



## Full wwPDB EM Validation Report ⓘ

Oct 7, 2024 – 05:33 PM EDT

PDB ID : 8V1T  
EMDB ID : EMD-42890  
Title : Herpes simplex virus 1 polymerase holoenzyme bound to DNA and acyclovir triphosphate in closed conformation  
Authors : Pan, J.; Abraham, J.; Coen, D.M.; Shankar, S.; Yang, P.; Hogle, J.  
Deposited on : 2023-11-21  
Resolution : 2.80 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.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

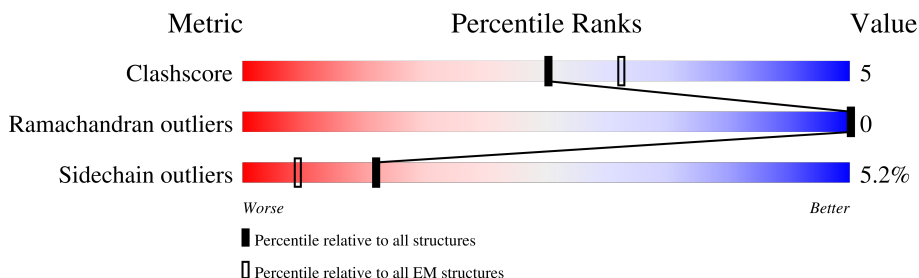
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1199	
2	B	340	
3	P	32	
4	T	50	

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
3	DOC	P	-1	X	-	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11645 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1064	Total	C	N	O	S	4	0
			8425	5401	1480	1505	39		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	HIS	-	expression tag	UNP H9E937
A	38	HIS	-	expression tag	UNP H9E937
A	39	HIS	-	expression tag	UNP H9E937
A	40	HIS	-	expression tag	UNP H9E937
A	41	HIS	-	expression tag	UNP H9E937
A	42	HIS	-	expression tag	UNP H9E937

- Molecule 2 is a protein called DNA polymerase processivity factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	265	Total	C	N	O	S	0	0
			2041	1299	359	376	7		

- Molecule 3 is a DNA chain called PRIMER DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	26	Total	C	N	O	P	0	0
			535	253	101	155	26		

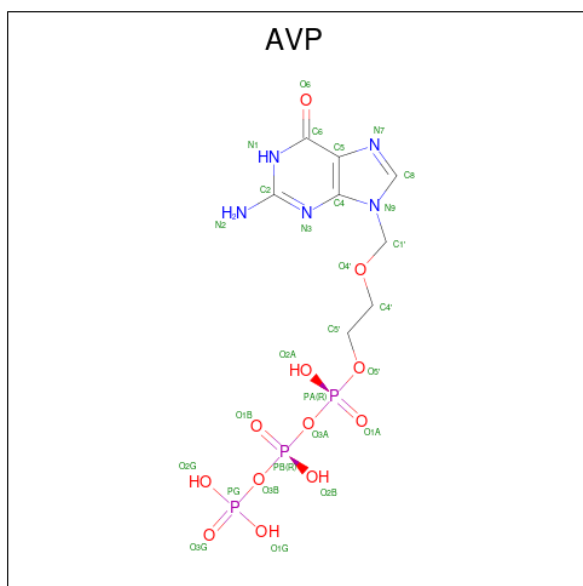
- Molecule 4 is a DNA chain called TEMPLATE DNA (50-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	30	Total	C	N	O	P	0	0
			608	288	111	179	30		

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

Mol	Chain	Residues	Atoms		AltConf
5	A	4	Total	Mg	0
			4	4	

- Molecule 6 is ACYCLOVIR TRIPHOSPHATE (three-letter code: AVP) (formula:  $C_8H_{14}N_5O_{12}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			28	8	5	12	3	

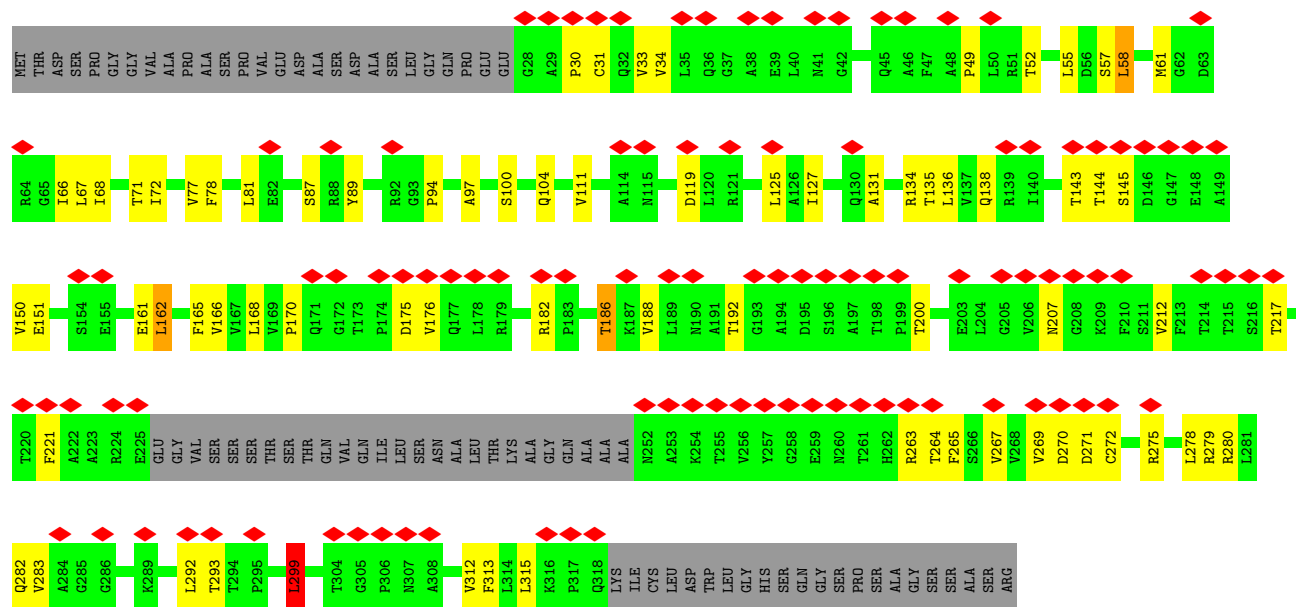
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	4	Total	O	0
			4	4	

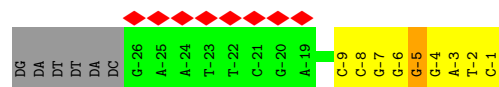




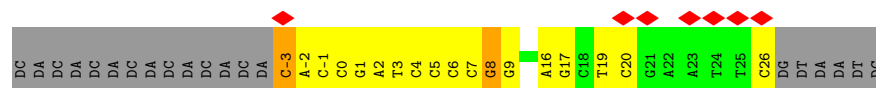
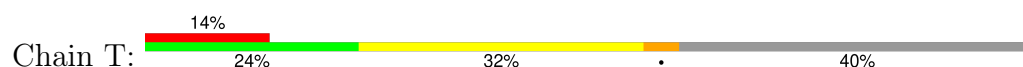
• Molecule 2: DNA polymerase processivity factor



• Molecule 3: PRIMER DNA (32-MER)



• Molecule 4: TEMPLATE DNA (50-MER)



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	187300	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 ( $e^-/\text{\AA}^2$ )	53.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	60606	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.167	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size ( $\text{\AA}$ )	264.0, 264.0, 264.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.825, 0.825, 0.825	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AVP, DOC, 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	1.07	23/8623 (0.3%)	0.88	8/11687 (0.1%)
2	B	0.59	0/2079	0.88	3/2830 (0.1%)
3	P	2.21	29/580 (5.0%)	1.16	2/894 (0.2%)
4	T	2.36	36/680 (5.3%)	1.46	12/1045 (1.1%)
All	All	1.20	88/11962 (0.7%)	0.95	25/16456 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
2	B	0	2
3	P	1	0
All	All	1	8

