



Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 12:32 PM EDT

PDB ID : 9NSP / pdb_00009nsp
EMDB ID : EMD-49747
Title : MPXV replisome bound to ssDNA
Authors : Yu, Z.; Abraham, J.
Deposited on : 2025-03-17
Resolution : 4.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

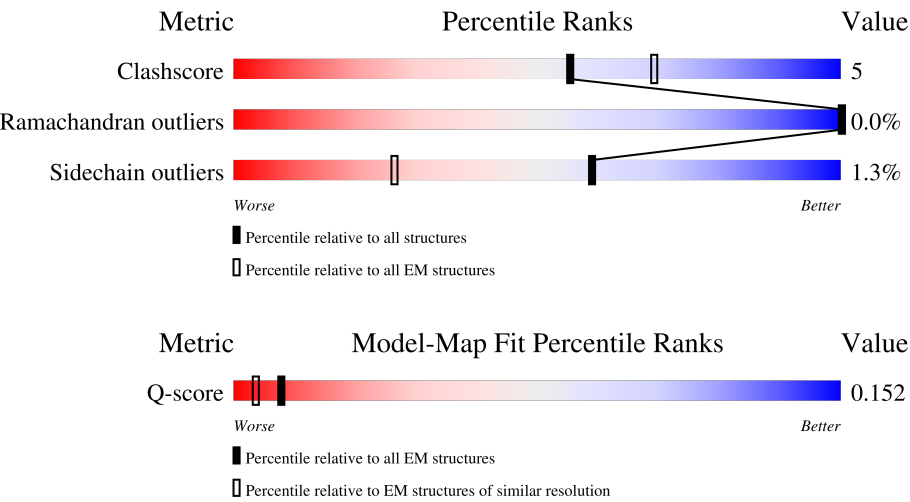
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 4.10 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	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	D	785	15% 74% 12% 14%
1	E	785	36% 57% 14% • 28%
1	H	785	13% 40% 5% 55%
1	I	785	12% 41% • 55%

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Mol	Chain	Length	Quality of chain
1	J	785	11%36%5%59%
1	K	785	13%39%5%55%
2	A	1006	84%13%
3	C	426	8%73%18%10%
4	B	218	11%79%20%
5	T	29	14%52%28%21%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 34677 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 Uncoating factor OPG117.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	674	Total	C	N	O	S	0	0
			5469	3479	932	1027	31		
1	E	566	Total	C	N	O	S	0	0
			4599	2923	779	869	28		
1	I	351	Total	C	N	O	S	0	0
			2857	1831	482	529	15		
1	H	351	Total	C	N	O	S	0	0
			2855	1832	482	526	15		
1	J	324	Total	C	N	O	S	0	0
			2635	1684	452	485	14		
1	K	351	Total	C	N	O	S	0	0
			2856	1831	483	528	14		

- Molecule 2 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	981	Total	C	N	O	S	0	0
			8031	5134	1340	1504	53		

- Molecule 3 is a protein called DNA polymerase processivity factor component OPG148.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	385	Total	C	N	O	S	0	0
			3141	2028	513	590	10		

- Molecule 4 is a protein called Uracil-DNA glycosylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	218	Total	C	N	O	S	0	0
			1773	1149	292	326	6		

- Molecule 5 is a DNA chain called DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
5	T	23	Total	C	N	O	P	0	0
			460	230	46	161	23		

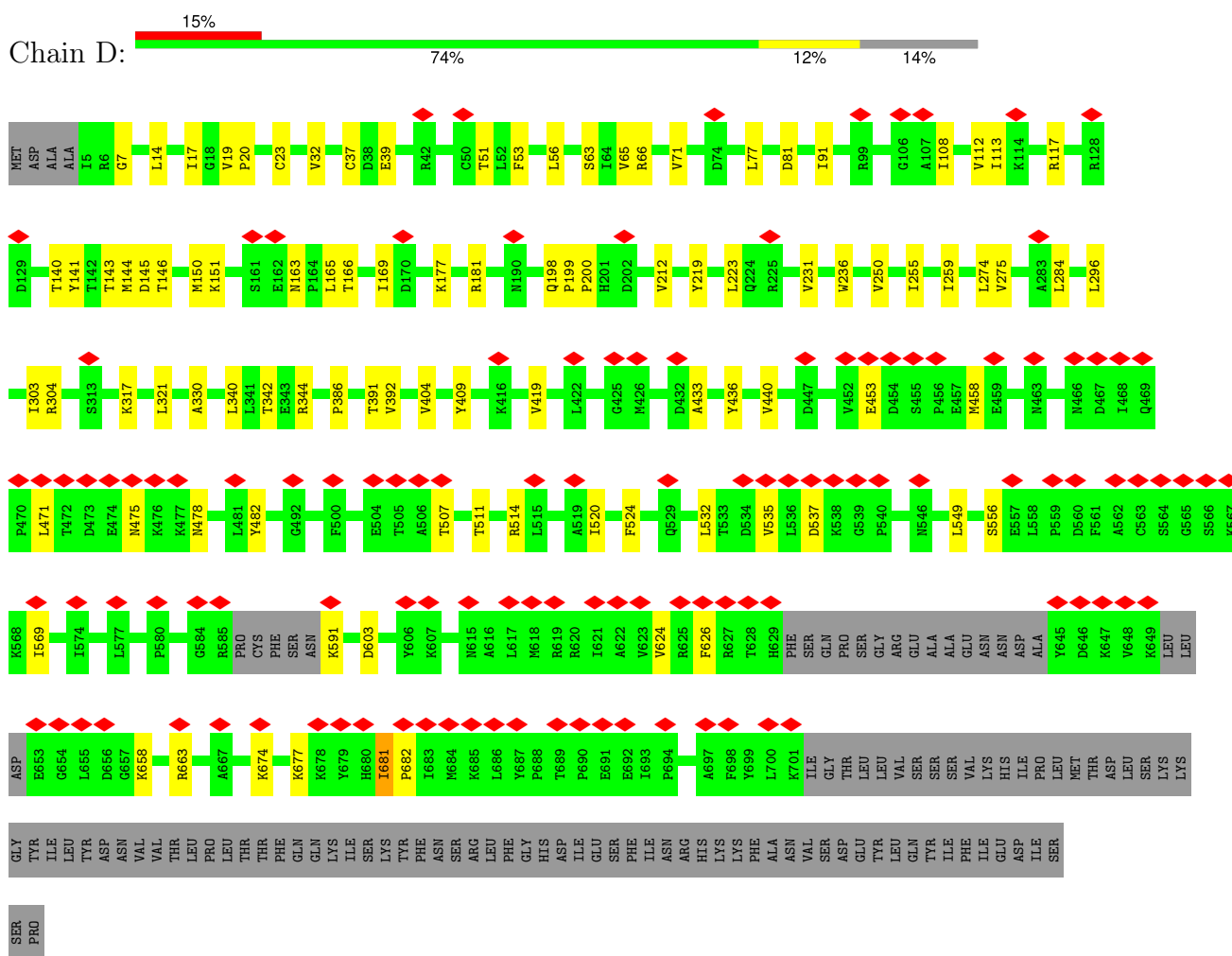
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	D	1	Total	Zn	0
			1	1	

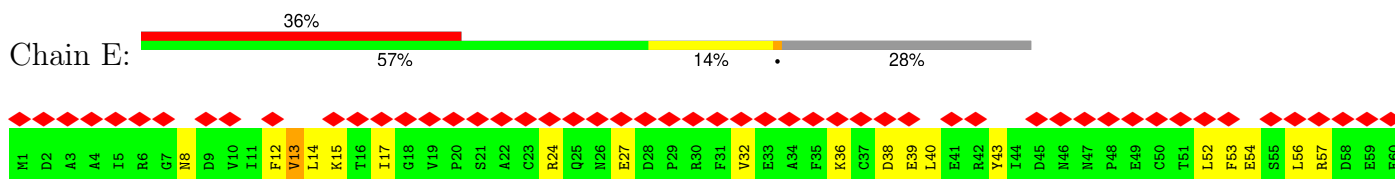
3 Residue-property plots

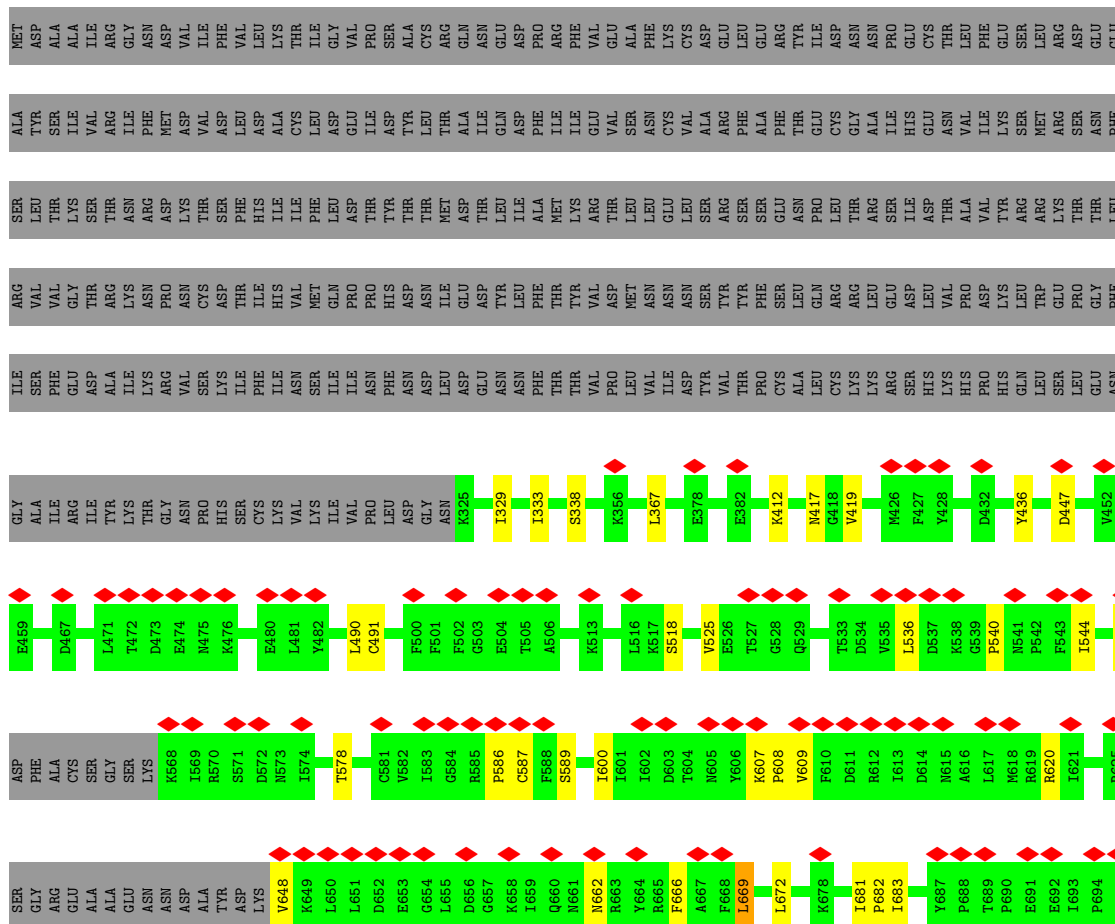
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Uncoating factor OPG117



