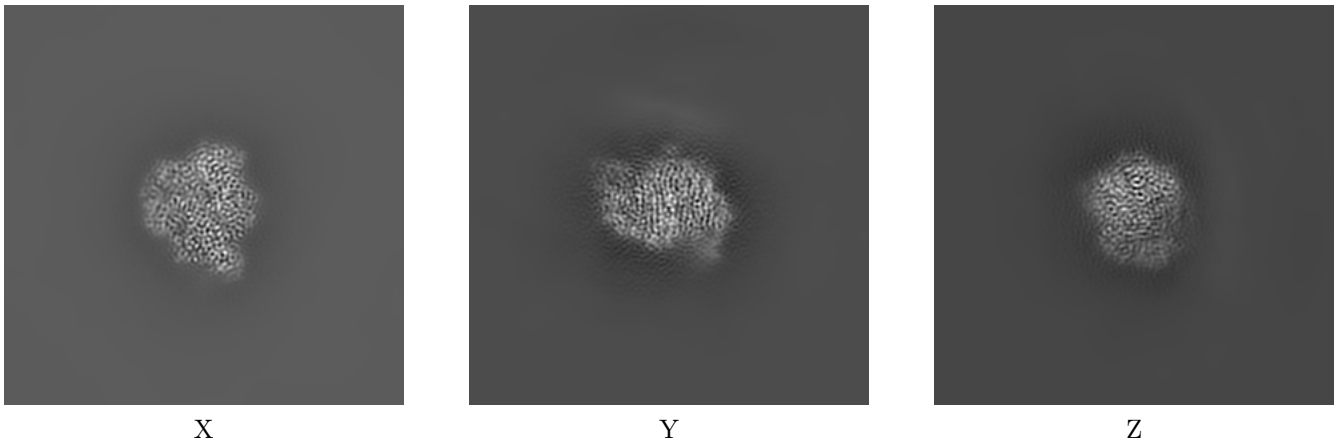
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16430. These allow visual inspection of the internal detail of the map and identification of artifacts.

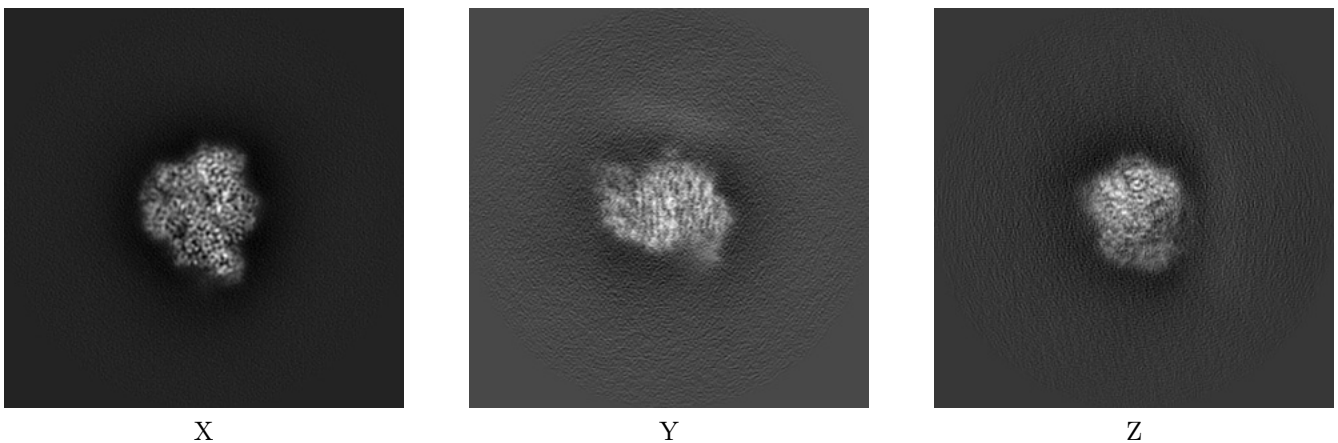
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



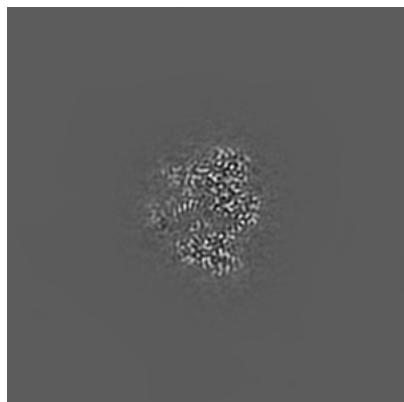
#### 6.1.2 Raw map



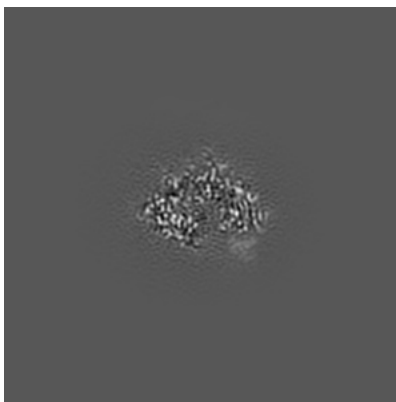
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