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	0	DC	C2-O2	-9.22	1.16	1.24
3	P	-4	DG	C3'-O3'	-8.55	1.32	1.44
4	T	3	DT	C3'-O3'	-7.85	1.33	1.44
1	A	1000	ALA	C-N	-7.84	1.16	1.34
1	A	320	PRO	CG-CD	-7.39	1.26	1.50
4	T	0	DC	N1-C2	-7.36	1.32	1.40
4	T	1	DG	C3'-O3'	-7.24	1.34	1.44
4	T	0	DC	N3-C4	-7.23	1.28	1.33
1	A	624	CYS	CB-SG	-7.14	1.70	1.82
3	P	-3	DA	C3'-O3'	-7.07	1.34	1.44
3	P	-5	DG	N7-C5	-6.98	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	1	DG	C8-N7	-6.93	1.26	1.30
4	T	2	DA	C6-N1	-6.72	1.30	1.35
3	P	-5	DG	C8-N7	-6.65	1.26	1.30
3	P	-7	DG	C8-N7	-6.61	1.26	1.30
3	P	-5	DG	C5-C4	-6.55	1.33	1.38
3	P	-2	DT	P-O5'	-6.51	1.53	1.59
3	P	-4	DG	C5-C4	-6.43	1.33	1.38
1	A	396	CYS	CB-SG	-6.28	1.71	1.82
3	P	-5	DG	C6-N1	-6.27	1.35	1.39
1	A	117	VAL	CB-CG2	-6.27	1.39	1.52
4	T	5	DC	N3-C4	-6.23	1.29	1.33
4	T	1	DG	O3'-P	-6.21	1.53	1.61
4	T	2	DA	C5-C4	-6.21	1.34	1.38
3	P	-7	DG	C5-C4	-6.20	1.34	1.38
3	P	-6	DG	C6-N1	-6.19	1.35	1.39
4	T	1	DG	C5-C4	-6.09	1.34	1.38
4	T	1	DG	N9-C4	-6.07	1.33	1.38
3	P	-6	DG	C5-C4	-5.99	1.34	1.38
1	A	320	PRO	N-CD	5.97	1.56	1.47
4	T	7	DC	N3-C4	-5.89	1.29	1.33
4	T	7	DC	C4-C5	-5.88	1.38	1.43
3	P	-6	DG	C2-N3	-5.88	1.28	1.32
1	A	259	TYR	CD2-CE2	-5.86	1.30	1.39
4	T	1	DG	C6-N1	-5.86	1.35	1.39
4	T	5	DC	C3'-O3'	-5.86	1.36	1.44
3	P	-7	DG	C5-C6	-5.84	1.36	1.42
4	T	4	DC	C3'-O3'	-5.84	1.36	1.44
3	P	-7	DG	N7-C5	-5.84	1.35	1.39
3	P	-3	DA	C5-C4	-5.79	1.34	1.38
3	P	-9	DC	N3-C4	-5.78	1.29	1.33
4	T	1	DG	C2-N3	-5.76	1.28	1.32
3	P	-7	DG	C3'-O3'	-5.75	1.36	1.44
1	A	263	THR	C-N	-5.73	1.20	1.34
4	T	0	DC	P-O5'	-5.72	1.54	1.59
3	P	-8	DC	N3-C4	-5.64	1.29	1.33
3	P	-5	DG	C2-N3	-5.63	1.28	1.32
1	A	362	TYR	CD1-CE1	-5.61	1.30	1.39
1	A	1055	TYR	CD1-CE1	-5.61	1.30	1.39
3	P	-3	DA	N9-C4	-5.60	1.34	1.37
4	T	26	DC	C1'-N1	5.58	1.56	1.49
3	P	-6	DG	N1-C2	-5.57	1.33	1.37
4	T	8	DG	C5-C4	-5.57	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	-1	DC	O3'-P	-5.54	1.54	1.61
3	P	-8	DC	N1-C6	-5.53	1.33	1.37
4	T	8	DG	N7-C5	-5.53	1.35	1.39
4	T	2	DA	C3'-O3'	-5.50	1.36	1.44
4	T	2	DA	N3-C4	-5.49	1.31	1.34
4	T	0	DC	C2-N3	-5.46	1.31	1.35
4	T	-1	DC	C3'-O3'	-5.44	1.36	1.44
1	A	696	TYR	CD1-CE1	-5.44	1.31	1.39
4	T	8	DG	C3'-O3'	-5.43	1.36	1.44
3	P	-4	DG	C8-N7	-5.40	1.27	1.30
3	P	-2	DT	C5-C6	-5.35	1.30	1.34
4	T	6	DC	C4-C5	-5.35	1.38	1.43
4	T	7	DC	C3'-O3'	-5.35	1.36	1.44
4	T	1	DG	N1-C2	-5.34	1.33	1.37
3	P	-4	DG	C2-N3	-5.31	1.28	1.32
4	T	9	DG	C3'-O3'	-5.30	1.37	1.44
4	T	2	DA	C8-N7	-5.29	1.27	1.31
1	A	818	TYR	CD2-CE2	-5.27	1.31	1.39
1	A	614	TYR	CD2-CE2	-5.26	1.31	1.39
1	A	490	TYR	CD1-CE1	-5.21	1.31	1.39
4	T	9	DG	C5-C4	-5.20	1.34	1.38
3	P	-8	DC	C4-C5	-5.18	1.38	1.43
3	P	-7	DG	C6-N1	-5.18	1.35	1.39
4	T	8	DG	N9-C8	-5.16	1.34	1.37
1	A	963	CYS	CB-SG	-5.15	1.73	1.81
1	A	366	CYS	CB-SG	-5.15	1.73	1.81
1	A	884	TYR	CD2-CE2	-5.14	1.31	1.39
1	A	345	CYS	CB-SG	-5.13	1.73	1.81
3	P	-5	DG	N1-C2	-5.09	1.33	1.37
1	A	196	VAL	CB-CG1	-5.07	1.42	1.52
1	A	316	TYR	CD1-CE1	-5.07	1.31	1.39
4	T	4	DC	C4-C5	-5.06	1.39	1.43
1	A	538	TYR	CD2-CE2	-5.04	1.31	1.39
1	A	362	TYR	CE1-CZ	-5.04	1.32	1.38
1	A	564	TYR	CD1-CE1	-5.01	1.31	1.39

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	PRO	CA-N-CD	-17.97	86.35	111.50
1	A	320	PRO	N-CD-CG	-12.21	84.89	103.20
4	T	-3	DC	P-O3'-C3'	11.84	133.91	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	16	DA	P-O3'-C3'	10.40	132.18	119.70
3	P	-4	DG	O4'-C1'-N9	10.29	115.20	108.00
4	T	3	DT	P-O3'-C3'	9.21	130.75	119.70
2	B	30	PRO	CA-N-CD	-8.28	99.91	111.50
4	T	0	DC	P-O3'-C3'	7.87	129.15	119.70
3	P	-9	DC	O4'-C1'-N1	7.85	113.49	108.00
4	T	1	DG	P-O3'-C3'	7.83	129.10	119.70
4	T	-2	DA	O3'-P-O5'	-7.63	89.51	104.00
4	T	2	DA	P-O3'-C3'	7.16	128.30	119.70
2	B	162	LEU	CA-CB-CG	7.16	131.77	115.30
4	T	4	DC	P-O3'-C3'	7.08	128.20	119.70
1	A	320	PRO	CA-CB-CG	-6.78	91.12	104.00
4	T	16	DA	O3'-P-O5'	6.67	116.67	104.00
4	T	19	DT	P-O3'-C3'	6.48	127.48	119.70
1	A	777	LEU	CA-CB-CG	6.38	129.96	115.30
1	A	823	VAL	CG1-CB-CG2	-6.37	100.71	110.90
1	A	581	ASP	CB-CG-OD1	6.22	123.90	118.30
4	T	4	DC	O4'-C1'-N1	5.83	112.08	108.00
4	T	17	DG	O5'-P-OP2	-5.79	100.49	105.70
1	A	1234	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	360	PRO	C-N-CA	5.44	135.31	121.70
2	B	299	LEU	CA-CB-CG	5.30	127.49	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	P	-1	DOC	C4'

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1001	ARG	Sidechain
1	A	1025	GLU	Peptide
1	A	128	ARG	Sidechain
1	A	259	TYR	Peptide
1	A	323	ASN	Peptide
1	A	789	ARG	Sidechain
2	B	207	ASN	Peptide
2	B	49	PRO	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8425	0	8428	92	0
2	B	2041	0	2087	39	0
3	P	535	0	291	1	0
4	T	608	0	336	3	0
5	A	4	0	0	0	0
6	A	28	0	10	0	0
7	A	4	0	0	1	0
All	All	11645	0	11152	122	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 5.