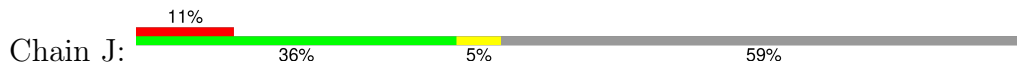
• Molecule 1: Uncoating factor OPG117





ARG	HIS	LYS	LYS	PHE	ALA	ASN	VAL	ASP	ASP	GLU	THR	LEU	GLN	THR	ILE	ILE	ILE	ILE	GLU	ASP	SER	SER	PRO
ILE	GLY	THR	LEU	LEU	VAL	SER	SER	SER	VAL	HIS	ILE	PRO	LEU	MET	THR	THR	ASP	LEU	SER	SER	LYS	GLY	THR
ASN	VAL	THR	THR	GLN	PHE	ASN	SER	ARG	LEU	PHE	GLY	HIS	ASP	ILE	LYS	LYS	THR	LEU	PRO	THR	LEU	THR	

- Molecule 1: Uncoating factor OPG117



Met	ASP	ALA	ALA	ALA	ARG	GLY	ASN	ASP	VAL	ILE	PHE	VAL	LEU	LYS	THR	ILE	GLY	VAL	PRO	PRO	ALA	SER	ALA	CYS	ARG	GLN	ASN	GLU	ASP	PRO	ARG	PHE	VAL	GLU	ALA	PHE	LYS	CYS	ASP	GLU	LEU	GLU	ARG	TYR	ILE	ASP	ASN	ASN	PRO	GLU	CYS	THR	PHE	GLU	SER	GLU	LEU	ARG	ASP	GLU	GLU
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ALA TYR SER ILE VAL ARG ILE PHE MET ASP VAL ASP ALA LEU ASP ALA CYS ASP GLY ILE ASP TYR THR ALA ILE GLN ASP PHE ILE ILE ILE GLU VAL ASN CYS VAL ALA ARG PHE ALA PHE THR GLU CYS GLY ILE HIS GLU ASN VAL ILE LYS SER MET ARG SER ASN PHE

SER	LEU	THR	LYS	SER	THR	ASN	ARG	ASP	LYS	THR	SER	PHE	HIS	ILE	ILE	PHE	LEU	ASP	THR	TYR	THR	THR	THR	MET	ASP	THR	LEU	ILE	ALA	ALA	MET	LYS	ARG	THR	LEU	LEU	GLU	LEU	LEU	SER	SER	ARG	ARG	SER	SER	GLU	ASN	PRO	THR	LEU	THR	THR	ARG	SER	ILE	ASP	THR	ALA	ALA	VAL	TYR	ARG	ARG	LYS	THR	THR	THR	LEU
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ARG	VAL	VAL	GLY	THR	ARG	LYS	ASN	PRO	ASN	CYS	ASP	THR	ILE	HIS	VAL	MET	GLN	PRO	PRO	ASP	HIS	ASN	ILE	GLU	ASP	Tyr	PHE	THR	THR	TYR	VAL	ASP	MET	MET	ASN	ASN	ASN	SER	TYR	TYR	PHE	SER	SER	LEU	GLN	ARG	ARG	LEU	LEU	GLU	ASP	GLY	PHE
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ILE	SER	PHE	GLU	ASP	ALA	ILE	LYS	ARG	VAL	SER	SER	LYS	ILE	PHE	ILE	ILE	SER	ASN	ASN	PHE	ASN	ASP	LEU	ASP	GLU	ASN	ASN	ASN	PHE	PHE	THR	THR	VAL	PRO	LEU	VAL	ILE	ASP	TYR	VAL	VAL	THR	THR	PRO	CYS	ALA	LEU	CYS	LYS	LYS	ARG	SER	HIS	LYS	HIS	HIS	HIS	GLN	LEU	SER	SER	LEU	GLU	CYS
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Residue	Position	Sequence	Conservation	Structure
GLY	1	GLY	0.00	
ALA	2	ALA	0.00	
ILE	3	ILE	0.00	
ARG	4	ARG	0.00	
ILE	5	ILE	0.00	
TYR	6	TYR	0.00	
LYS	7	LYS	0.00	
THR	8	THR	0.00	
GLY	9	GLY	0.00	
ASN	10	ASN	0.00	
PRO	11	PRO	0.00	
HIS	12	HIS	0.00	
SER	13	SER	0.00	
CYS	14	CYS	0.00	
VAL	15	VAL	0.00	
LYS	16	LYS	0.00	
ILE	17	ILE	0.00	
VAL	18	VAL	0.00	
PRO	19	PRO	0.00	
LEU	20	LEU	0.00	
ASP	21	ASP	0.00	
G323	22	G323	0.00	
N328	23	N328	0.00	
I333	24	I333	0.00	
L334	25	L334	0.00	
D335	26	D335	0.00	
I336	27	I336	0.00	
I351	28	I351	0.00	
K356	29	K356	0.00	
E361	30	E361	0.00	
I371	31	I371	0.00	
Q374	32	Q374	0.00	
K377	33	K377	0.00	
E378	34	E378	0.00	
Y379	35	Y379	0.00	
K412	36	K412	0.00	
D424	37	D424	0.00	
G425	38	G425	0.00	
M426	39	M426	0.00	
F427	40	F427	0.00	
Y428	41	Y428	0.00	
S429	42	S429	0.00	
G430	43	G430	0.00	
D431	44	D431	0.00	
D432	45	D432	0.00	
Y436	46	Y436	0.00	
F446	47	F446	0.00	

D447	D448	T449	K450	F451	V452	E453	D454	L471	T472	D473	E474	M475	K476	K477	D478	D479	Y482	L490	L498	T499	F500	F501	F502	G503	E504	T505	A506	A507	G508	S509	S510	A519	I520	G528	Q529	T530	G530	I531	L532	L533	D534	VAL	LEU	ASP	LYS	GLY	PRO	ASN	P542	F543	I544	M547
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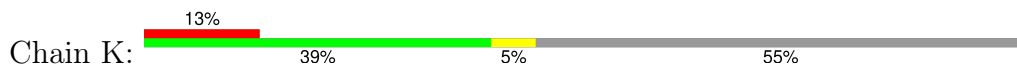
K550		S556	E557	L568	P569	D660	F661	ALA	CYS	CYS	GLY	SER	SER	SER	LYS	K568	I569	R570	S571	E579	L583	G584	R585	P586	CYS	PHE	SER	SER	ASN	K591	I592	N593	D603	Y606	K607	F610	D611	R612	T613	D614	M615	M618	R619	R620	T621	A622	V623	V624	R625	F626	G627	T628	H629	PHE	SER	GLN
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PRO	SER	GLY	ARG	GLU	ALA	ALA	GLU	ASN	ASP	ALA	TYP	ASP	LYS	VAL	LYS	LEU	LEU	ASP	GLU	G654	G657	G658	G659	G664	R665	F666	A667	F668	L672	V673	K674	K677	G678	P681	P682	V687	PRO	THR	PRO	GLU	ILE	ILE	PRO	ASP	PHE	ALA	PHE	TYR	LEU	LYS	I F
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GLY THR LEU LEU VAL SER SER VAL HIS PRO TYR LEU SER LYS LYS GLY TYR ILE LEU TYR ASP ASN VAL VAL THR LEU PRO PRO LEU THR THR PHE GLN GLN LYS ILE SER SER TYR PHE ASN SER ARG LEU PHE GLY HIS ASP ILE GLU SER PHE ILE ASN ARG

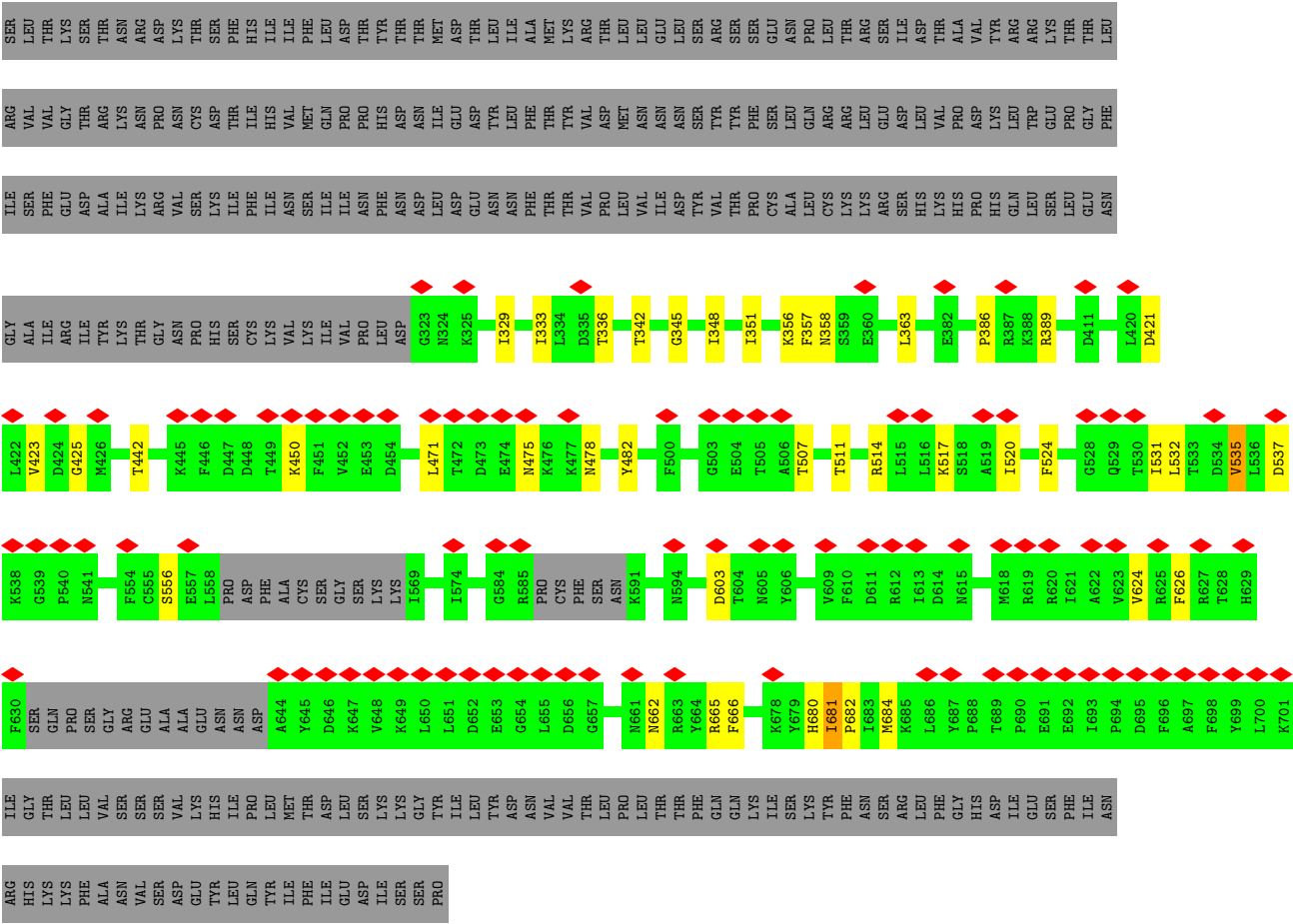
HIS	LYS	LYS	PHE	ALA	ASN	VAL	SER	ASP	GLU	TYR	LEU	GLN	TYR	ILE	PHE	ILE	GLU	ASP	ILE	SER	SER	PRO
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- Molecule 1: Uncoating factor OPG117