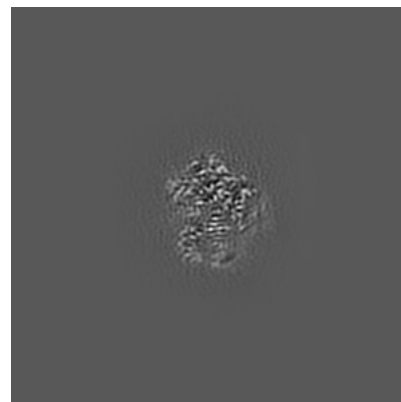
### 6.2.1 Primary map



X Index: 130

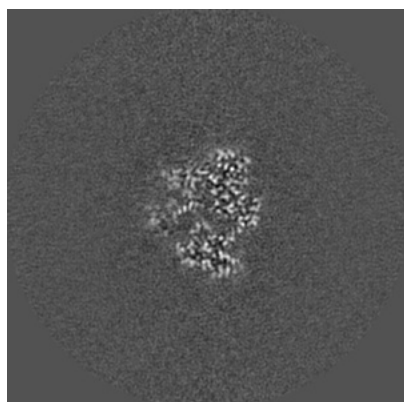


Y Index: 130

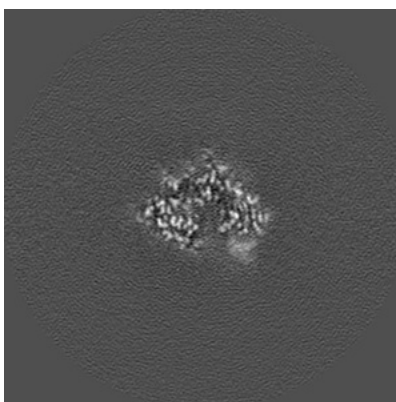


Z Index: 130

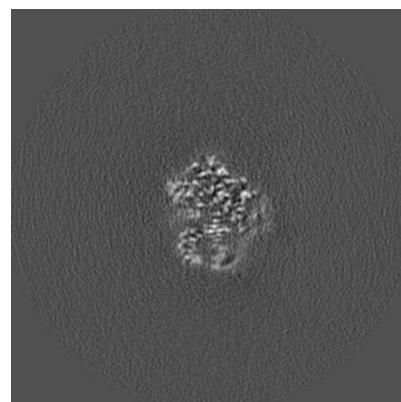
### 6.2.2 Raw map



X Index: 130



Y Index: 130

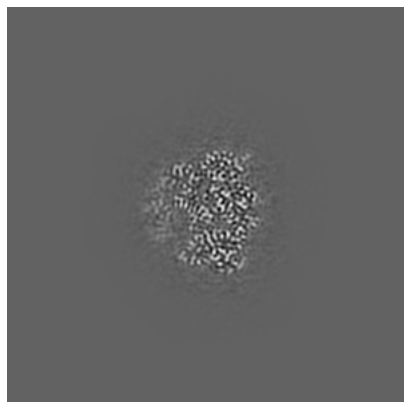


Z Index: 130

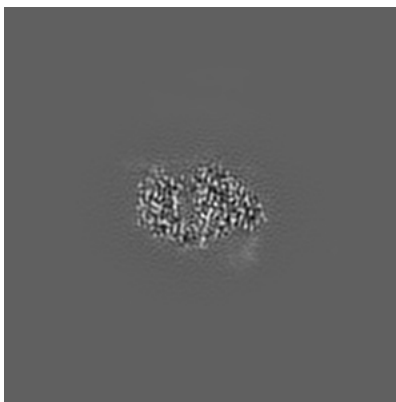
The images above show central slices of the map in three orthogonal directions.