All (122) 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:771:GLU:OE2	1:A:779:ARG:NH2	2.13	0.80
1:A:977:LEU:O	1:A:984:SER:OG	2.01	0.79
1:A:319:LYS:NZ	1:A:348:ASP:O	2.15	0.78
1:A:767:ALA:O	1:A:768:HIS:ND1	2.17	0.77
2:B:111:VAL:HG21	2:B:138:GLN:HE22	1.51	0.75
1:A:692:ARG:NH2	3:P:-5:DG:N7	2.34	0.75
2:B:55:LEU:O	2:B:100:SER:OG	2.06	0.74
1:A:855:ARG:O	1:A:861:GLN:NE2	2.21	0.74
1:A:1054:VAL:HG21	1:A:1074:TYR:HB3	1.70	0.73
1:A:1054:VAL:HG22	1:A:1143:ALA:O	1.90	0.71
1:A:476:LEU:O	1:A:480:THR:OG1	2.08	0.71
1:A:644:ARG:O	4:T:-3:DC:N4	2.26	0.69
1:A:1037:LEU:O	1:A:1044:TYR:OH	2.10	0.69
1:A:1016:ASP:OD1	1:A:1019:ARG:NH1	2.25	0.69
1:A:986:ALA:HB1	1:A:1007:LEU:HD22	1.73	0.68
2:B:192:THR:O	2:B:275:ARG:NH2	2.26	0.67
1:A:1038:SER:N	1:A:1068:ILE:O	2.28	0.66
1:A:996:GLU:HG3	1:A:1183:ILE:HD11	1.77	0.66
1:A:476:LEU:HD22	1:A:487:LEU:HD13	1.77	0.65
1:A:1194:GLU:HG2	2:B:162:LEU:HD12	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1219:THR:OG1	1:A:1222:GLU:OE1	2.15	0.65
1:A:721:LEU:HD22	1:A:888:ASP:HB3	1.78	0.65
2:B:279:ARG:NH2	4:T:20:DC:OP2	2.33	0.62
2:B:34:VAL:O	2:B:87:SER:N	2.34	0.61
1:A:262:GLU:HB3	1:A:742:ALA:HB2	1.82	0.60
1:A:720:SER:OG	7:A:1402:HOH:O	2.09	0.59
1:A:120:GLY:O	1:A:125:ARG:NH2	2.35	0.59
1:A:1213:ALA:HB1	2:B:166:VAL:CG2	2.32	0.59
1:A:1164:HIS:NE2	4:T:8:DG:OP1	2.36	0.59
1:A:911:SER:OG	1:A:915:ARG:NH2	2.36	0.58
1:A:273:VAL:HG11	1:A:279:LEU:HD22	1.85	0.58
1:A:193:ARG:NH2	1:A:458:GLY:O	2.37	0.57
1:A:832:HIS:O	1:A:836:THR:OG1	2.22	0.57
1:A:1016:ASP:OD2	1:A:1020:ARG:NH1	2.37	0.56
1:A:323:ASN:OD1	1:A:324:ASN:N	2.35	0.56
1:A:873:ARG:NH2	1:A:876:GLY:O	2.39	0.56
1:A:888:ASP:N	1:A:888:ASP:OD1	2.39	0.55
1:A:1196:TRP:HE1	2:B:58:LEU:HD13	1.72	0.55
1:A:1194:GLU:CG	2:B:162:LEU:HD12	2.37	0.55
1:A:1234:LEU:HD21	2:B:78:PHE:CG	2.41	0.55
1:A:1201:ASP:O	1:A:1205:ARG:NE	2.40	0.55
1:A:1221:GLU:OE2	1:A:1224:ARG:NH1	2.39	0.55
1:A:476:LEU:HD22	1:A:487:LEU:CD1	2.38	0.54
1:A:1054:VAL:HG21	1:A:1074:TYR:CB	2.35	0.54
2:B:134:ARG:NE	2:B:161:GLU:OE1	2.35	0.54
2:B:299:LEU:HB3	2:B:315:LEU:HD11	1.89	0.54
2:B:267:VAL:CG1	2:B:292:LEU:HD11	2.37	0.53
2:B:270:ASP:OD1	2:B:271:ASP:N	2.42	0.53
2:B:188:VAL:HG13	2:B:212:VAL:HG21	1.90	0.53
2:B:182:ARG:O	2:B:186:THR:OG1	2.25	0.52
1:A:1061:ARG:NH1	1:A:1144:GLU:OE2	2.40	0.52
1:A:787:GLN:OE1	1:A:791:ARG:NH1	2.43	0.51
1:A:1234:LEU:HD21	2:B:78:PHE:CD2	2.45	0.51
1:A:303:PHE:O	1:A:307:ASN:ND2	2.43	0.51
1:A:698:GLY:O	1:A:842:ARG:NH1	2.41	0.51
1:A:337:THR:OG1	1:A:342:GLU:OE2	2.28	0.50
1:A:293:TYR:CD2	1:A:635:ILE:HD12	2.47	0.49
2:B:119:ASP:O	2:B:143:THR:HG23	2.12	0.49
2:B:127:ILE:HD11	2:B:136:LEU:HD13	1.93	0.49
2:B:125:LEU:HG	2:B:136:LEU:HD11	1.95	0.49
1:A:504:ILE:HG21	1:A:1068:ILE:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:LEU:HD13	1:A:613:ILE:HG12	1.94	0.48
2:B:278:LEU:HD13	2:B:283:VAL:HG21	1.96	0.48
1:A:330:ARG:NH1	1:A:334:ALA:O	2.47	0.48
2:B:97:ALA:O	2:B:162:LEU:N	2.40	0.48
1:A:1222:GLU:OE1	1:A:1222:GLU:N	2.47	0.48
1:A:315:TRP:NE1	1:A:358:ASP:O	2.40	0.47
1:A:928:LYS:HE3	1:A:951:LEU:HD22	1.96	0.47
1:A:526:TYR:O	1:A:530:THR:HG23	2.15	0.46
1:A:818:TYR:O	1:A:821:THR:OG1	2.30	0.46
1:A:882:ILE:HD12	1:A:890:ILE:HD12	1.97	0.46
1:A:175:ILE:HG22	1:A:179:GLY:HA3	1.97	0.46
1:A:615:ASP:OD1	1:A:615:ASP:N	2.47	0.46
2:B:176:VAL:HG11	2:B:265:PHE:HE1	1.79	0.46
1:A:1050:ALA:O	1:A:1054:VAL:HG23	2.15	0.46
1:A:1180:ASN:OD1	1:A:1183:ILE:HD12	2.16	0.46
1:A:1216:ALA:N	2:B:165:PHE:O	2.42	0.46
1:A:1214:VAL:HG21	1:A:1227:LEU:HD21	1.98	0.45
1:A:1041:PRO:HB3	1:A:1052:LEU:HD22	1.98	0.45
1:A:1206:LEU:HD23	1:A:1211:PHE:HD2	1.82	0.45
1:A:298:ASP:OD1	1:A:298:ASP:N	2.51	0.44
1:A:268:PHE:CZ	1:A:635:ILE:HD11	2.52	0.44
1:A:1234:LEU:HD13	2:B:170:PRO:HG2	2.00	0.44
1:A:463:THR:OG1	1:A:523:ILE:O	2.23	0.44
1:A:823:VAL:O	1:A:829:PRO:HB3	2.17	0.44
1:A:995:ALA:HB2	1:A:1177:PHE:O	2.18	0.44
1:A:936:ILE:HA	1:A:1175:ALA:HB2	1.99	0.44
2:B:68:ILE:HD11	2:B:81:LEU:HD11	1.99	0.44
1:A:983:VAL:HG22	1:A:1006:GLY:O	2.18	0.44
1:A:216:LEU:HD21	1:A:287:CYS:SG	2.58	0.43
2:B:269:VAL:HG22	2:B:315:LEU:HD23	1.99	0.43
2:B:170:PRO:HG3	2:B:312:VAL:HG21	1.99	0.43
1:A:182:ILE:HG13	1:A:201:THR:HG21	2.00	0.43
2:B:72:ILE:HD12	2:B:77:VAL:HG11	1.99	0.43
1:A:1040:HIS:HA	1:A:1068:ILE:HD12	2.01	0.43
1:A:1202:VAL:HG12	1:A:1206:LEU:HD13	2.00	0.43
2:B:97:ALA:O	2:B:162:LEU:HB2	2.19	0.43
2:B:94:PRO:HG2	2:B:131:ALA:HB1	2.01	0.42
1:A:1018:HIS:O	1:A:1021:ILE:HG22	2.19	0.42
1:A:859:PHE:CE2	1:A:863:LEU:HD13	2.54	0.42
2:B:33:VAL:HG22	2:B:89:TYR:CD2	2.55	0.42
2:B:144:THR:CG2	2:B:150:VAL:HG23	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:TYR:HD1	1:A:282:LEU:HD12	1.85	0.42
1:A:384:ALA:HB1	1:A:477:ALA:HB3	2.02	0.42
1:A:465:TYR:OH	1:A:543:VAL:HG21	2.19	0.42
2:B:175:ASP:OD1	2:B:176:VAL:N	2.53	0.41
1:A:281:TYR:O	1:A:285:ASN:N	2.50	0.41
2:B:61:MET:HG3	2:B:66:ILE:HG23	2.03	0.41
1:A:122:PHE:HB3	1:A:438:LEU:HD21	2.01	0.41
1:A:293:TYR:CG	1:A:635:ILE:HD12	2.55	0.41
1:A:447:LEU:HD22	1:A:475:LEU:CD2	2.50	0.41
1:A:739:ARG:NH2	1:A:741:ASP:OD2	2.54	0.41
1:A:789:ARG:HA	1:A:792:ILE:HD12	2.03	0.41
1:A:600:ALA:HB1	1:A:784:MET:CE	2.51	0.41
1:A:624:CYS:CB	1:A:777:LEU:HD13	2.51	0.41
1:A:1213:ALA:HB1	2:B:166:VAL:HG23	2.01	0.41
2:B:71:THR:HG23	2:B:71:THR:O	2.21	0.40
1:A:292:LYS:N	1:A:292:LYS:HD3	2.36	0.40
2:B:52:THR:HG23	2:B:55:LEU:HD22	2.03	0.40
2:B:144:THR:HG21	2:B:150:VAL:HG23	2.03	0.40
1:A:206:TYR:HA	1:A:269:TYR:O	2.22	0.40
1:A:404:THR:O	1:A:404:THR:HG22	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1060/1199 (88%)	1053 (99%)	7 (1%)	0	100	100
2	B	261/340 (77%)	261 (100%)	0	0	100	100
All	All	1321/1539 (86%)	1314 (100%)	7 (0%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	880/977 (90%)	844 (96%)	36 (4%)	26	59
2	B	226/282 (80%)	205 (91%)	21 (9%)	7	23
All	All	1106/1259 (88%)	1049 (95%)	57 (5%)	22	50

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	THR
1	A	64	ARG
1	A	72	ASP
1	A	87	PRO
1	A	110	ASP
1	A	180	THR
1	A	256	THR
1	A	277	ARG
1	A	292	LYS
1	A	333	MET
1	A	345	CYS
1	A	390	LEU
1	A	414	LEU
1	A	442	SER
1	A	471	ASP
1	A	499	PHE
1	A	545	GLU
1	A	556	SER
1	A	578	CYS
1	A	693	HIS
1	A	717	ASP
1	A	739	ARG
1	A	760	ARG
1	A	794	GLN
1	A	868	GLU
1	A	888	ASP
1	A	907	ASP

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Mol	Chain	Res	Type
1	A	911	SER
1	A	990	LEU
1	A	1034	THR
1	A	1042	ARG
1	A	1062	ARG
1	A	1145	ASP
1	A	1164	HIS
1	A	1194	GLU
1	A	1201	ASP
2	B	31	CYS
2	B	57	SER
2	B	58	LEU
2	B	67	LEU
2	B	104	GLN
2	B	135	THR
2	B	145	SER
2	B	151	GLU
2	B	168	LEU
2	B	186	THR
2	B	200	THR
2	B	217	THR
2	B	221	PHE
2	B	263	ARG
2	B	264	THR
2	B	272	CYS
2	B	280	ARG
2	B	282	GLN
2	B	293	THR
2	B	299	LEU
2	B	313	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	138	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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
3	DOC	P	-1	3,4	16,19,20	2.81	10 (62%)	20,26,29	3.78	7 (35%)