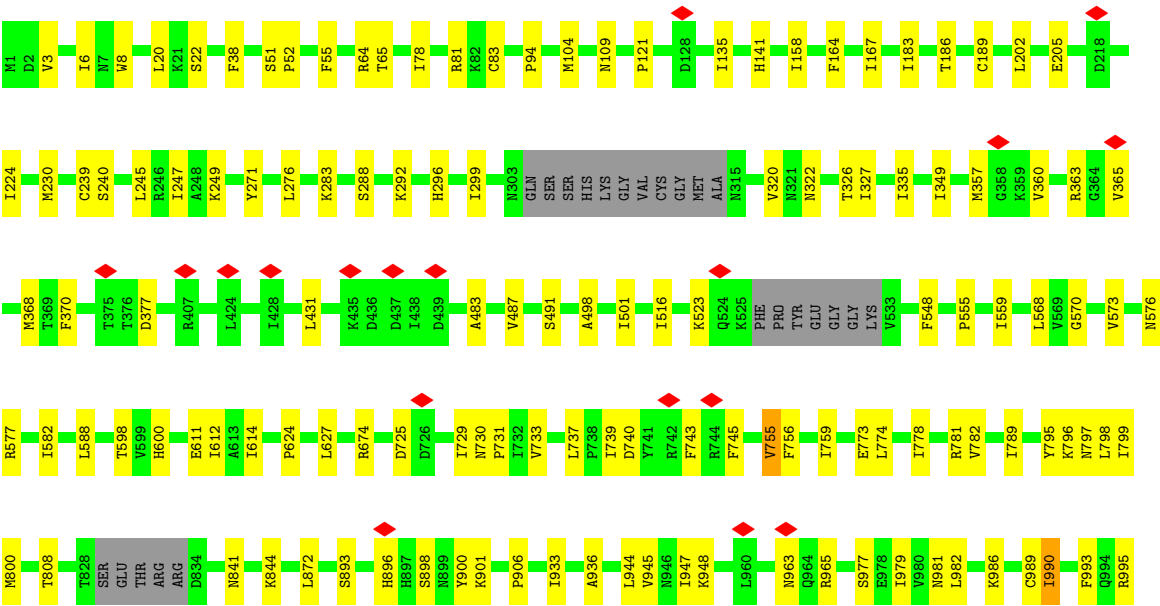
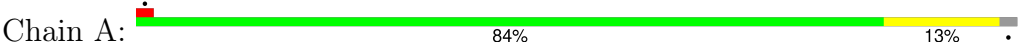


MET	ASP	ALA	ALA	ALA	ILE	ARG	GLY	ASN	ASP	VAL	ILE	PHE	VAL	LEU	LYS	THR	ILE	GLY	VAL	PRO	SER	ALA	CYS	ARG	GLN	ASN	GLU	GLU	ASP	PRO	ARG	PHE	VAL	GLU	ALA	PHE	LYS	CYS	ASP	GLU	LEU	GLU	TYR	ILE	ASN	ASN	PRO	GLU	CYS	THR	PHE	GLU	SER	LEU	ARG	ASP	GLU
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ALA TYR SER ILE VAL ARG ILE PHE MET ASP VAL ASP ALA LEU LEU GLY ILE ASP TYR THR ALA ILE GLN ASP PHE ILE ILE ILE GLY VAL ASN CYS VAL ALA PHE THR GLU CYS GLY HIS GLU ASN ARG PHE PHE THR LEU LYS SER MET ARG SER ASN PHE



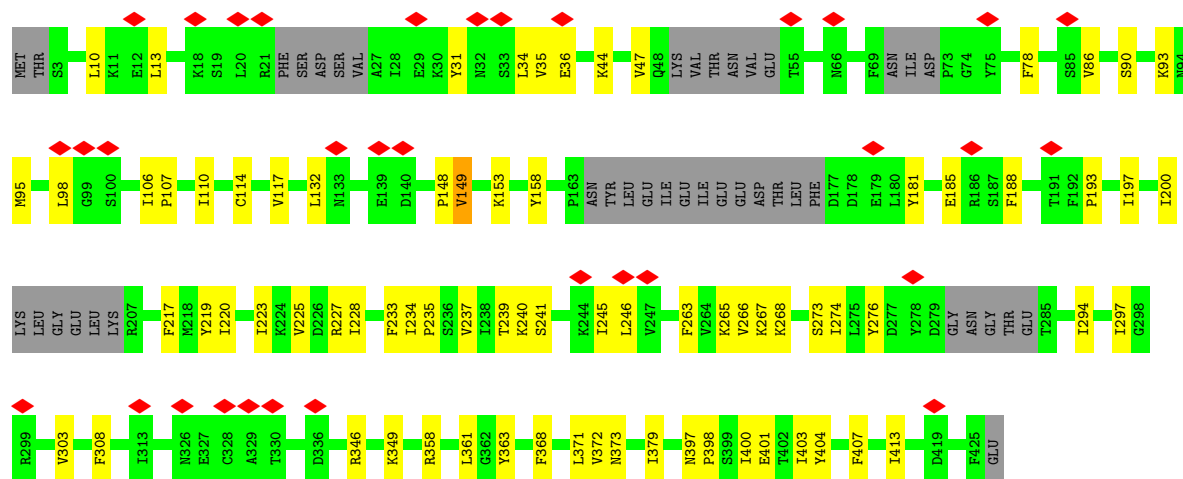
● Molecule 2: DNA polymerase





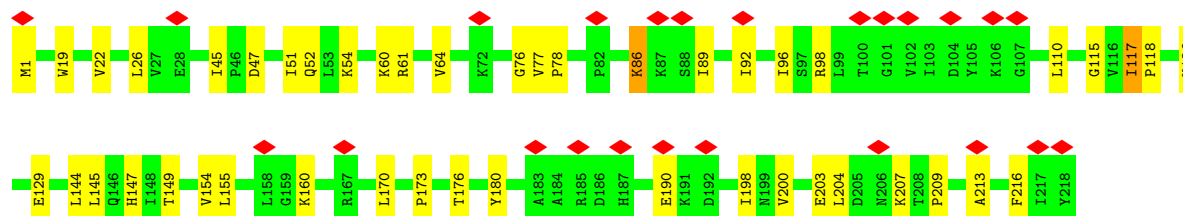
• Molecule 3: DNA polymerase processivity factor component OPG148

Chain C:



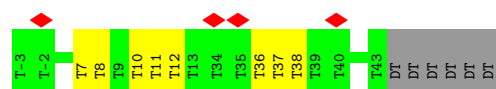
• Molecule 4: Uracil-DNA glycosylase

Chain B:



• Molecule 5: DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3')

Chain T:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56874	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.469	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.04	Depositor
Map size ($\text{\AA}$)	378.88, 378.88, 378.88	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.74, 0.74, 0.74	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	D	0.10	0/5579	0.25	0/7542
1	E	0.10	0/4684	0.25	0/6324
1	H	0.08	0/2914	0.23	0/3934
1	I	0.08	0/2915	0.22	0/3935
1	J	0.07	0/2684	0.22	0/3614
1	K	0.07	0/2912	0.21	0/3927
2	A	0.08	0/8199	0.24	1/11070 (0.0%)
3	C	0.09	0/3199	0.24	0/4306
4	B	0.09	0/1823	0.26	0/2479
5	T	0.28	0/503	0.83	0/770
All	All	0.09	0/35412	0.26	1/47901 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	948	LYS	N-CA-C	-5.18	108.71	114.62