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

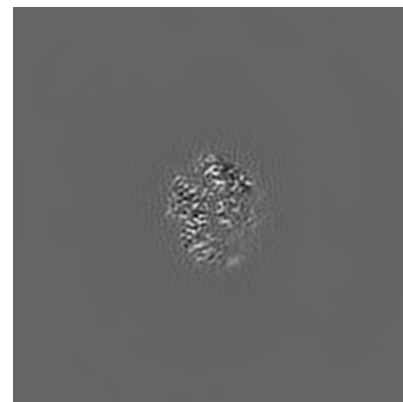
### 6.3.1 Primary map



X Index: 135

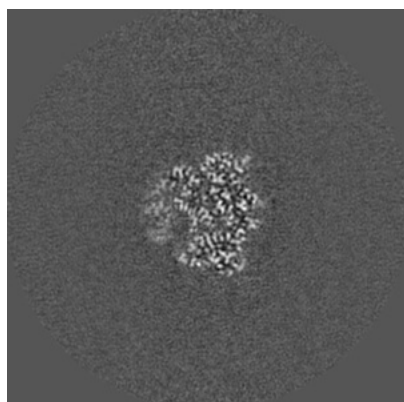


Y Index: 139

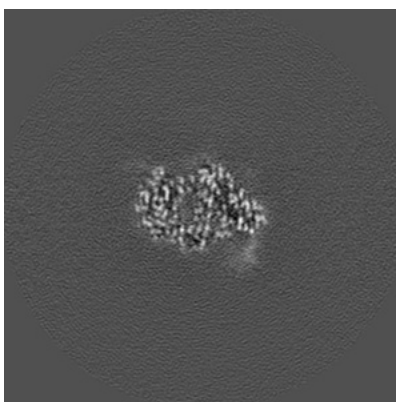


Z Index: 124

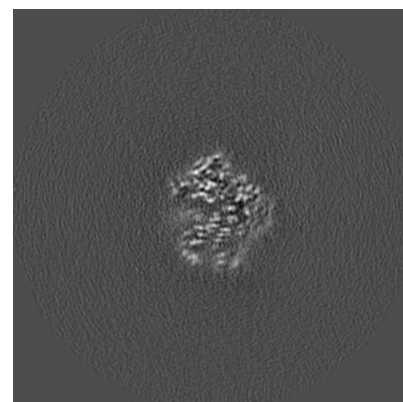
### 6.3.2 Raw map



X Index: 135



Y Index: 138

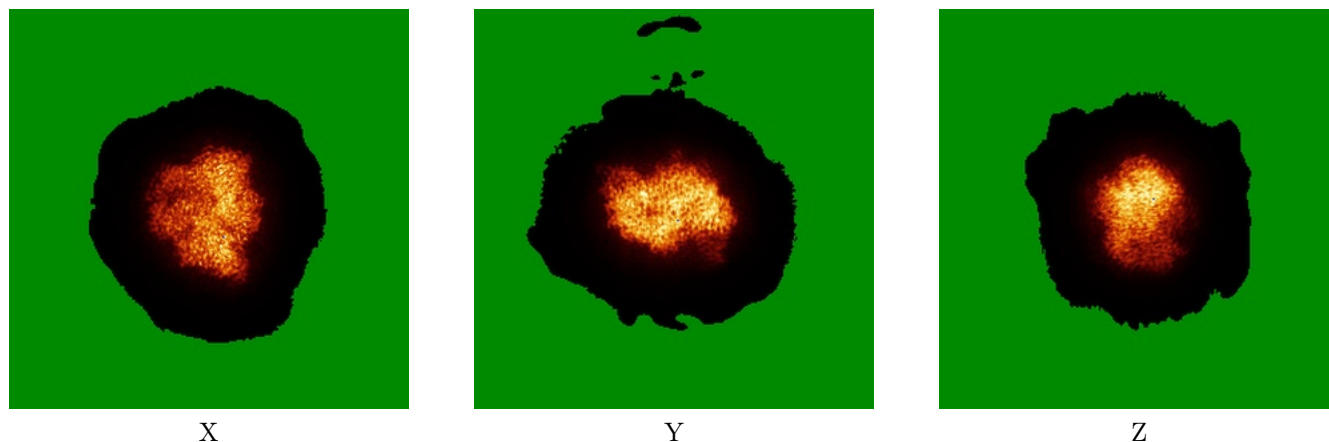


Z Index: 132

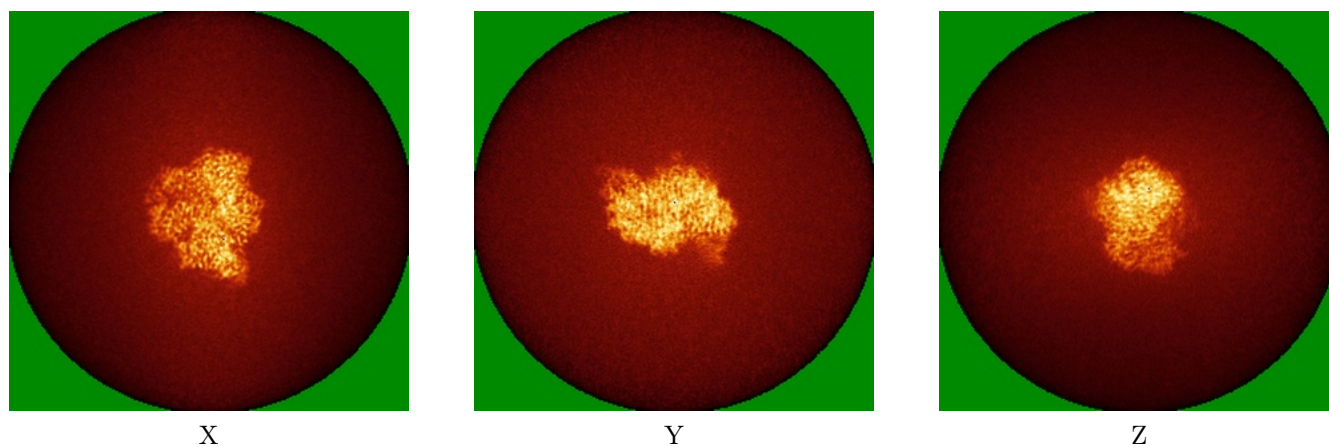
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map