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
3	DOC	P	-1	3,4	1/1/3/3	1/7/18/19	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	-1	DOC	C5-C4	-4.81	1.31	1.42
3	P	-1	DOC	C2-N1	-3.98	1.31	1.40
3	P	-1	DOC	O2-C2	-3.86	1.16	1.23
3	P	-1	DOC	C4-N4	3.64	1.42	1.33
3	P	-1	DOC	C3'-C2'	-3.47	1.44	1.54
3	P	-1	DOC	C4-N3	-3.21	1.28	1.34
3	P	-1	DOC	C6-N1	-3.19	1.30	1.38
3	P	-1	DOC	O4'-C4'	-3.03	1.38	1.44
3	P	-1	DOC	C2-N3	-2.27	1.31	1.36
3	P	-1	DOC	O5'-C5'	-2.13	1.37	1.44

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	-1	DOC	C4'-O4'-C1'	-11.53	98.92	109.81
3	P	-1	DOC	O4'-C4'-C5'	6.70	121.42	109.34
3	P	-1	DOC	O4'-C4'-C3'	6.11	114.87	104.81
3	P	-1	DOC	C2'-C3'-C4'	-4.44	94.50	102.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	-1	DOC	C3'-C2'-C1'	3.83	107.28	102.87
3	P	-1	DOC	O4'-C1'-N1	3.55	114.16	107.86
3	P	-1	DOC	O2-C2-N3	-2.05	119.10	122.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	P	-1	DOC	C4'

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	-1	DOC	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	AVP	A	1305	5	23,29,29	2.66	9 (39%)	28,44,44	2.37	10 (35%)

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
6	AVP	A	1305	5	-	10/19/21/21	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1305	AVP	PB-O3B	5.58	1.65	1.59
6	A	1305	AVP	PB-O3A	5.40	1.65	1.59
6	A	1305	AVP	C2-N2	4.79	1.43	1.33
6	A	1305	AVP	PA-O3A	4.56	1.64	1.59
6	A	1305	AVP	C4-N3	-3.12	1.31	1.35
6	A	1305	AVP	C5-C6	-2.69	1.36	1.41
6	A	1305	AVP	PG-O1G	-2.59	1.45	1.54
6	A	1305	AVP	PG-O2G	-2.41	1.45	1.54
6	A	1305	AVP	PB-O2B	-2.34	1.44	1.55

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1305	AVP	N3-C2-N1	-5.65	120.03	127.21
6	A	1305	AVP	O3A-PB-O1B	-5.22	95.00	110.70
6	A	1305	AVP	C2-N3-C4	4.42	120.25	115.48
6	A	1305	AVP	O2B-PB-O3A	3.82	117.60	107.27
6	A	1305	AVP	N2-C2-N3	3.81	123.74	117.79
6	A	1305	AVP	C5-C6-N1	-3.16	119.20	123.42
6	A	1305	AVP	C2-N1-C6	2.95	120.07	115.96
6	A	1305	AVP	C4-C5-N7	-2.85	106.32	109.34
6	A	1305	AVP	O3A-PA-O1A	-2.20	104.08	110.70
6	A	1305	AVP	O4'-C4'-C5'	-2.11	100.72	110.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1305	AVP	C5'-O5'-PA-O2A
6	A	1305	AVP	C5'-O5'-PA-O3A
6	A	1305	AVP	O4'-C4'-C5'-O5'
6	A	1305	AVP	PB-O3B-PG-O2G
6	A	1305	AVP	N9-C1'-O4'-C4'
6	A	1305	AVP	C5'-O5'-PA-O1A
6	A	1305	AVP	PB-O3B-PG-O1G

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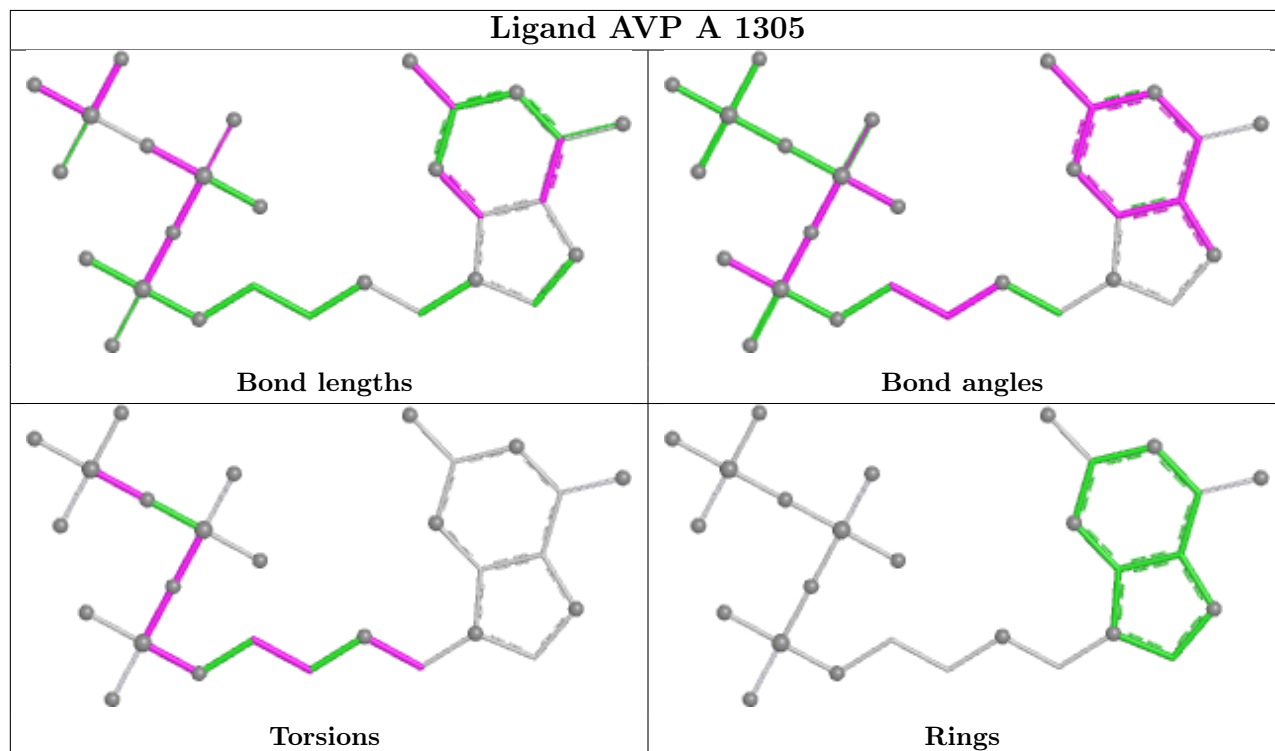
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Mol	Chain	Res	Type	Atoms
6	A	1305	AVP	PB-O3A-PA-O2A
6	A	1305	AVP	PB-O3A-PA-O1A
6	A	1305	AVP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1000:ALA	C	1001:ARG	N	1.16

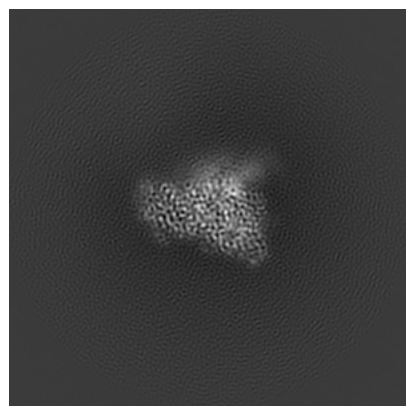
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42890. These allow visual inspection of the internal detail of the map and identification of artifacts.

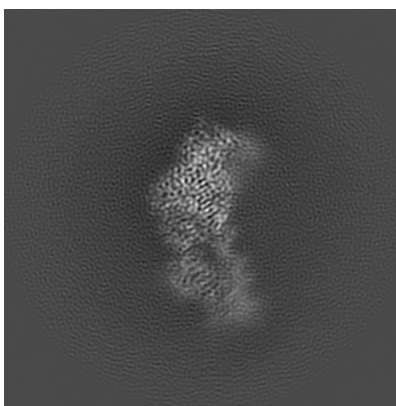
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