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	D	5469	0	5471	58	0
1	E	4599	0	4592	64	0
1	H	2855	0	2892	20	0
1	I	2857	0	2889	15	0
1	J	2635	0	2674	21	0
1	K	2856	0	2892	22	0
2	A	8031	0	7999	78	0
3	C	3141	0	3151	50	0
4	B	1773	0	1764	26	0
5	T	460	0	279	15	0
6	D	1	0	0	0	0
All	All	34677	0	34603	348	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 (348) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1000:ARG:NH1	5:T:11:DT:C7	1.69	1.56
2:A:1000:ARG:NH1	5:T:11:DT:H72	1.31	1.30
2:A:1000:ARG:NH1	5:T:11:DT:H73	1.45	1.07
1:D:151:LYS:NZ	5:T:12:DT:OP2	2.00	0.94
1:H:681:ILE:HG13	1:H:682:PRO:HD3	1.48	0.94
1:I:681:ILE:HG23	1:I:682:PRO:HD3	1.63	0.81
3:C:13:LEU:HD13	3:C:34:LEU:HD13	1.64	0.80
1:E:107:ALA:HB1	1:E:112:VAL:HG21	1.67	0.77
1:E:164:PRO:HA	1:E:167:ARG:HB2	1.67	0.77
2:A:38:PHE:HA	2:A:109:ASN:HD21	1.51	0.76
1:E:36:LYS:H	1:E:39:GLU:HB2	1.52	0.74
2:A:598:THR:HB	2:A:612:ILE:HD11	1.70	0.73
1:E:80:ILE:HG21	3:C:241:SER:HB3	1.69	0.72
2:A:1000:ARG:HH12	5:T:11:DT:C7	2.01	0.71
1:E:36:LYS:HD3	1:E:38:ASP:H	1.56	0.70
1:J:475:ASN:HD21	1:J:478:ASN:HD22	1.40	0.70
1:I:556:SER:HA	1:I:603:ASP:HB3	1.74	0.70
1:E:475:ASN:HD21	1:E:478:ASN:HD22	1.41	0.68
1:D:177:LYS:NZ	5:T:10:DT:OP1	2.27	0.68
1:D:475:ASN:HD21	1:D:478:ASN:HD22	1.42	0.67
3:C:217:PHE:HB3	3:C:263:PHE:HE1	1.60	0.67
1:H:490:LEU:HD22	1:H:672:LEU:HB3	1.75	0.67
1:E:52:LEU:HD22	1:E:182:VAL:HB	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:475:ASN:HD21	1:K:478:ASN:HD22	1.42	0.67
1:E:89:PHE:HB2	1:E:165:LEU:HD13	1.76	0.66
4:B:51:ILE:HD11	4:B:76:GLY:HA3	1.76	0.66
1:E:183:VAL:HB	1:E:204:ILE:HG23	1.78	0.66
4:B:203:GLU:HB3	4:B:209:PRO:HG3	1.78	0.66
1:E:329:ILE:HG21	1:E:383:LEU:HD21	1.78	0.65
1:E:52:LEU:HD13	1:E:182:VAL:HG11	1.79	0.65
2:A:81:ARG:HH21	2:A:568:LEU:HB3	1.62	0.64
3:C:267:LYS:HG3	3:C:276:TYR:HB2	1.80	0.64
1:E:54:GLU:HG2	1:E:208:LEU:HD22	1.79	0.64
1:D:391:THR:HG23	1:E:386:PRO:HG2	1.79	0.64
1:D:681:ILE:HG23	1:D:682:PRO:HD3	1.80	0.64
1:D:20:PRO:HG2	1:D:23:CYS:HB2	1.80	0.64
1:E:681:ILE:HG23	1:E:682:PRO:HD3	1.80	0.63
2:A:183:ILE:HG12	2:A:271:TYR:HE2	1.63	0.63
1:H:629:HIS:HB3	1:H:648:VAL:HG22	1.81	0.63
2:A:104:MET:HE3	2:A:516:ILE:HG12	1.80	0.62
1:I:498:LEU:HD22	1:I:600:ILE:HB	1.82	0.62
2:A:3:VAL:HB	2:A:22:SER:HB3	1.81	0.61
1:E:197:MET:HE2	1:E:201:HIS:HB2	1.81	0.61
1:E:123:THR:HB	1:E:195:HIS:HB3	1.81	0.61
3:C:397:ASN:HD22	3:C:400:ILE:HG12	1.65	0.61
1:K:681:ILE:HG23	1:K:682:PRO:HD3	1.82	0.61
2:A:733:VAL:HG12	2:A:781:ARG:HD3	1.82	0.60
2:A:135:ILE:HD13	2:A:141:HIS:HB2	1.84	0.60
1:J:544:ILE:HG21	1:J:584:GLY:HA3	1.83	0.60
4:B:26:LEU:HD12	4:B:144:LEU:HD11	1.85	0.59
3:C:219:TYR:HB3	3:C:240:LYS:HB2	1.85	0.59
1:D:143:THR:HG22	1:D:145:ASP:H	1.67	0.59
3:C:90:SER:HB3	3:C:93:LYS:HD2	1.83	0.59
2:A:523:LYS:HB3	2:A:674:ARG:HH12	1.68	0.59
1:E:90:ILE:HD11	1:E:122:LEU:HD22	1.83	0.59
1:D:177:LYS:NZ	5:T:10:DT:P	2.75	0.58
2:A:121:PRO:HB2	2:A:483:ALA:HB1	1.84	0.58
2:A:78:ILE:HD13	2:A:570:GLY:HA3	1.84	0.58
3:C:13:LEU:HB2	3:C:34:LEU:HD22	1.84	0.58
1:H:540:PRO:HB2	1:H:587:CYS:HA	1.84	0.58
4:B:51:ILE:HG13	4:B:52:GLN:HE21	1.69	0.58
2:A:582:ILE:HG22	3:C:379:ILE:HG21	1.86	0.57
4:B:45:ILE:HG22	4:B:47:ASP:H	1.68	0.57
2:A:900:TYR:HA	2:A:906:PRO:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:6:ILE:HD11	2:A:158:ILE:HD11	1.86	0.57
1:H:578:THR:HG21	1:H:620:ARG:HD3	1.86	0.57
1:H:607:LYS:HD3	1:H:608:PRO:HD2	1.86	0.57
1:K:507:THR:HG21	1:K:626:PHE:HB3	1.87	0.56
1:J:681:ILE:HG23	1:J:682:PRO:HD3	1.88	0.56
4:B:78:PRO:HB2	4:B:118:PRO:HB2	1.87	0.56
4:B:126:LYS:HB3	4:B:129:GLU:HB2	1.88	0.56
1:J:655:LEU:HA	1:J:658:LYS:HE2	1.87	0.56
2:A:756:PHE:HE2	2:A:800:MET:HE1	1.69	0.56
1:K:556:SER:HA	1:K:603:ASP:HB3	1.87	0.56
1:D:520:ILE:HD11	1:D:524:PHE:HB2	1.86	0.56
1:D:440:VAL:HG22	1:D:549:LEU:HD23	1.86	0.56
1:E:96:CYS:HB3	1:E:157:LEU:HD21	1.88	0.56
2:A:944:LEU:HB3	2:A:947:ILE:HD11	1.87	0.56
1:E:520:ILE:HD11	1:E:524:PHE:HB2	1.87	0.56
1:K:520:ILE:HD11	1:K:524:PHE:HB2	1.88	0.56
1:J:585:ARG:HH11	1:J:586:PRO:HD2	1.71	0.56
2:A:576:ASN:HD22	3:C:372:VAL:HG11	1.71	0.56
1:D:556:SER:HA	1:D:603:ASP:HB3	1.88	0.55
3:C:268:LYS:HD3	3:C:273:SER:HB3	1.89	0.55
1:E:14:LEU:HB2	1:E:53:PHE:HB2	1.89	0.55
1:H:490:LEU:HD13	1:H:672:LEU:HD23	1.88	0.55
1:D:77:LEU:HG	1:D:81:ASP:HB3	1.89	0.55
1:D:532:LEU:HD12	1:D:569:ILE:HG23	1.88	0.55
2:A:598:THR:HG22	2:A:614:ILE:HG12	1.89	0.55
1:E:556:SER:HA	1:E:603:ASP:HB3	1.87	0.55
2:A:357:MET:HE3	2:A:377:ASP:HB2	1.88	0.55
1:D:151:LYS:NZ	5:T:12:DT:P	2.81	0.54
1:E:180:LEU:HD22	1:E:209:PHE:HB3	1.89	0.54
1:J:507:THR:HG21	1:J:626:PHE:HB3	1.89	0.54
2:A:555:PRO:HA	2:A:627:LEU:HD13	1.90	0.54
1:E:127:ASN:HB2	1:E:193:THR:HG22	1.89	0.54
3:C:86:VAL:HG23	3:C:98:LEU:HB3	1.89	0.53
3:C:346:ARG:HA	3:C:349:LYS:HE2	1.90	0.53
3:C:358:ARG:HG2	3:C:363:TYR:HB2	1.91	0.53
1:D:14:LEU:HD22	1:D:32:VAL:HG12	1.90	0.53
2:A:167:ILE:HG22	2:A:186:THR:HG22	1.90	0.52
1:E:358:ASN:HB3	1:E:363:LEU:HD22	1.91	0.52
1:D:259:ILE:HD12	1:D:275:VAL:HG12	1.92	0.52
2:A:8:TRP:CE2	2:A:20:LEU:HD13	2.44	0.52
3:C:398:PRO:HA	3:C:401:GLU:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:155:LEU:HB3	4:B:176:THR:HG22	1.90	0.52
1:E:181:ARG:HH11	1:E:187:LYS:H	1.58	0.52
4:B:19:TRP:HA	4:B:147:HIS:HE1	1.74	0.52
1:J:556:SER:HA	1:J:603:ASP:HB3	1.91	0.52
1:D:198:GLN:HB3	1:D:200:PRO:HD2	1.90	0.52
1:H:412:LYS:HG3	1:H:436:TYR:HE2	1.75	0.52
2:A:245:LEU:HB3	2:A:276:LEU:HD13	1.90	0.52
2:A:299:ILE:HG12	2:A:320:VAL:HG22	1.92	0.52
1:K:421:ASP:HB3	1:K:425:GLY:HA3	1.92	0.51
1:D:53:PHE:HE1	1:D:181:ARG:HG2	1.76	0.51
1:E:53:PHE:HZ	1:E:187:LYS:HA	1.76	0.51
4:B:60:LYS:HG2	4:B:117:ILE:HB	1.93	0.51
1:H:558:LEU:HD12	1:H:559:PRO:HD2	1.92	0.51
1:E:377:LYS:HA	1:E:380:SER:HB3	1.93	0.51
1:E:386:PRO:HA	1:E:389:ARG:HE	1.75	0.51
1:D:507:THR:HG21	1:D:626:PHE:HB3	1.92	0.51
1:I:547:MET:HG3	1:I:553:VAL:HG21	1.93	0.51
2:A:283:LYS:HE2	2:A:296:HIS:CG	2.46	0.50
5:T:37:DT:H2''	5:T:38:DT:O5'	2.11	0.50
2:A:249:LYS:HD3	2:A:276:LEU:HD21	1.93	0.50
1:E:532:LEU:HD12	1:E:569:ILE:HG23	1.93	0.50
2:A:322:ASN:HD21	2:A:326:THR:HB	1.76	0.50
1:K:386:PRO:HA	1:K:389:ARG:HE	1.75	0.50
1:D:658:LYS:HD2	1:D:663:ARG:HD3	1.94	0.50
3:C:223:ILE:HG22	3:C:297:ILE:HD11	1.94	0.50
3:C:245:ILE:HD13	3:C:266:VAL:HG21	1.92	0.50
1:D:274:LEU:HD11	1:D:296:LEU:HG	1.94	0.50
2:A:55:PHE:HB2	2:A:94:PRO:HD3	1.94	0.50
2:A:65:THR:HG22	2:A:516:ILE:HB	1.93	0.50
2:A:737:LEU:HD13	2:A:773:GLU:HG3	1.94	0.50
1:J:664:TYR:HB2	1:J:667:ALA:HB3	1.92	0.49
3:C:220:ILE:HD12	3:C:237:VAL:HG12	1.94	0.49
1:J:532:LEU:HD12	1:J:569:ILE:HG23	1.94	0.49
1:H:447:ASP:HB2	1:H:666:PHE:CZ	2.47	0.49
3:C:246:LEU:HB2	3:C:274:ILE:HG22	1.95	0.49
2:A:288:SER:HB3	2:A:292:LYS:H	1.78	0.49
3:C:404:TYR:HA	3:C:407:PHE:HB2	1.94	0.49
1:E:507:THR:HG21	1:E:626:PHE:HB3	1.94	0.49
2:A:548:PHE:HB3	2:A:789:ILE:HD11	1.95	0.49
2:A:872:LEU:HD13	2:A:979:ILE:HD13	1.95	0.49
3:C:114:CYS:HA	3:C:117:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:841:ASN:HA	2:A:844:LYS:HE3	1.94	0.49
3:C:234:ILE:HD12	3:C:235:PRO:HD2	1.94	0.49
1:D:453:GLU:HG2	1:D:458:MET:HB2	1.94	0.49
1:E:658:LYS:HD2	1:E:663:ARG:HD3	1.94	0.49
1:E:219:TYR:HE2	1:E:221:PHE:HB3	1.78	0.48
1:E:24:ARG:HA	1:E:32:VAL:HG11	1.95	0.48
1:D:284:LEU:HD21	1:D:317:LYS:HD2	1.95	0.48
1:D:17:ILE:HD11	1:D:51:THR:HG21	1.94	0.48
1:K:329:ILE:O	1:K:333:ILE:HG12	2.14	0.48
1:K:535:VAL:HG22	1:K:537:ASP:H	1.78	0.48
1:D:56:LEU:HD13	1:D:63:SER:HA	1.95	0.48
1:J:490:LEU:HD11	1:J:672:LEU:HD13	1.96	0.48
1:E:150:MET:SD	1:E:154:LEU:HB2	2.54	0.48
1:E:64:ILE:HG13	1:E:141:TYR:HB3	1.96	0.47
1:K:358:ASN:HB3	1:K:363:LEU:HD11	1.95	0.47
3:C:10:LEU:HB3	4:B:200:VAL:HG11	1.96	0.47
1:D:535:VAL:HG22	1:D:537:ASP:H	1.79	0.47
1:H:586:PRO:HB2	1:H:589:SER:HB3	1.95	0.47
1:E:535:VAL:HG22	1:E:537:ASP:H	1.78	0.47
2:A:368:MET:HE2	2:A:368:MET:HB2	1.80	0.47
2:A:986:LYS:HA	2:A:989:CYS:HB2	1.96	0.47
5:T:36:DT:H2''	5:T:37:DT:O5'	2.14	0.47
1:I:419:VAL:HG12	1:I:433:ALA:HB1	1.95	0.47
1:D:177:LYS:HZ1	5:T:10:DT:P	2.37	0.47
2:A:335:ILE:HD13	2:A:349:ILE:HD13	1.96	0.47
3:C:148:PRO:HG2	3:C:200:ILE:HD13	1.97	0.47
1:E:13:VAL:O	1:E:14:LEU:HD13	2.15	0.47
1:E:421:ASP:HB2	1:E:428:TYR:HE2	1.80	0.47
3:C:227:ARG:HG2	3:C:233:PHE:CE1	2.49	0.47
1:H:553:VAL:HG23	1:H:600:ILE:HA	1.97	0.47