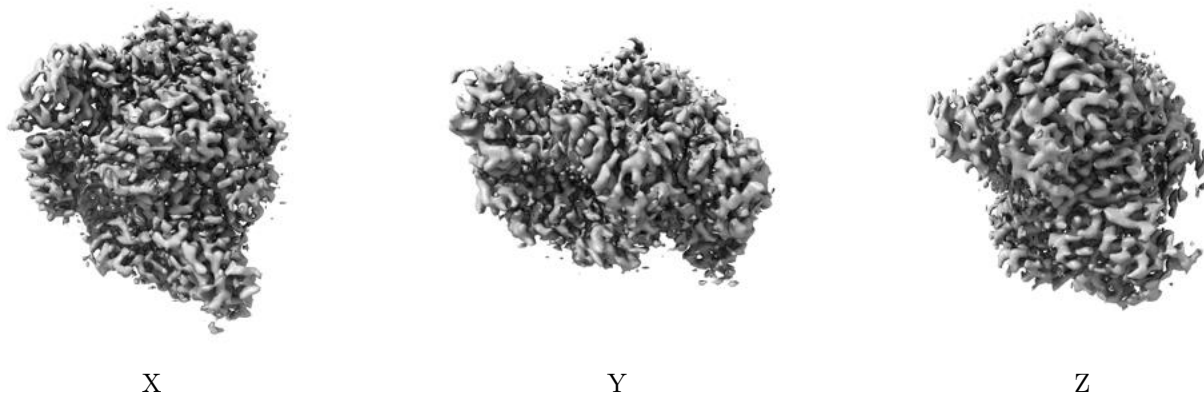


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



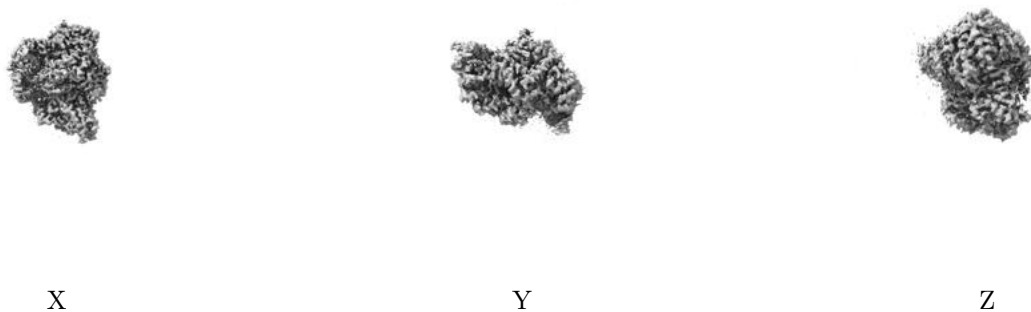
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0271. 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.

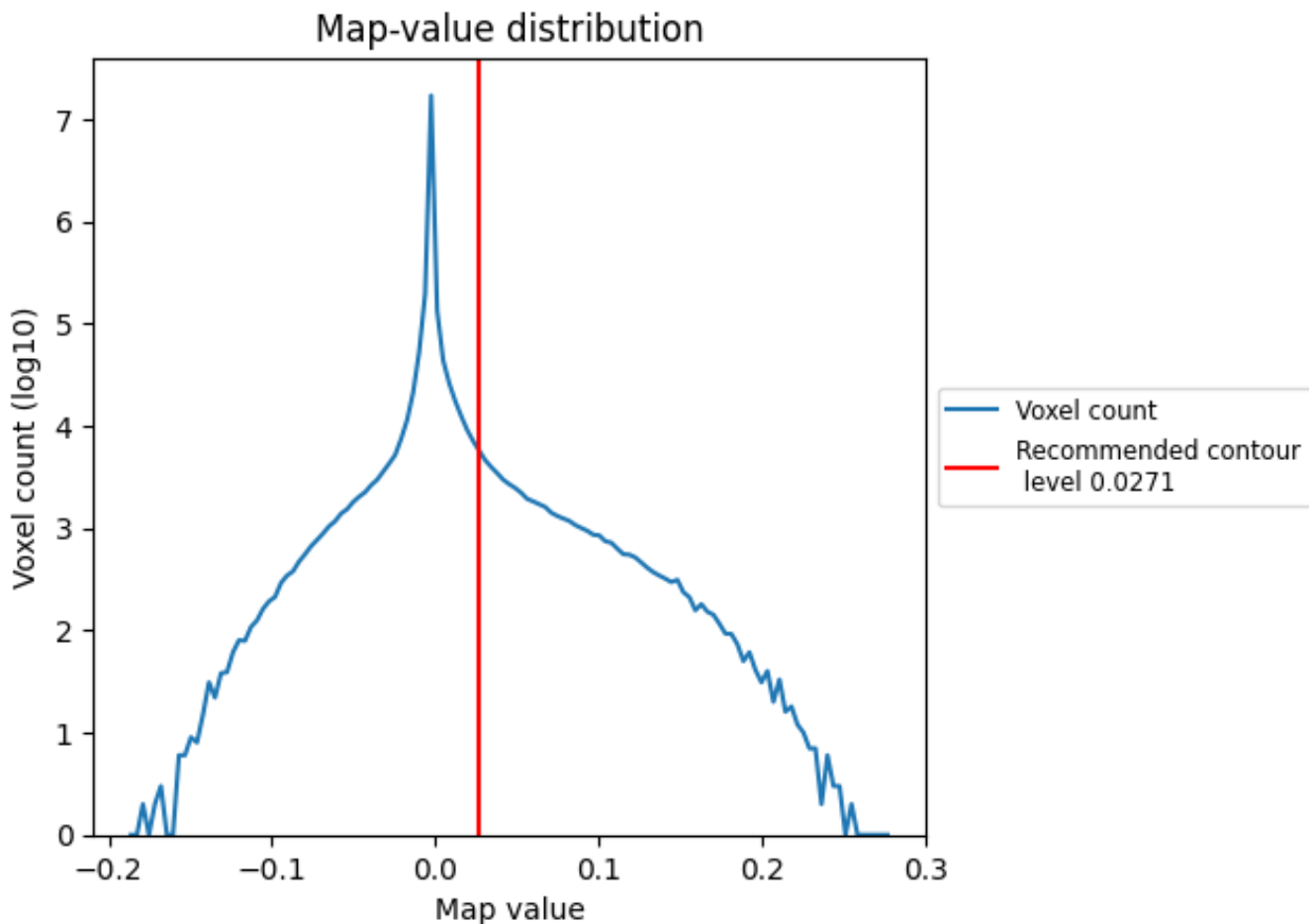
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