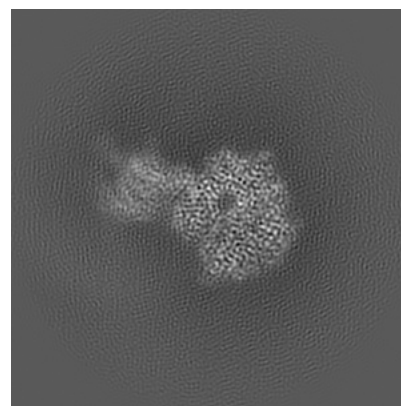
#### 6.1.1 Primary map



X

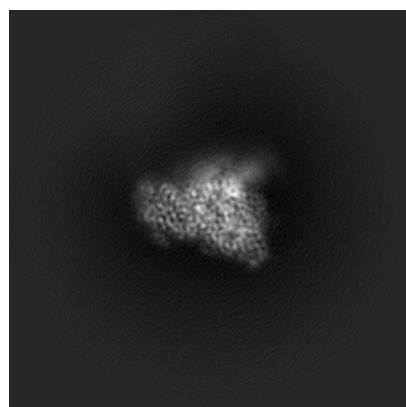


Y

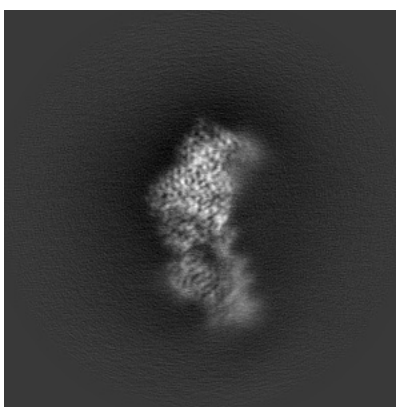


Z

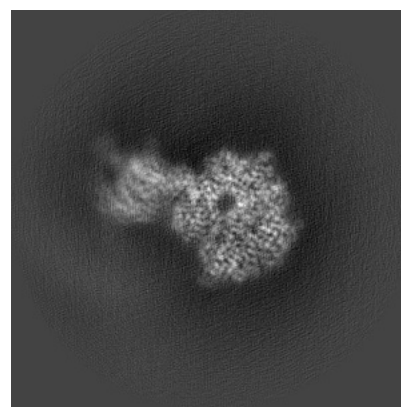
#### 6.1.2 Raw map



X



Y

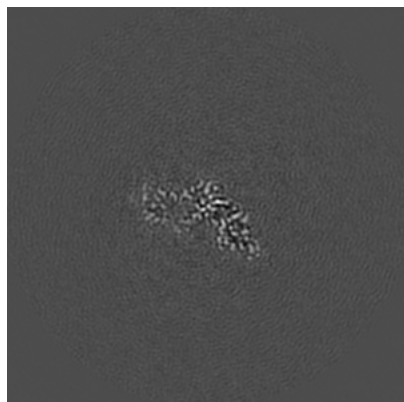


Z

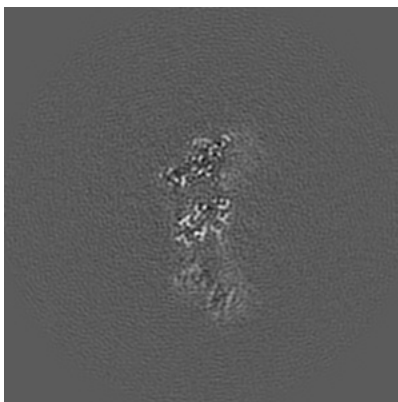
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

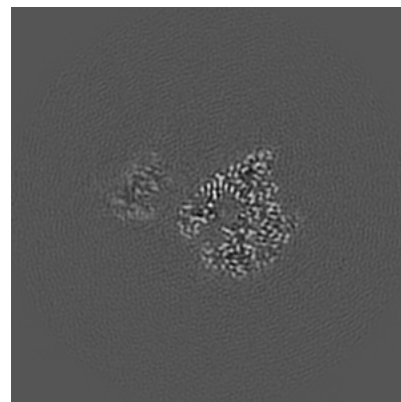
### 6.2.1 Primary map



X Index: 160

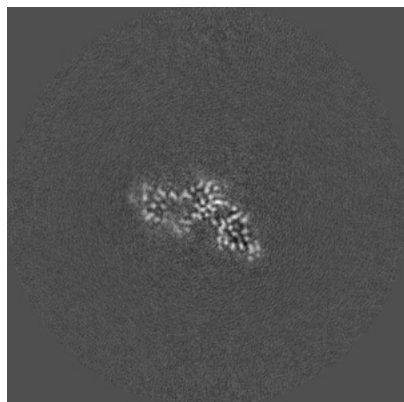


Y Index: 160

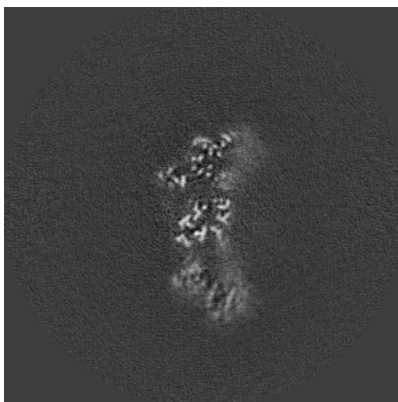


Z Index: 160

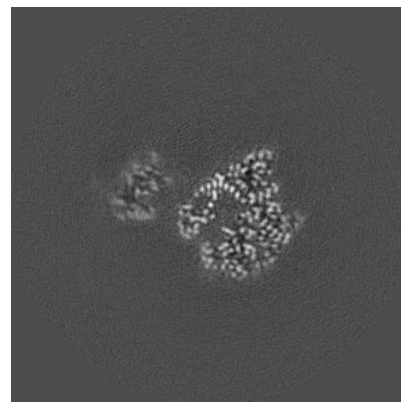
### 6.2.2 Raw map



X Index: 160



Y Index: 160

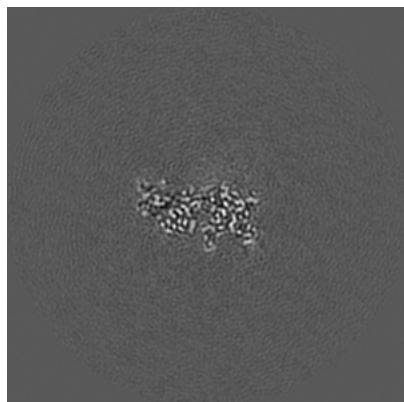


Z Index: 160

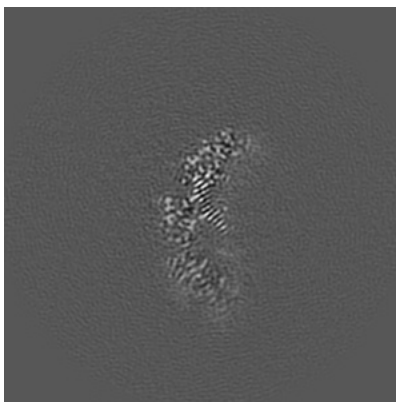
The images above show central slices of the map in three orthogonal directions.

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

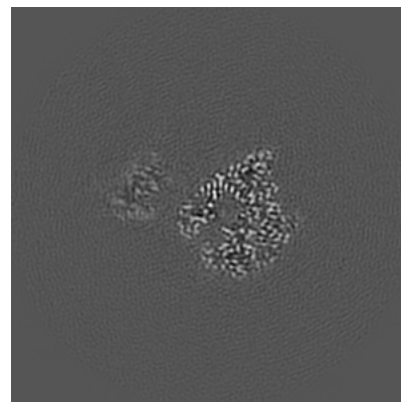
### 6.3.1 Primary map



X Index: 184

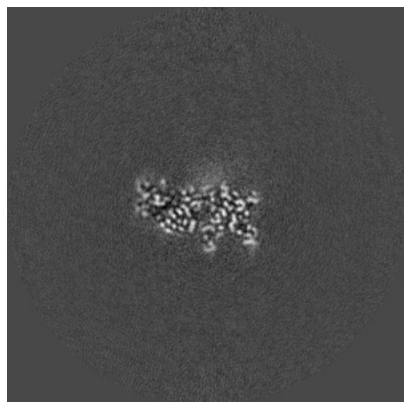


Y Index: 174

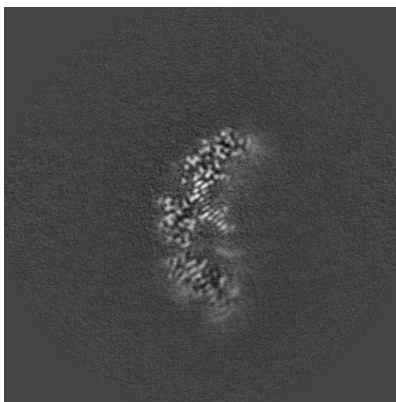


Z Index: 160

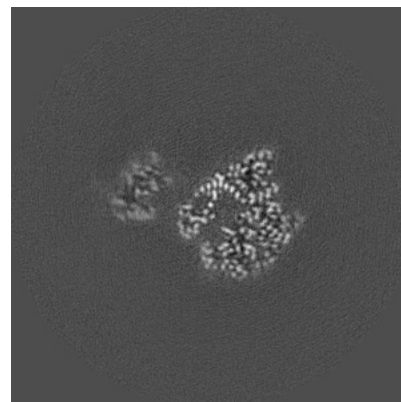
### 6.3.2 Raw map



X Index: 184



Y Index: 174

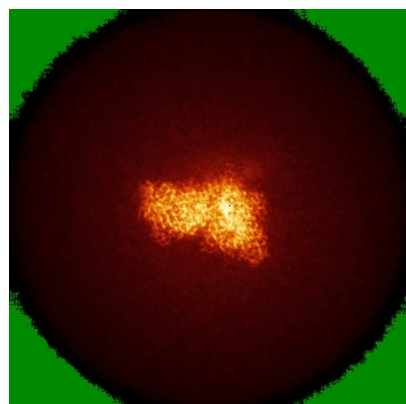


Z Index: 160

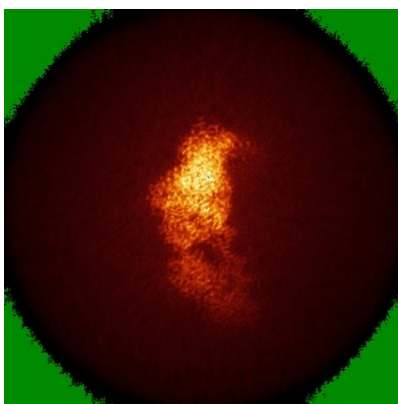
The images above show the largest variance slices of the map in three orthogonal directions.