4:B:145:LEU:HG	4:B:170:LEU:HD21	1.96	0.47
1:J:471:LEU:H	1:J:471:LEU:HD23	1.79	0.47
2:A:327:ILE:HG12	2:A:491:SER:HB3	1.97	0.46
1:H:666:PHE:HA	1:H:669:LEU:HB2	1.98	0.46
2:A:51:SER:HB3	2:A:52:PRO:HD3	1.97	0.46
2:A:990:ILE:HD12	2:A:1001:PRO:HD2	1.96	0.46
2:A:577:ARG:HG2	3:C:373:ASN:HA	1.96	0.46
5:T:7:DT:H2''	5:T:8:DT:O5'	2.15	0.46
1:D:91:ILE:HA	1:D:117:ARG:HH12	1.80	0.46
1:D:113:ILE:HG23	1:D:117:ARG:HE	1.79	0.46
1:E:69:MET:HG3	1:E:135:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:357:MET:HB3	2:A:377:ASP:HB2	1.96	0.46
1:K:662:ASN:HB3	1:K:665:ARG:HD3	1.96	0.46
3:C:303:VAL:HG22	3:C:308:PHE:HE1	1.81	0.46
1:E:67:ILE:HD11	1:E:147:LEU:HD21	1.98	0.46
2:A:778:ILE:HA	2:A:782:VAL:HG12	1.96	0.46
1:J:351:ILE:HD11	1:J:356:LYS:HD2	1.98	0.46
1:K:531:ILE:HG13	1:K:532:LEU:HG	1.97	0.46
1:D:71:VAL:HG22	1:D:169:ILE:HG22	1.97	0.46
2:A:739:ILE:HG13	2:A:740:ASP:H	1.80	0.46
3:C:363:TYR:CZ	3:C:403:ILE:HG23	2.51	0.46
1:J:519:ALA:HB2	1:J:668:PHE:HD2	1.81	0.46
1:D:386:PRO:HG2	1:I:391:THR:HG23	1.96	0.46
1:E:155:LEU:HG	1:E:159:ARG:HH12	1.81	0.46
3:C:228:ILE:HD13	3:C:234:ILE:HB	1.98	0.45
1:D:177:LYS:HZ3	5:T:10:DT:P	2.38	0.45
1:E:181:ARG:HE	1:E:195:HIS:CE1	2.33	0.45
3:C:44:LYS:HG3	4:B:173:PRO:HB2	1.97	0.45
1:H:681:ILE:HG13	1:H:682:PRO:CD	2.33	0.45
1:K:348:ILE:HG22	1:K:357:PHE:HB3	1.98	0.45
1:D:340:LEU:HB3	1:D:404:VAL:HG21	1.98	0.45
1:H:536:LEU:HD13	1:H:544:ILE:HG21	1.99	0.45
1:D:199:PRO:N	1:D:200:PRO:HD2	2.32	0.45
1:D:419:VAL:HG12	1:D:433:ALA:HB1	1.98	0.45
2:A:205:GLU:HG2	2:A:240:SER:HA	1.99	0.45
2:A:573:VAL:HG12	2:A:611:GLU:HG3	1.98	0.45
4:B:64:VAL:HG21	4:B:110:LEU:HD13	1.99	0.45
1:D:108:ILE:O	1:D:112:VAL:HG23	2.17	0.45
3:C:78:PHE:HB2	3:C:188:PHE:CZ	2.52	0.45
1:D:344:ARG:NH2	1:D:591:LYS:HB3	2.33	0.44
3:C:371:LEU:HB2	3:C:400:ILE:HD12	1.99	0.44
2:A:548:PHE:HB2	2:A:755:VAL:HG13	1.98	0.44
3:C:363:TYR:HB3	3:C:368:PHE:HB2	1.99	0.44
1:D:146:THR:O	1:D:150:MET:HG2	2.18	0.44
2:A:896:HIS:CE1	2:A:898:SER:HB2	2.52	0.44
4:B:19:TRP:HE3	4:B:22:VAL:HG11	1.82	0.44
2:A:933:ILE:HG13	2:A:965:ARG:O	2.17	0.44
3:C:78:PHE:HB2	3:C:188:PHE:CE1	2.53	0.44
3:C:225:VAL:HB	3:C:233:PHE:HB3	1.98	0.44
4:B:60:LYS:HA	4:B:115:GLY:HA2	1.99	0.44
1:E:155:LEU:HB2	1:E:171:THR:HG21	1.98	0.44
1:H:518:SER:HB2	1:H:662:ASN:HD22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:TRP:HD1	2:A:995:ARG:HD3	1.82	0.44
1:D:482:TYR:HD1	1:D:624:VAL:HG11	1.82	0.44
1:E:420:LEU:HB2	1:E:427:PHE:HD1	1.83	0.44
4:B:154:VAL:HG11	4:B:198:ILE:HG23	1.99	0.44
1:J:482:TYR:HD1	1:J:624:VAL:HG11	1.83	0.44
1:D:7:GLY:HA3	1:D:212:VAL:HG11	2.00	0.44
3:C:107:PRO:HG2	3:C:110:ILE:HD12	2.00	0.44
3:C:223:ILE:HG13	3:C:237:VAL:HG13	1.98	0.44
2:A:64:ARG:HE	2:A:83:CYS:HB3	1.83	0.44
2:A:798:LEU:HD11	2:A:800:MET:HE3	2.00	0.44
1:I:475:ASN:HB3	1:I:479:ARG:HB2	1.99	0.44
1:H:338:SER:HB3	1:H:367:LEU:HD21	1.99	0.44
2:A:900:TYR:HD2	2:A:901:LYS:HG3	1.83	0.43
1:I:363:LEU:HG	1:I:366:LYS:HD2	2.00	0.43
1:D:163:ASN:HD21	1:D:165:LEU:HB3	1.83	0.43
2:A:202:LEU:HD21	2:A:247:ILE:HD12	2.00	0.43
2:A:559:ILE:HA	2:A:624:PRO:HB3	1.99	0.43
3:C:181:TYR:O	3:C:185:GLU:HG3	2.18	0.43
1:E:195:HIS:HB2	1:E:207:TYR:CE2	2.53	0.43
1:I:556:SER:C	1:I:557:GLU:HG3	2.43	0.43
1:H:329:ILE:O	1:H:333:ILE:HG12	2.19	0.43
2:A:936:ALA:HB3	2:A:963:ASN:HA	2.01	0.43
4:B:213:ALA:HA	4:B:216:PHE:HD2	1.83	0.43
1:D:674:LYS:HD2	1:D:677:LYS:HE3	2.00	0.43
2:A:370:PHE:CG	2:A:431:LEU:HD11	2.53	0.43
2:A:993:PHE:CG	2:A:1001:PRO:HB3	2.53	0.43
3:C:265:LYS:HE2	3:C:276:TYR:CD2	2.53	0.43
1:I:329:ILE:O	1:I:333:ILE:HG12	2.18	0.43
1:H:412:LYS:HG3	1:H:436:TYR:CE2	2.54	0.43
1:D:250:VAL:HG11	1:D:296:LEU:HD21	2.01	0.43
4:B:92:ILE:O	4:B:96:ILE:HG12	2.18	0.43
2:A:796:LYS:HG2	2:A:797:ASN:HD22	1.84	0.43
1:K:342:THR:HG23	1:K:345:GLY:H	1.84	0.43
1:D:163:ASN:HB3	1:D:166:THR:HG22	1.99	0.43
1:E:72:ASP:HA	1:E:132:SER:HA	2.01	0.43
3:C:239:THR:HG23	3:C:241:SER:H	1.84	0.43
1:E:471:LEU:H	1:E:471:LEU:HD23	1.84	0.43
1:E:12:PHE:CD2	1:E:57:ARG:HA	2.54	0.42
4:B:1:MET:HE1	4:B:54:LYS:HG2	2.01	0.42
1:J:543:PHE:O	1:J:547:MET:HG2	2.19	0.42
1:K:471:LEU:HD23	1:K:471:LEU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:482:TYR:HD1	1:K:624:VAL:HG11	1.83	0.42
2:A:360:VAL:HG21	2:A:363:ARG:NH2	2.34	0.42
3:C:31:TYR:O	3:C:35:VAL:HG22	2.19	0.42
1:I:675:TRP:HA	1:I:678:LYS:HB2	2.01	0.42
1:J:674:LYS:HA	1:J:677:LYS:HG2	2.01	0.42
1:D:163:ASN:ND2	1:D:165:LEU:HB3	2.34	0.42
1:D:330:ALA:HB2	1:D:392:VAL:HG13	2.01	0.42
4:B:86:LYS:HZ3	4:B:89:ILE:N	2.17	0.42
2:A:743:PHE:HB3	2:A:759:ILE:HD11	2.01	0.42
3:C:132:LEU:HD21	3:C:193:PRO:HD2	2.02	0.42
4:B:160:LYS:HG2	4:B:180:TYR:HA	2.01	0.42
1:I:390:LYS:HE2	1:I:390:LYS:HB2	1.92	0.42
1:D:146:THR:HG22	1:D:223:LEU:HB2	2.00	0.42
1:D:303:ILE:HG12	1:D:321:LEU:HD11	2.01	0.42
1:E:461:LEU:HD12	1:E:464:ILE:HD11	2.01	0.42
3:C:188:PHE:CZ	3:C:197:ILE:HD12	2.54	0.42
4:B:149:THR:HG21	4:B:170:LEU:HD13	2.00	0.42
1:J:412:LYS:HE2	1:J:436:TYR:CE1	2.55	0.42
1:D:342:THR:HG23	1:D:344:ARG:HG2	2.02	0.42
1:E:181:ARG:HD3	1:E:187:LYS:N	2.35	0.42
3:C:294:ILE:HD12	3:C:398:PRO:HB2	2.02	0.42
3:C:361:LEU:HD11	3:C:413:ILE:HG21	2.01	0.42
1:D:37:CYS:C	1:D:39:GLU:H	2.27	0.42
1:D:471:LEU:HD23	1:D:471:LEU:H	1.84	0.42
3:C:47:VAL:HG23	4:B:204:LEU:HD21	2.01	0.42
5:T:36:DT:H2''	5:T:37:DT:O4'	2.19	0.42
1:J:519:ALA:HB2	1:J:668:PHE:CD2	2.55	0.42
1:K:450:LYS:HB2	1:K:666:PHE:HD2	1.85	0.42
1:E:40:LEU:HG	1:E:52:LEU:HG	2.01	0.42
1:E:103:THR:HG22	1:E:104:GLU:HG2	2.01	0.42
1:E:211:TYR:CE2	1:E:213:ASP:HB2	2.55	0.42
1:E:482:TYR:HD1	1:E:624:VAL:HG11	1.83	0.42
2:A:739:ILE:HG23	2:A:740:ASP:OD2	2.19	0.42
1:I:386:PRO:HG3	1:I:389:ARG:HH21	1.85	0.42
1:H:525:VAL:HG21	1:H:550:LYS:HG3	2.00	0.42
1:K:333:ILE:O	1:K:336:THR:HG22	2.19	0.41
1:D:304:ARG:HD3	5:T:12:DT:H71	2.01	0.41
1:E:27:GLU:HA	1:E:32:VAL:HG23	2.01	0.41
2:A:936:ALA:HA	2:A:965:ARG:HD3	2.02	0.41
1:I:558:LEU:HD22	1:I:602:ILE:HG21	2.03	0.41
1:E:101:ALA:O	1:E:105:CYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:544:ILE:HG21	1:E:584:GLY:HA3	2.02	0.41
3:C:117:VAL:HG23	3:C:158:TYR:HD2	1.85	0.41
1:E:15:LYS:HD2	1:E:43:TYR:CE2	2.55	0.41
2:A:498:ALA:HA	2:A:501:ILE:HG12	2.03	0.41
1:K:514:ARG:HA	1:K:517:LYS:HG2	2.03	0.41
1:K:680:HIS:HB3	1:K:684:MET:HG3	2.02	0.41
1:D:65:VAL:HG21	1:D:144:MET:HE2	2.03	0.41
3:C:149:VAL:O	3:C:153:LYS:HG2	2.20	0.41
2:A:164:PHE:HB2	2:A:189:CYS:HB3	2.02	0.41
1:E:198:GLN:HB3	1:E:200:PRO:HD2	2.03	0.41
2:A:730:ASN:HA	2:A:731:PRO:HD3	1.95	0.41
2:A:795:TYR:CD2	2:A:808:THR:HG21	2.56	0.41
1:J:333:ILE:HG13	1:J:371:ILE:HD13	2.02	0.41
1:K:351:ILE:HD11	1:K:356:LYS:HD2	2.02	0.41
1:E:62:TYR:HB3	1:E:212:VAL:HG21	2.03	0.41
3:C:217:PHE:CE2	3:C:265:LYS:HB3	2.56	0.41
1:I:350:TRP:CZ2	1:I:353:ASN:HA	2.56	0.41
1:D:112:VAL:HG22	1:D:219:TYR:CE1	2.56	0.40
4:B:61:ARG:HD2	4:B:207:LYS:HE2	2.03	0.40
4:B:98:ARG:HH12	4:B:190:GLU:HB3	1.86	0.40
1:D:66:ARG:HG2	1:D:141:TYR:CE1	2.56	0.40
1:D:409:TYR:CE2	1:D:436:TYR:HA	2.56	0.40
2:A:322:ASN:ND2	2:A:326:THR:HB	2.35	0.40
2:A:745:PHE:HE2	2:A:774:LEU:HD11	1.86	0.40
1:J:333:ILE:O	1:J:336:THR:HG22	2.21	0.40
1:E:543:PHE:O	1:E:547:MET:HG2	2.22	0.40
1:K:511:THR:HG22	1:K:514:ARG:HH22	1.86	0.40
2:A:600:HIS:CE1	2:A:612:ILE:HD13	2.56	0.40
1:J:501:PHE:HD1	1:J:501:PHE:HA	1.79	0.40
1:D:511:THR:HG22	1:D:514:ARG:HH22	1.85	0.40
1:E:17:ILE:HG22	1:E:53:PHE:CE2	2.56	0.40
1:E:413:LEU:HD12	1:E:414:PRO:HD2	2.04	0.40
1:E:419:VAL:HG23	1:E:433:ALA:HB1	2.04	0.40
2:A:224:ILE:HG12	2:A:239:CYS:HB3	2.04	0.40
2:A:230:MET:HE3	2:A:230:MET:HB3	1.97	0.40
2:A:799:ILE:HG21	2:A:982:LEU:HD12	2.03	0.40
2:A:977:SER:O	2:A:981:ASN:HB2	2.21	0.40
3:C:265:LYS:HE2	3:C:276:TYR:HD2	1.87	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	D	666/785 (85%)	648 (97%)	17 (3%)	1 (0%)	43	76
1	E	552/785 (70%)	537 (97%)	15 (3%)	0	100	100
1	H	345/785 (44%)	339 (98%)	6 (2%)	0	100	100
1	I	345/785 (44%)	338 (98%)	7 (2%)	0	100	100
1	J	314/785 (40%)	307 (98%)	7 (2%)	0	100	100
1	K	343/785 (44%)	336 (98%)	7 (2%)	0	100	100
2	A	973/1006 (97%)	944 (97%)	28 (3%)	1 (0%)	48	81
3	C	371/426 (87%)	359 (97%)	12 (3%)	0	100	100
4	B	216/218 (99%)	208 (96%)	8 (4%)	0	100	100
All	All	4125/6360 (65%)	4016 (97%)	107 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	255	ILE
2	A	487	VAL