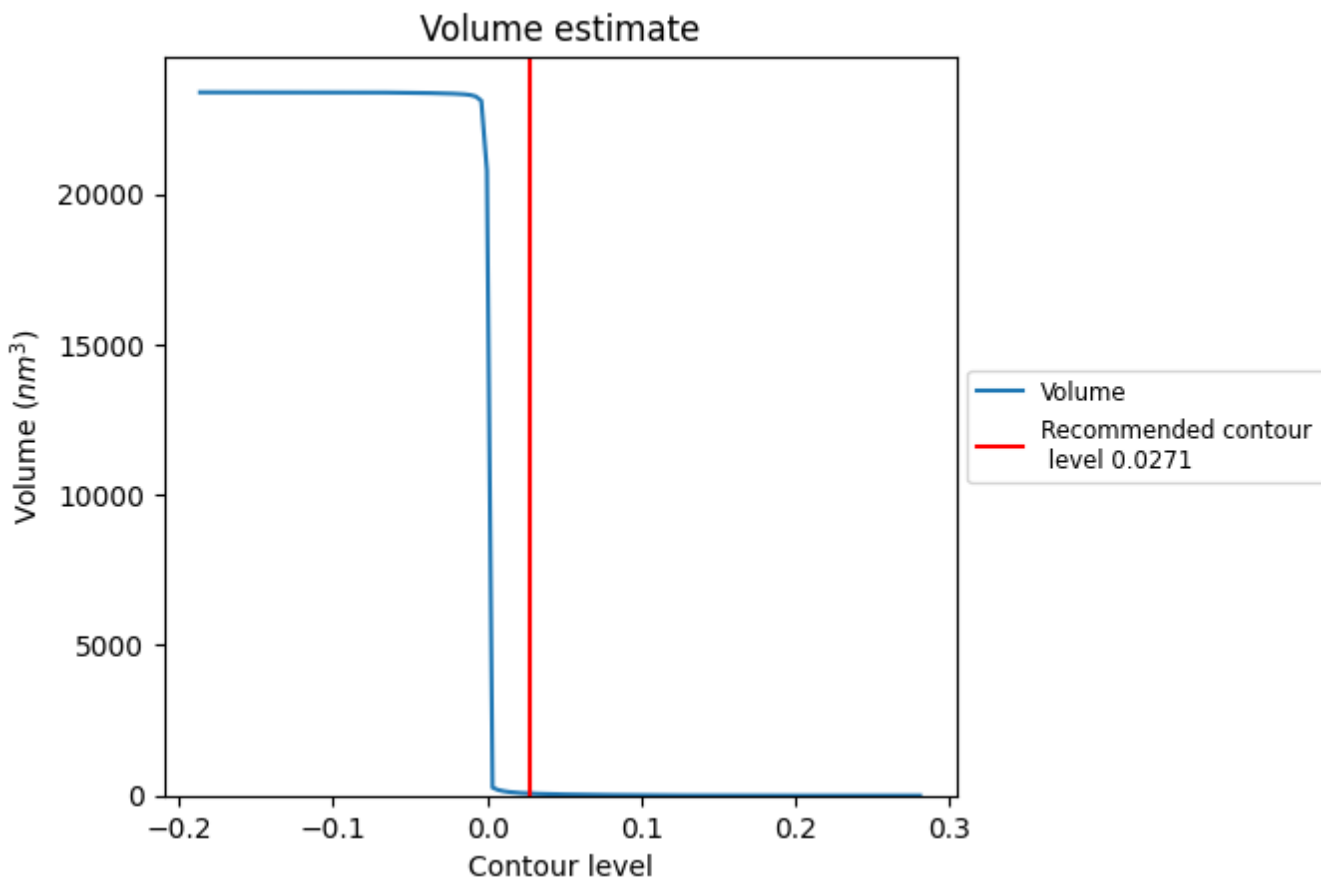
This section contains the results of statistical analysis of the map.