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

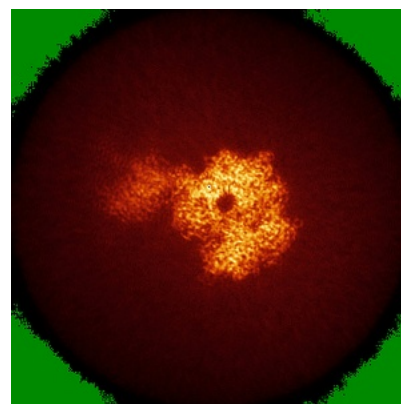
### 6.4.1 Primary map



X

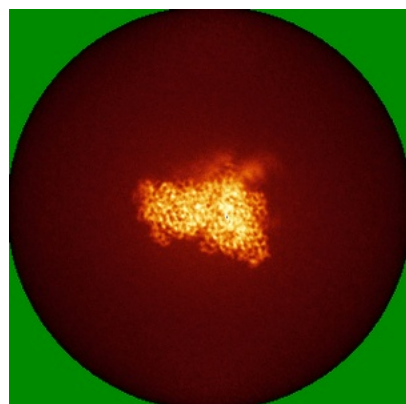


Y

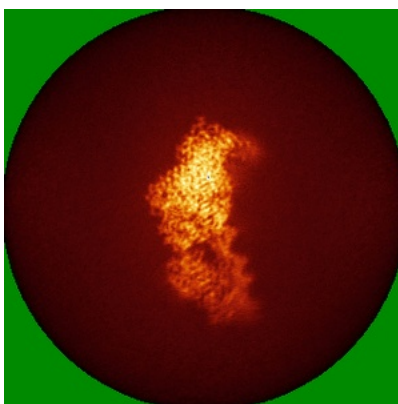


Z

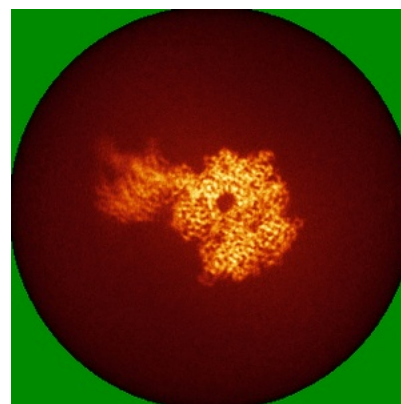
### 6.4.2 Raw map



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.

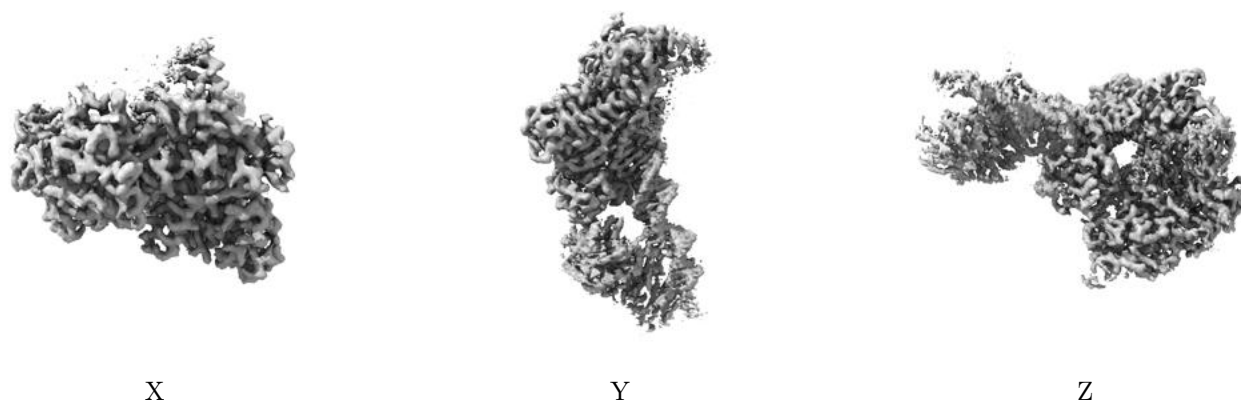
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

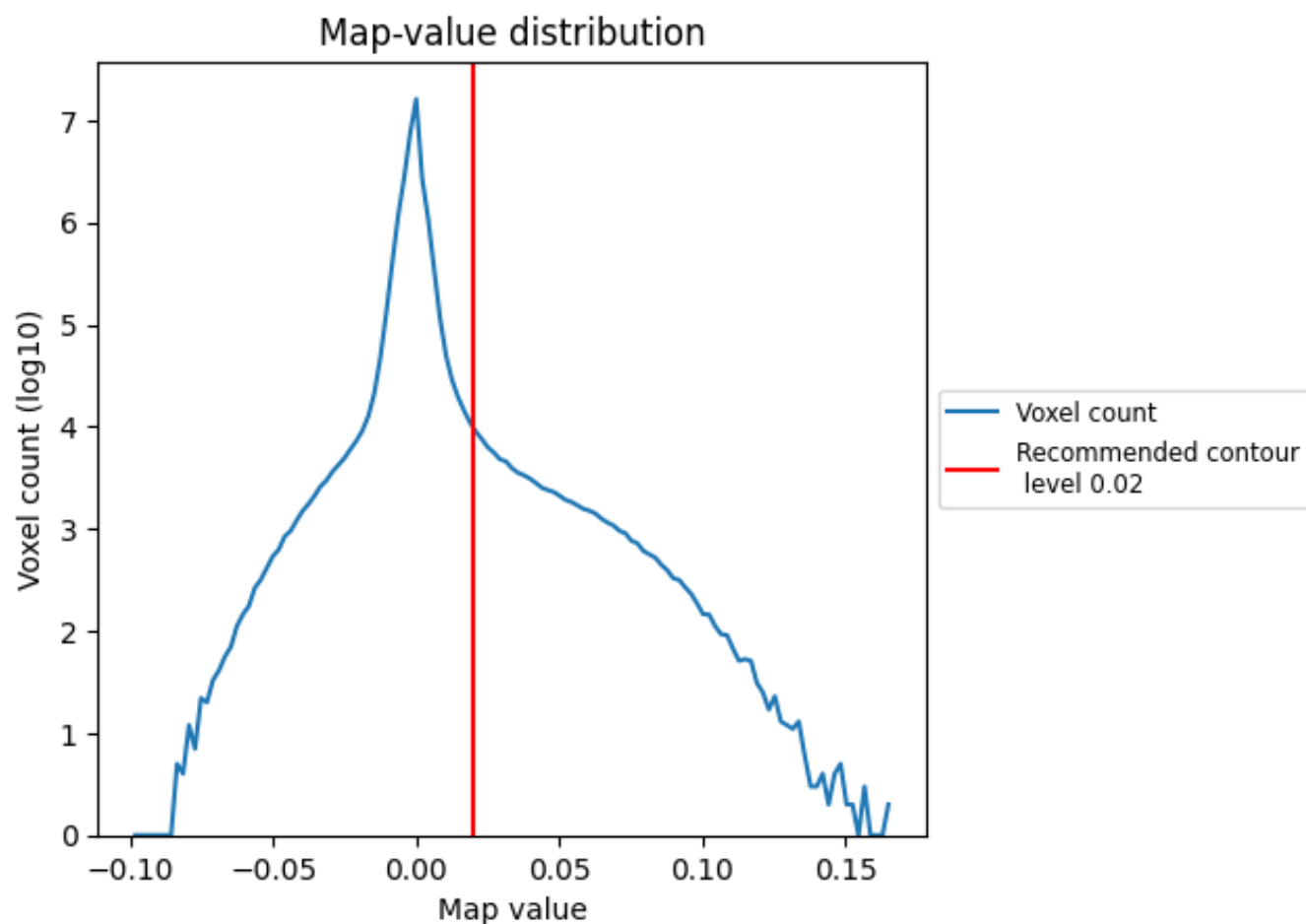
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

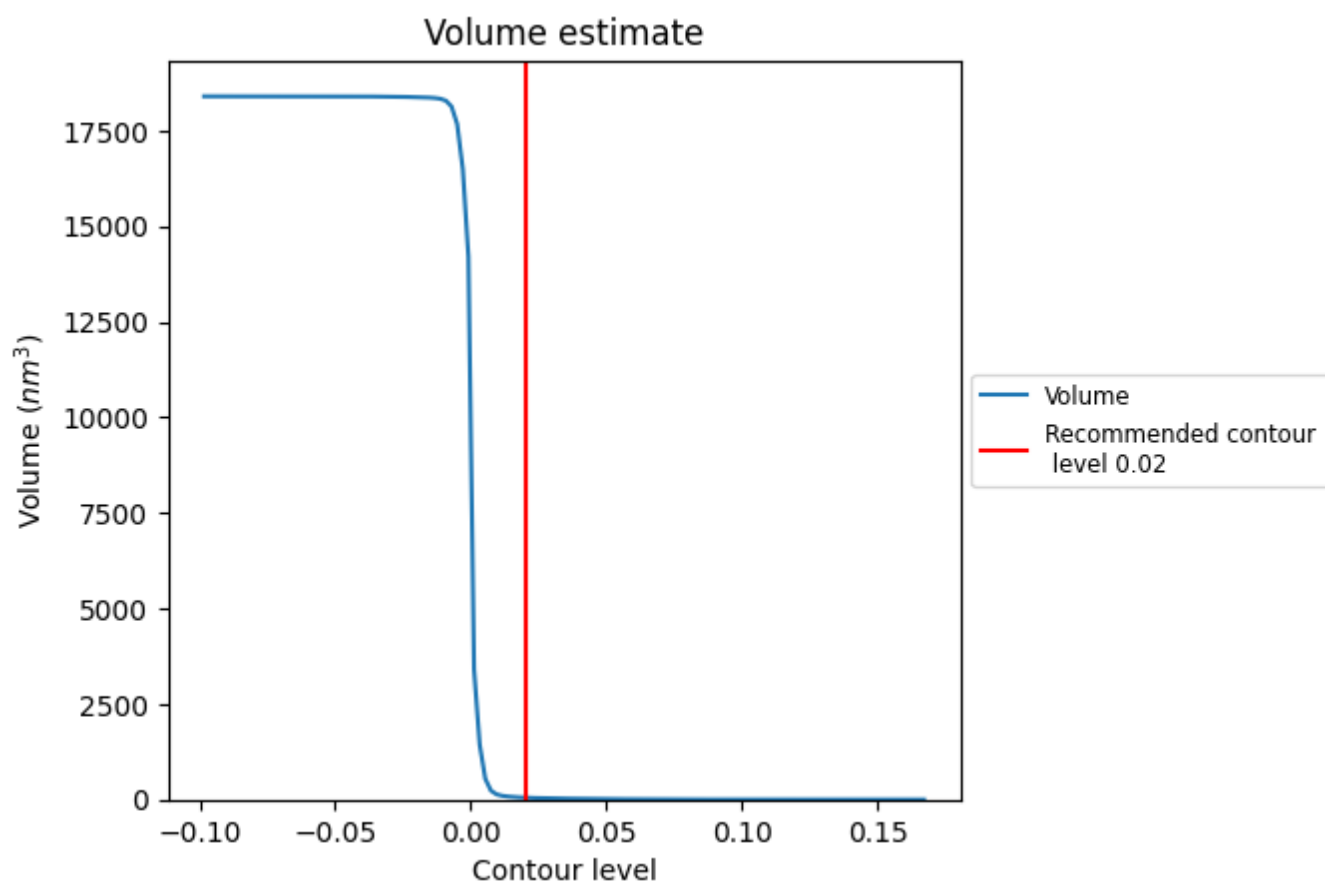
This section contains the results of statistical analysis of the map.