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	D	624/725 (86%)	620 (99%)	4 (1%)	78	80
1	E	522/725 (72%)	508 (97%)	14 (3%)	39	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	324/725 (45%)	318 (98%)	6 (2%)	50	67
1	I	324/725 (45%)	318 (98%)	6 (2%)	50	67
1	J	298/725 (41%)	296 (99%)	2 (1%)	76	79
1	K	322/725 (44%)	318 (99%)	4 (1%)	63	73
2	A	909/928 (98%)	901 (99%)	8 (1%)	70	76
3	C	358/396 (90%)	354 (99%)	4 (1%)	65	74
4	B	200/200 (100%)	197 (98%)	3 (2%)	57	70
All	All	3881/5874 (66%)	3830 (99%)	51 (1%)	59	72

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	19	VAL
1	D	140	THR
1	D	231	VAL
1	D	681	ILE
1	E	8	ASN
1	E	13	VAL
1	E	56	LEU
1	E	65	VAL
1	E	84	THR
1	E	86	ILE
1	E	93	VAL
1	E	123	THR
1	E	140	THR
1	E	165	LEU
1	E	182	VAL
1	E	210	THR
1	E	457	GLU
1	E	681	ILE
2	A	365	VAL
2	A	588	LEU
2	A	725	ASP
2	A	729	ILE
2	A	755	VAL
2	A	893	SER
2	A	945	VAL
2	A	990	ILE
3	C	36	GLU
3	C	95	MET

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Mol	Chain	Res	Type
3	C	106	ILE
3	C	149	VAL
4	B	77	VAL
4	B	86	LYS
4	B	117	ILE
1	I	363	LEU
1	I	471	LEU
1	I	507	THR
1	I	668	PHE
1	I	679	TYR
1	I	681	ILE
1	H	417	ASN
1	H	419	VAL
1	H	491	CYS
1	H	609	VAL
1	H	669	LEU
1	H	683	ILE
1	J	361	GLU
1	J	681	ILE
1	K	423	VAL
1	K	442	THR
1	K	535	VAL
1	K	681	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	256	ASN
1	D	312	HIS
1	D	469	GLN
1	D	475	ASN
1	E	26	ASN
1	E	47	ASN
1	E	163	ASN
1	E	195	HIS
1	E	469	GLN
1	E	475	ASN
1	E	629	HIS
2	A	36	HIS
2	A	225	GLN
2	A	303	ASN
2	A	319	HIS

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Mol	Chain	Res	Type
2	A	336	GLN
2	A	393	ASN
2	A	461	HIS
2	A	562	ASN
2	A	675	ASN
2	A	716	ASN
2	A	786	ASN
2	A	797	ASN
2	A	896	HIS
3	C	105	GLN
3	C	318	GLN
3	C	397	ASN
4	B	52	GLN
4	B	55	GLN
4	B	147	HIS
1	I	478	ASN
1	I	605	ASN
1	I	629	HIS
1	I	660	GLN
1	I	662	ASN
1	H	541	ASN
1	H	605	ASN
1	H	629	HIS
1	H	662	ASN
1	J	475	ASN
1	K	469	GLN
1	K	475	ASN
1	K	548	HIS
1	K	597	HIS
1	K	629	HIS
1	K	661	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	T	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	13:DT	O3'	34:DT	P	55.39
1	T	1:DT	O3'	6:DT	P	27.58

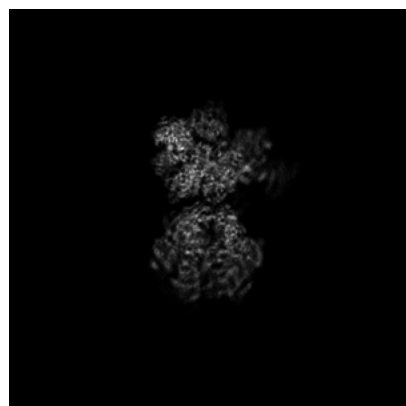
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49747. These allow visual inspection of the internal detail of the map and identification of artifacts.