### 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.

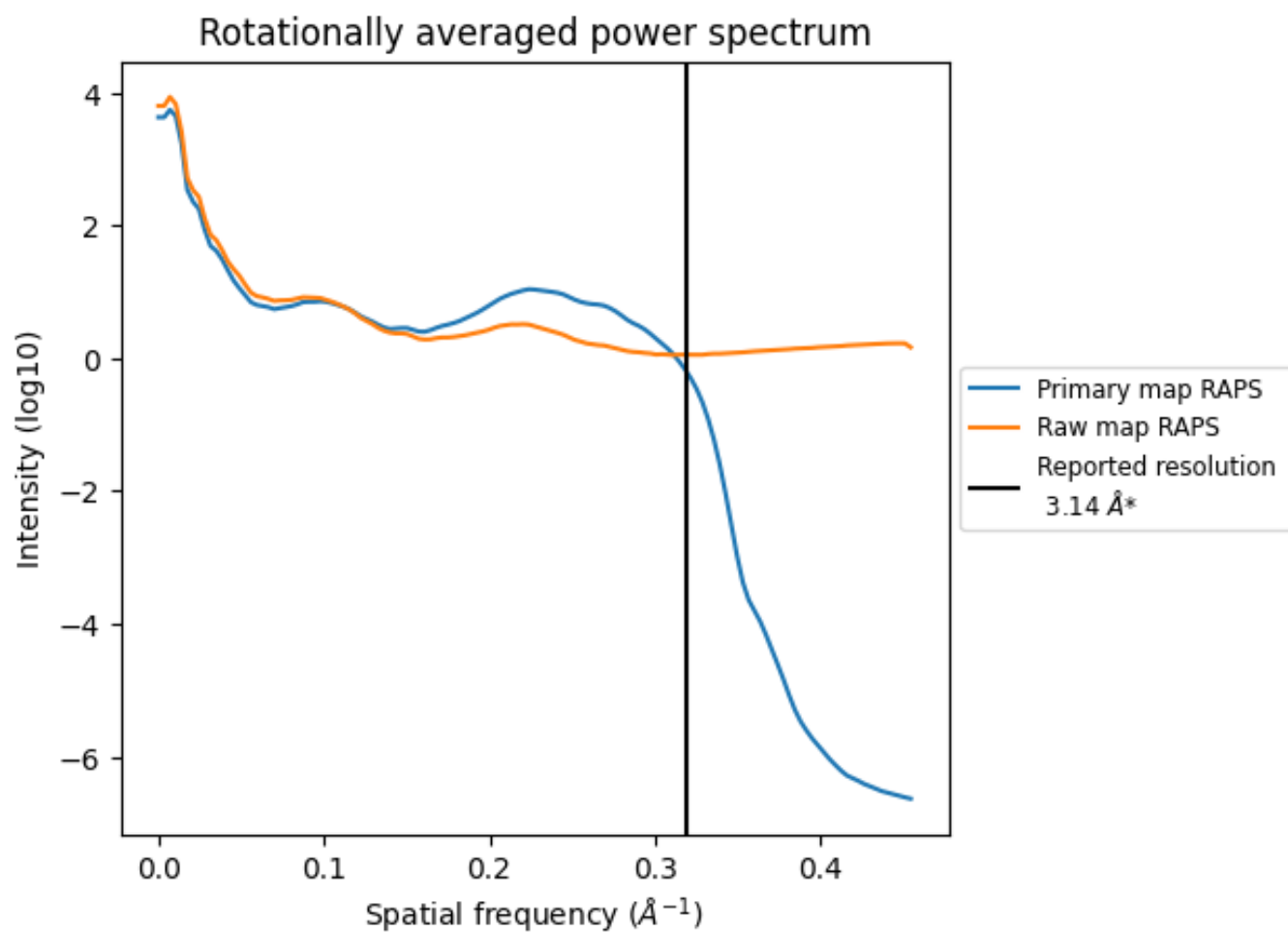
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 71 nm<sup>3</sup>; this corresponds to an approximate mass of 64 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](#)