### 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.

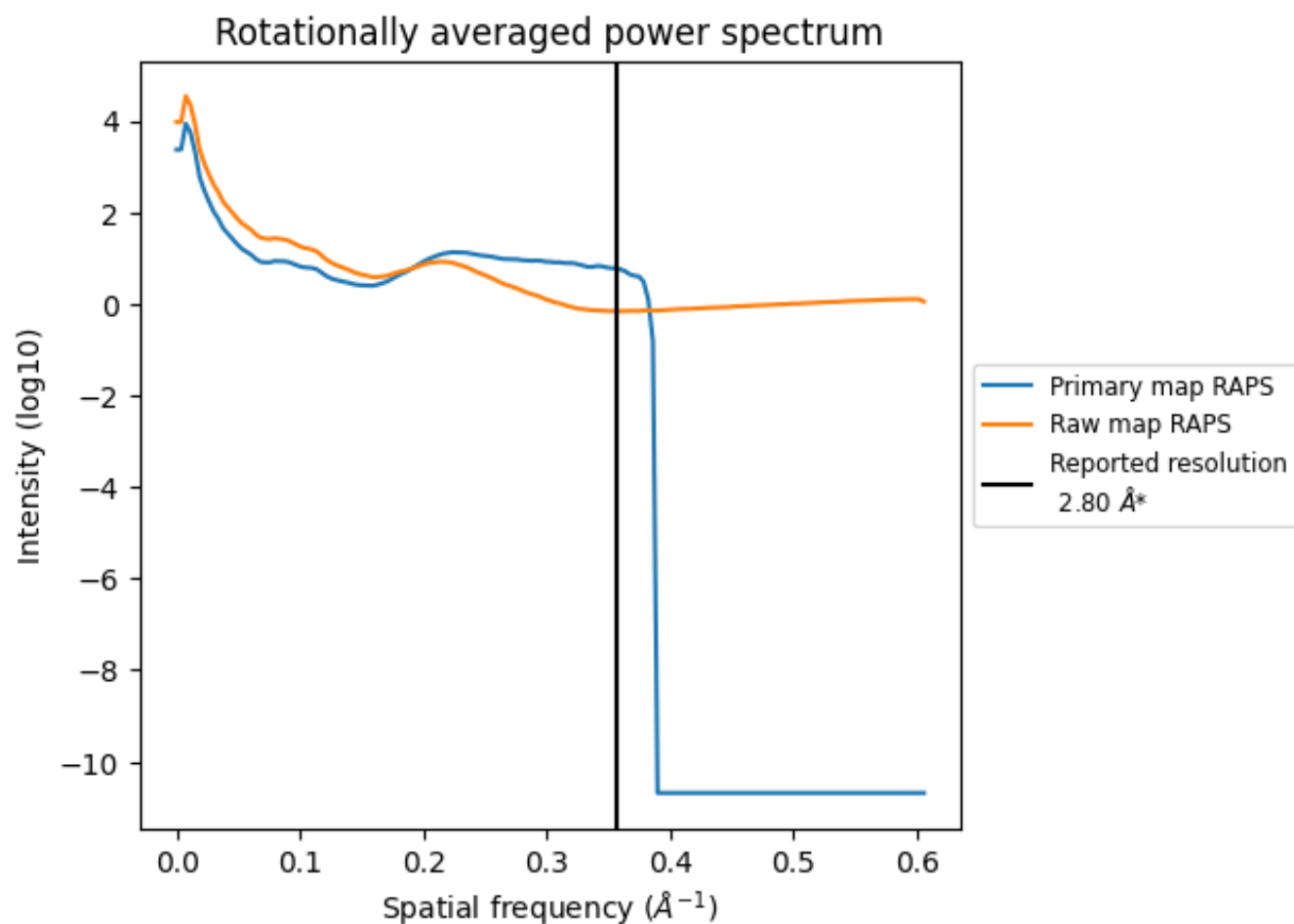
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 50  $\text{nm}^3$ ; this corresponds to an approximate mass of 45 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

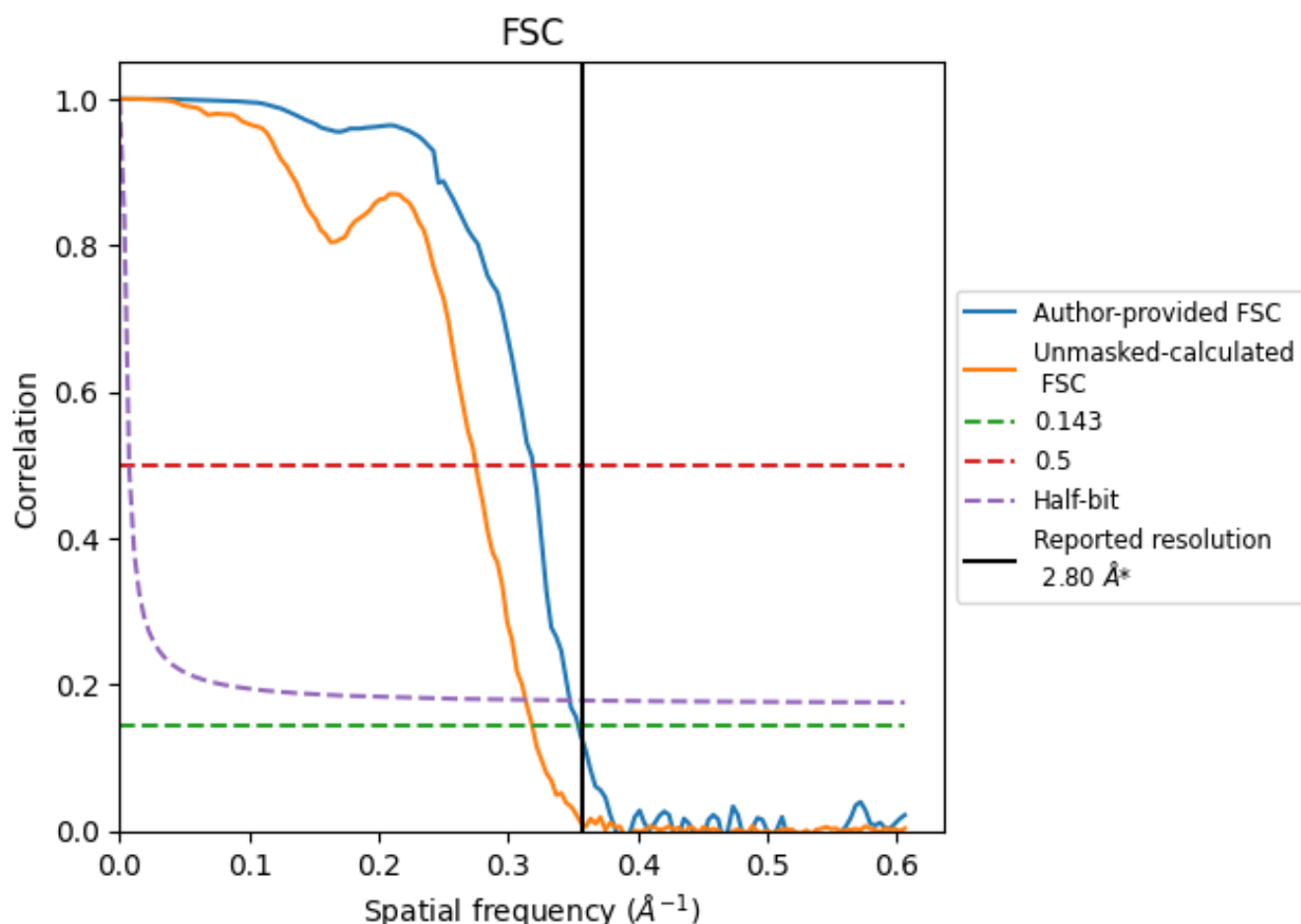


\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

## 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 0.357  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

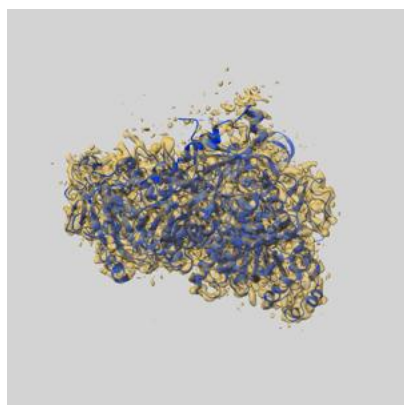
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.82	3.13	2.88
Unmasked-calculated*	3.14	3.64	3.19

\*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 3.14 differs from the reported value 2.8 by more than 10 %

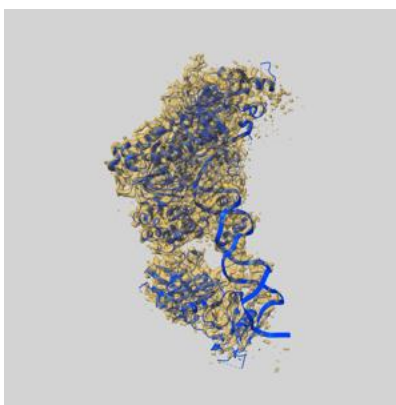
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42890 and PDB model 8V1T. Per-residue inclusion information can be found in section [3](#) on page [5](#).