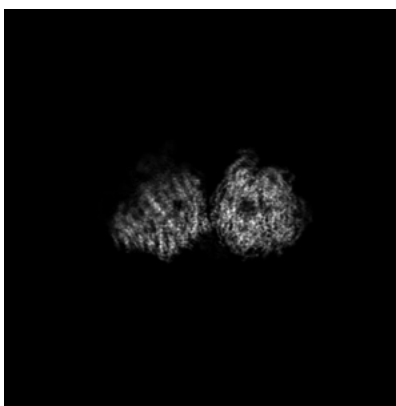
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

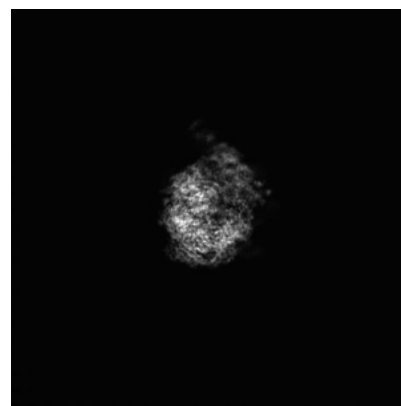
6.1.1 Primary map



X

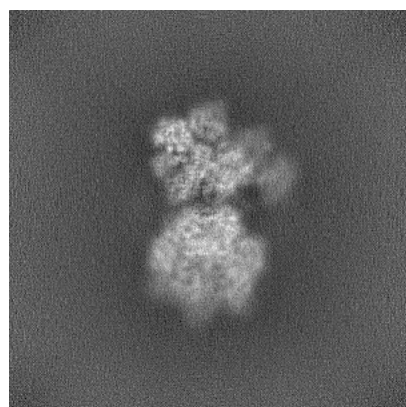


Y

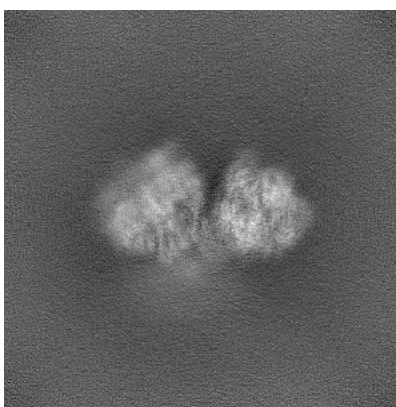


Z

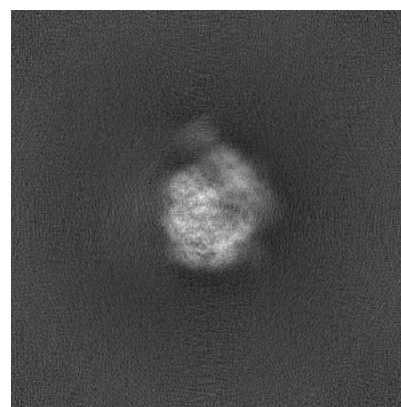
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

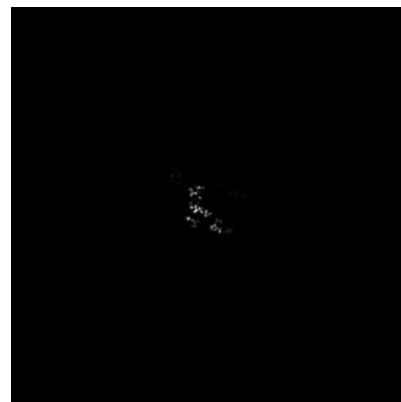
6.2.1 Primary map



X Index: 256

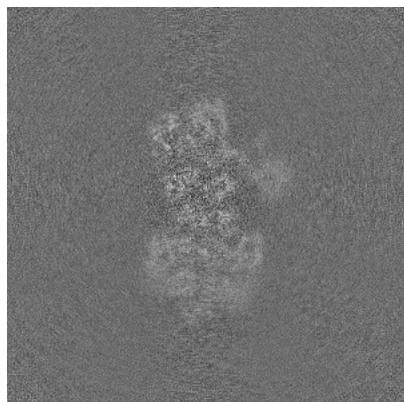


Y Index: 256

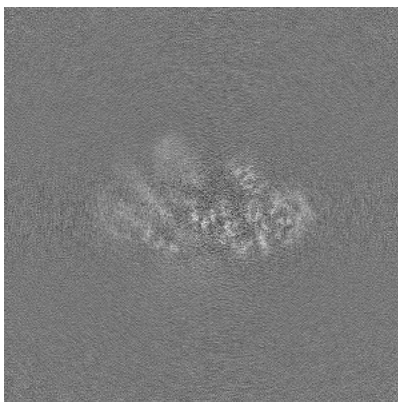


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

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

6.3 Largest variance slices [i](#)

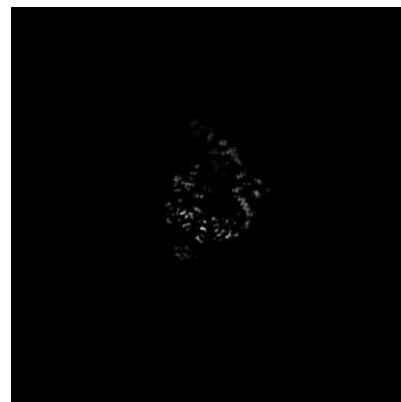
6.3.1 Primary map



X Index: 239

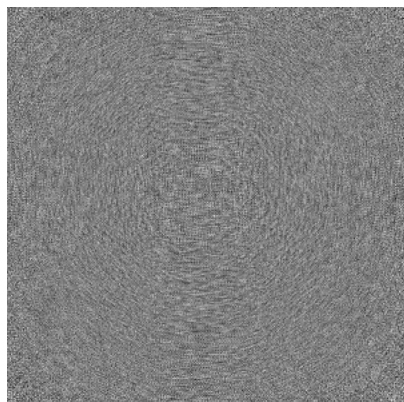


Y Index: 240

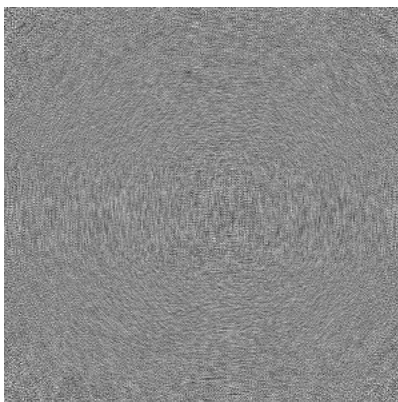


Z Index: 299

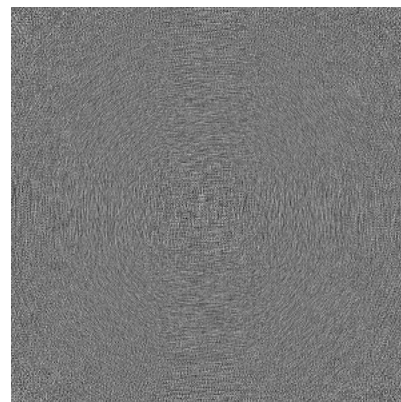
6.3.2 Raw map



X Index: 0



Y Index: 0

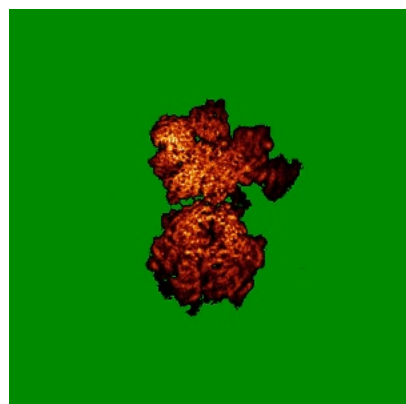


Z Index: 0

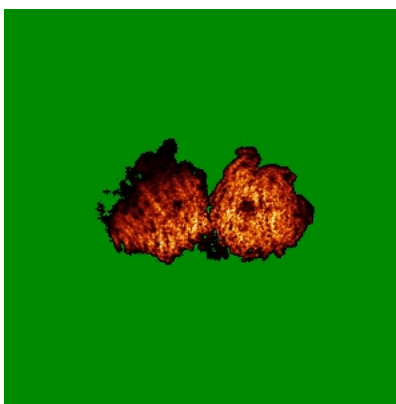
The images above show the largest variance slices of the map in three orthogonal directions.