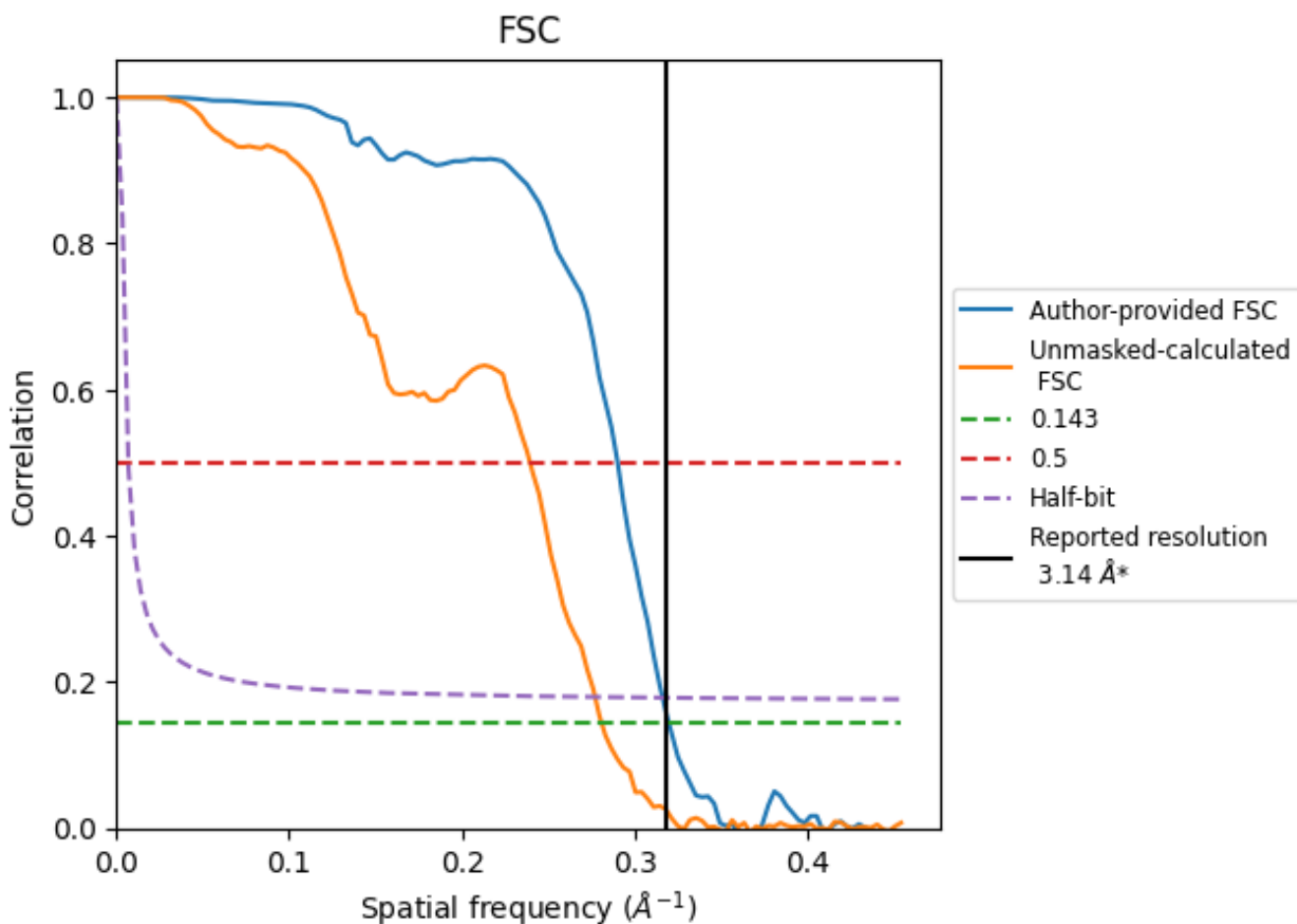


\*Reported resolution corresponds to spatial frequency of 0.318 Å<sup>-1</sup>

## 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 0.318 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

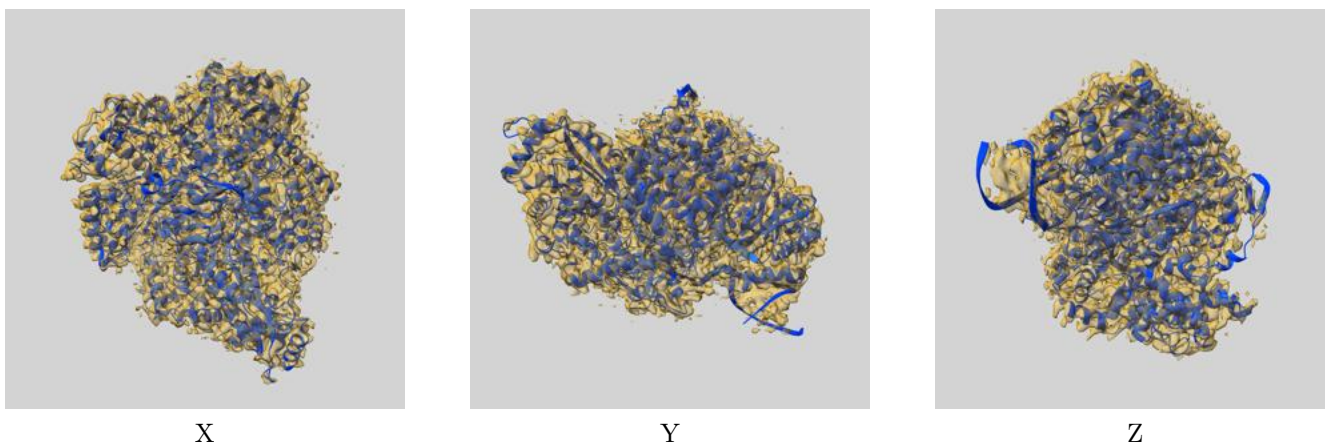
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	3.12	3.44	3.16
Unmasked-calculated*	3.56	4.18	3.61

\*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 3.56 differs from the reported value 3.14 by more than 10 %

## 9 Map-model fit [i](#)

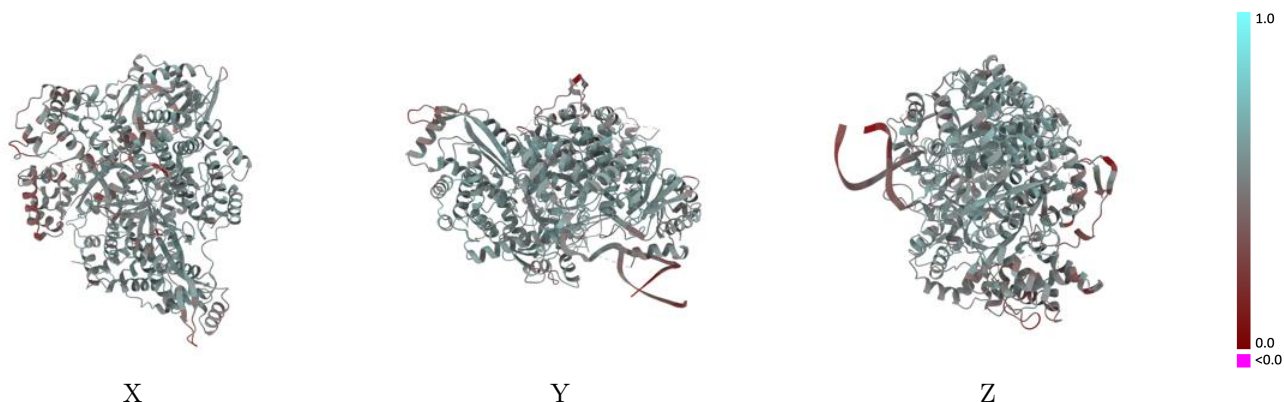
This section contains information regarding the fit between EMDB map EMD-16430 and PDB model 8C4V. Per-residue inclusion information can be found in section 3 on page 5.