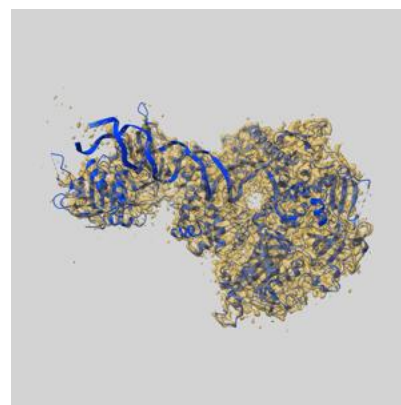
### 9.1 Map-model overlay [i](#)



X



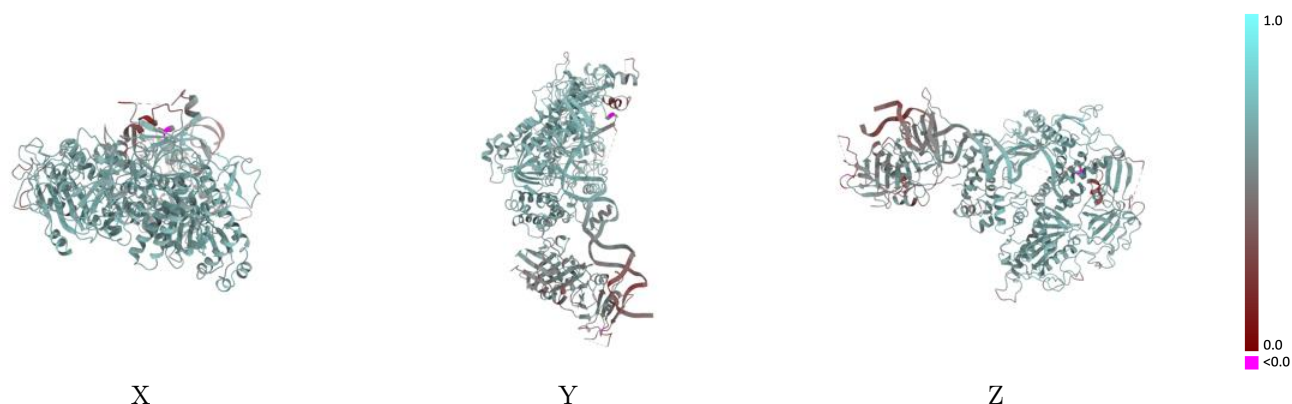
Y



Z

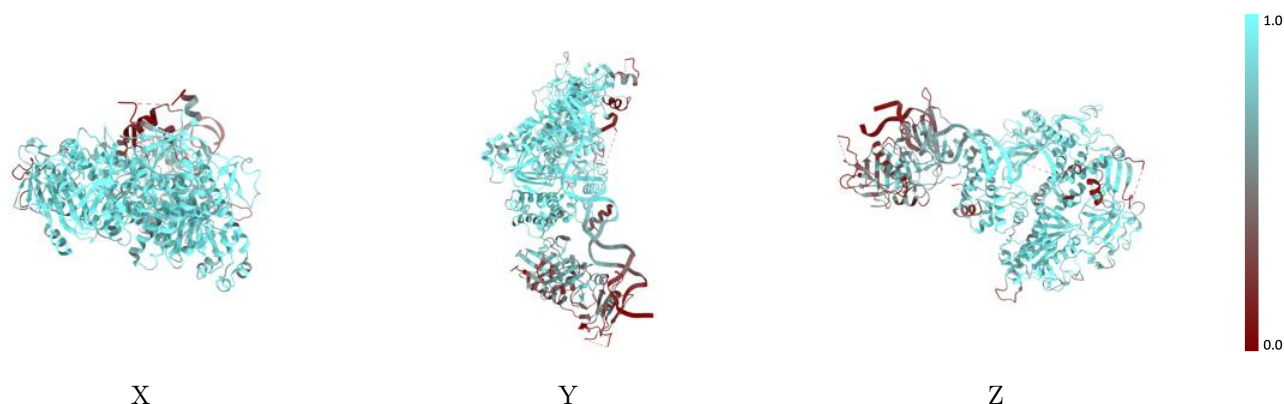
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



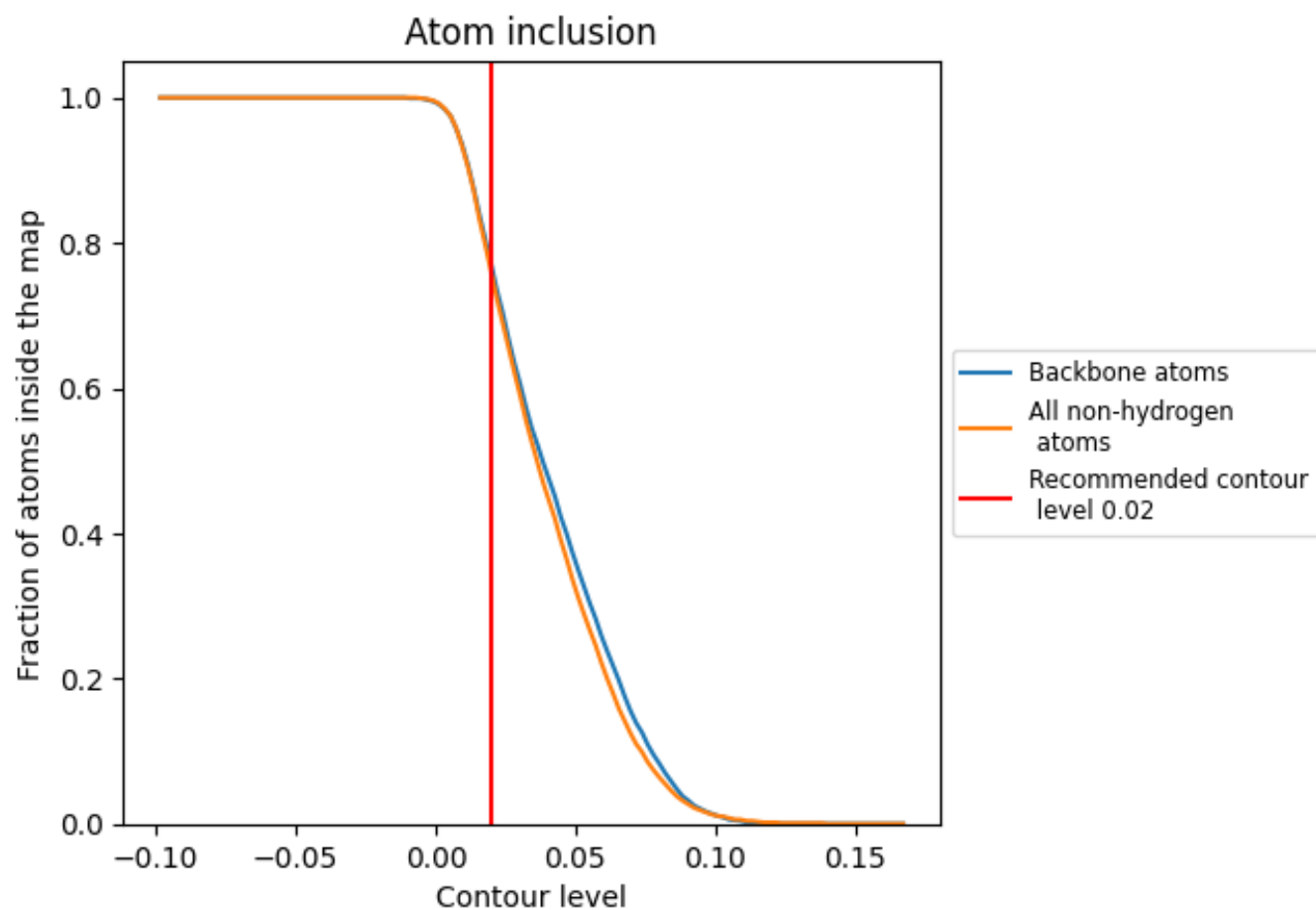
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 76% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7580	<div></div> 0.5790
A	<div></div> 0.8380	<div></div> 0.6080
B	<div></div> 0.5000	<div></div> 0.4960
P	<div></div> 0.5960	<div></div> 0.5050
T	<div></div> 0.6840	<div></div> 0.5350