### 9.1 Map-model overlay [i](#)



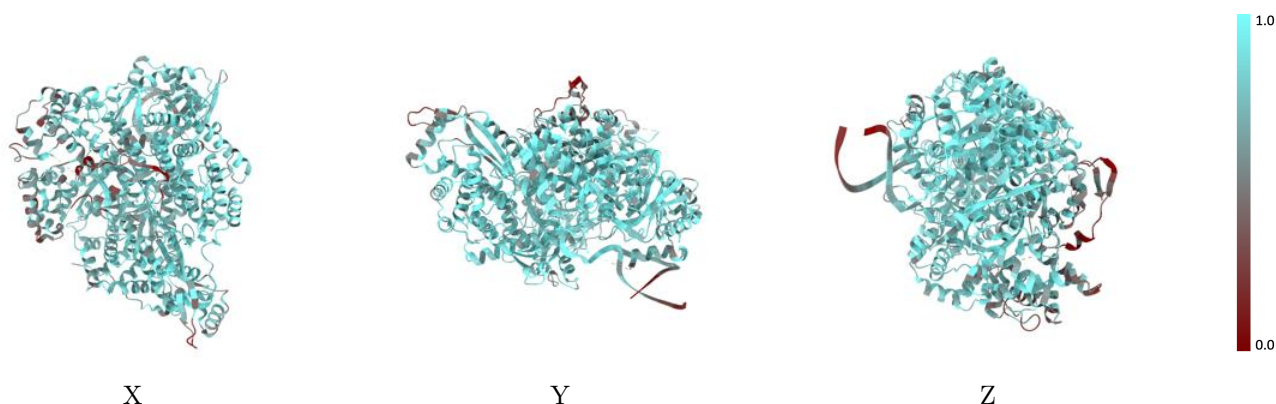
The images above show the 3D surface view of the map at the recommended contour level 0.0271 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

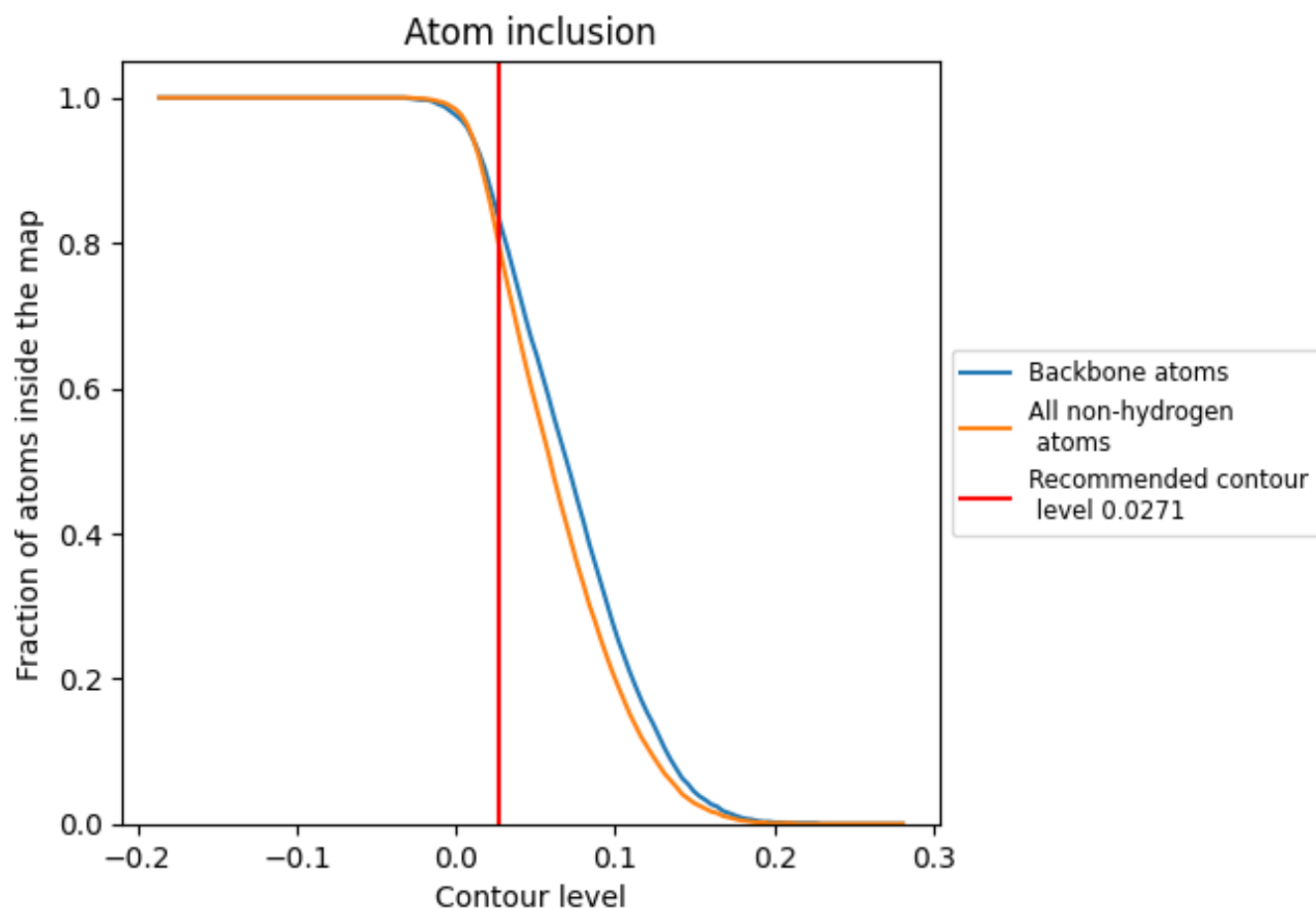
## 9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



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 (0.0271).

















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.0271) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7960	 0.5200
A	 0.8010	 0.5270
H	 0.7020	 0.4400
P	 0.8730	 0.5450
S	 0.9180	 0.5510
T	 0.8530	 0.5030
V	 0.4970	 0.3080