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

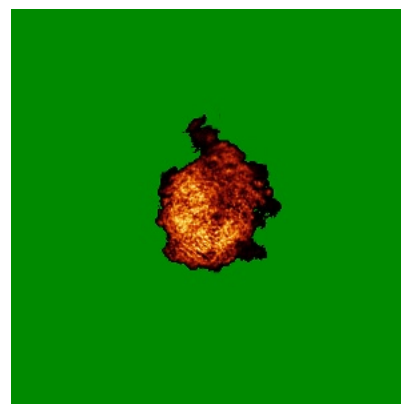
6.4.1 Primary map



X

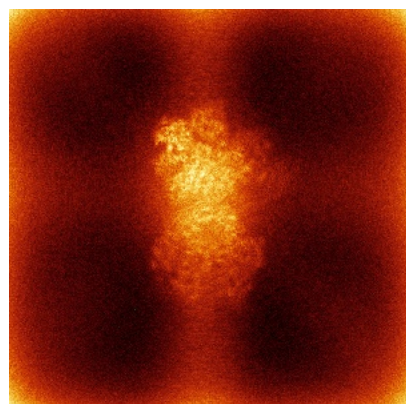


Y

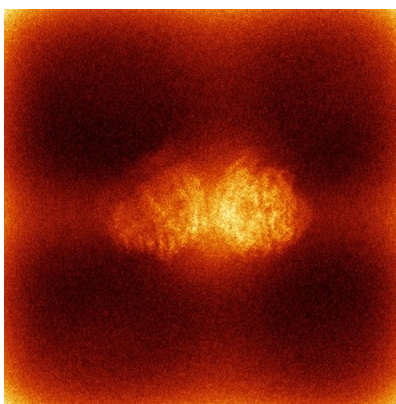


Z

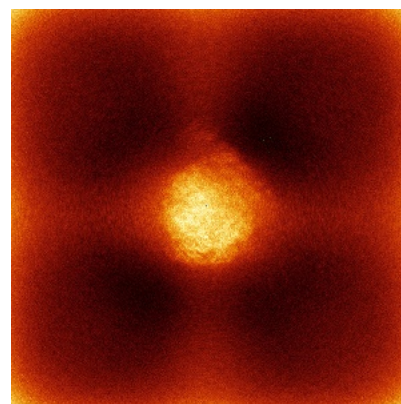
6.4.2 Raw map



X



Y



Z

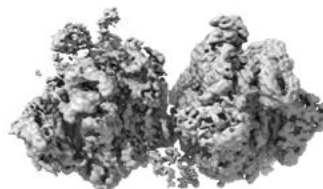
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



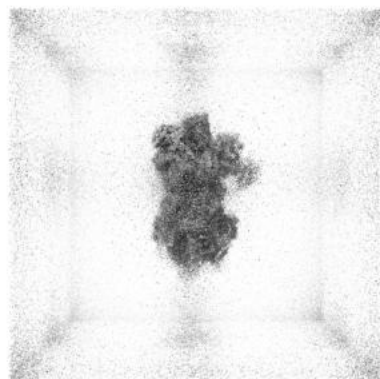
Y



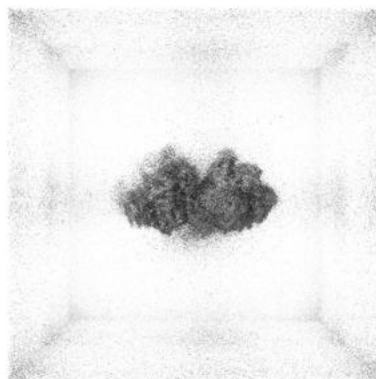
Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

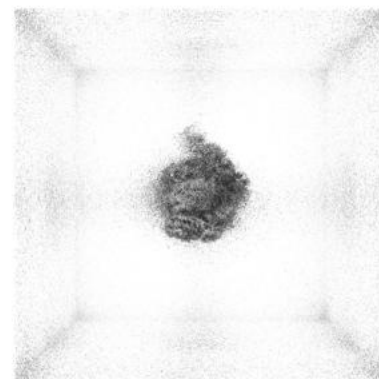
6.5.2 Raw map



X



Y



Z

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.

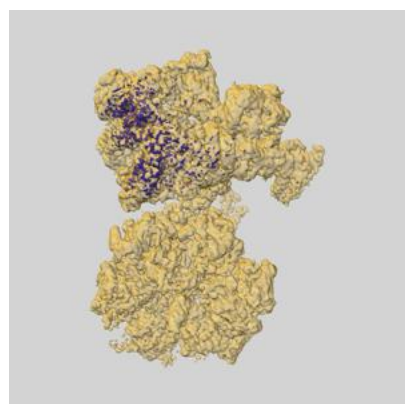
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

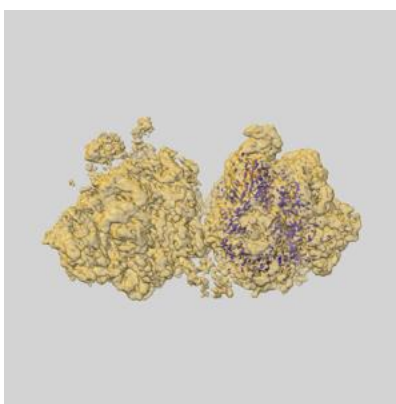
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

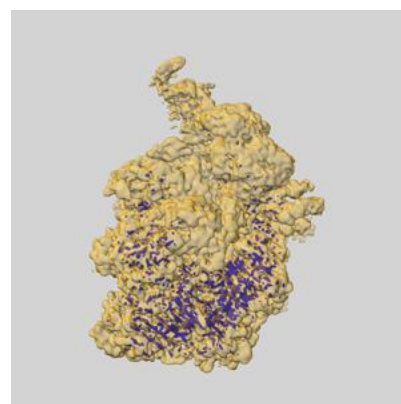
6.6.1 emd_49747_msk_1.map [i](#)



X

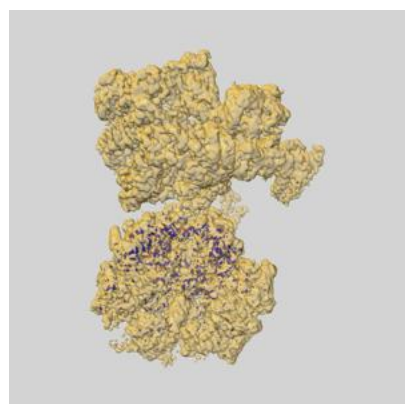


Y

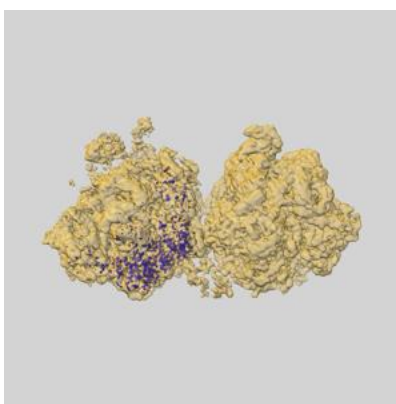


Z

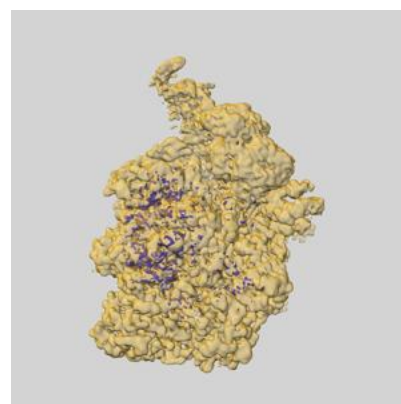
6.6.2 emd_49747_msk_2.map [i](#)



X



Y

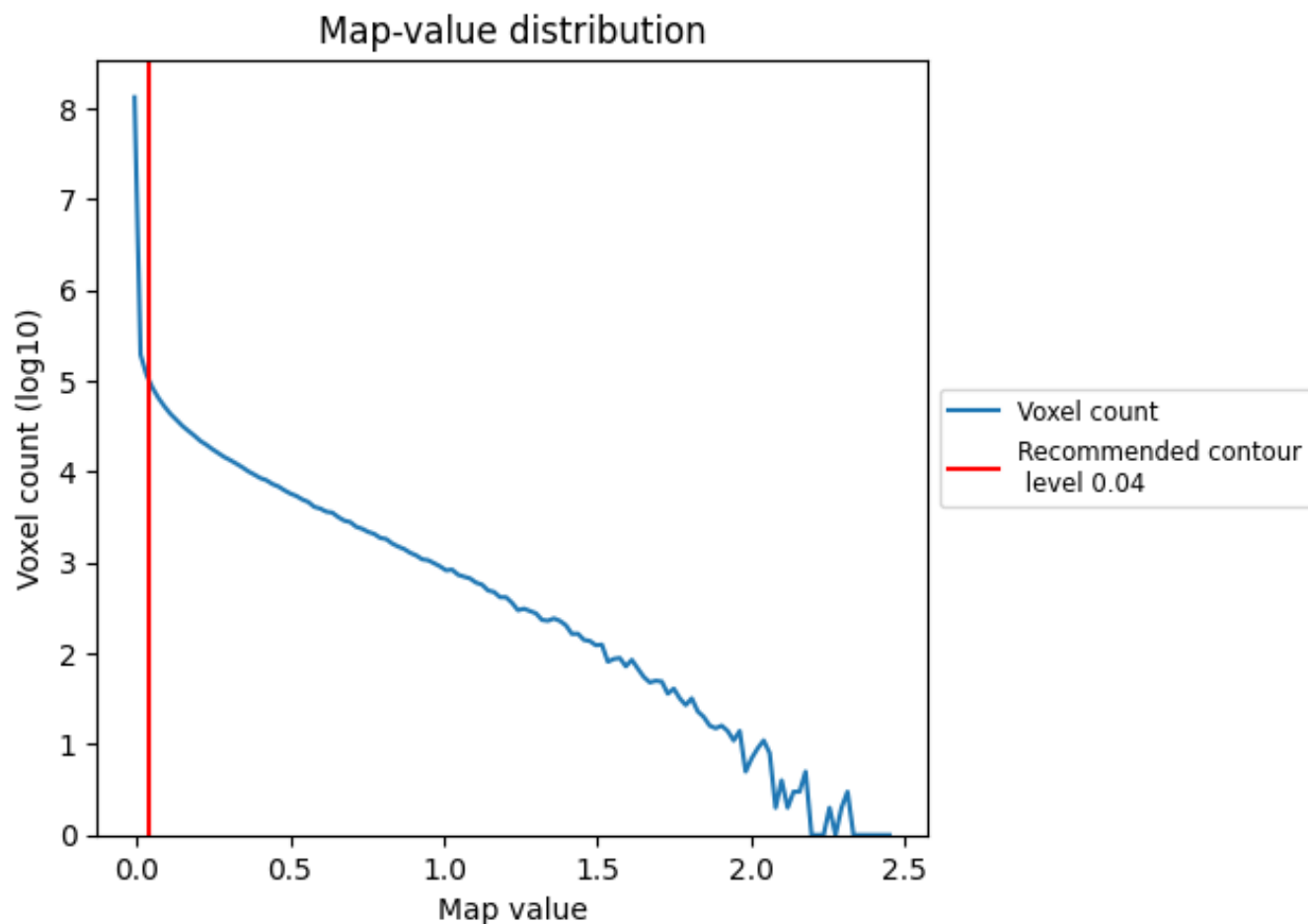


Z

7 Map analysis [i](#)

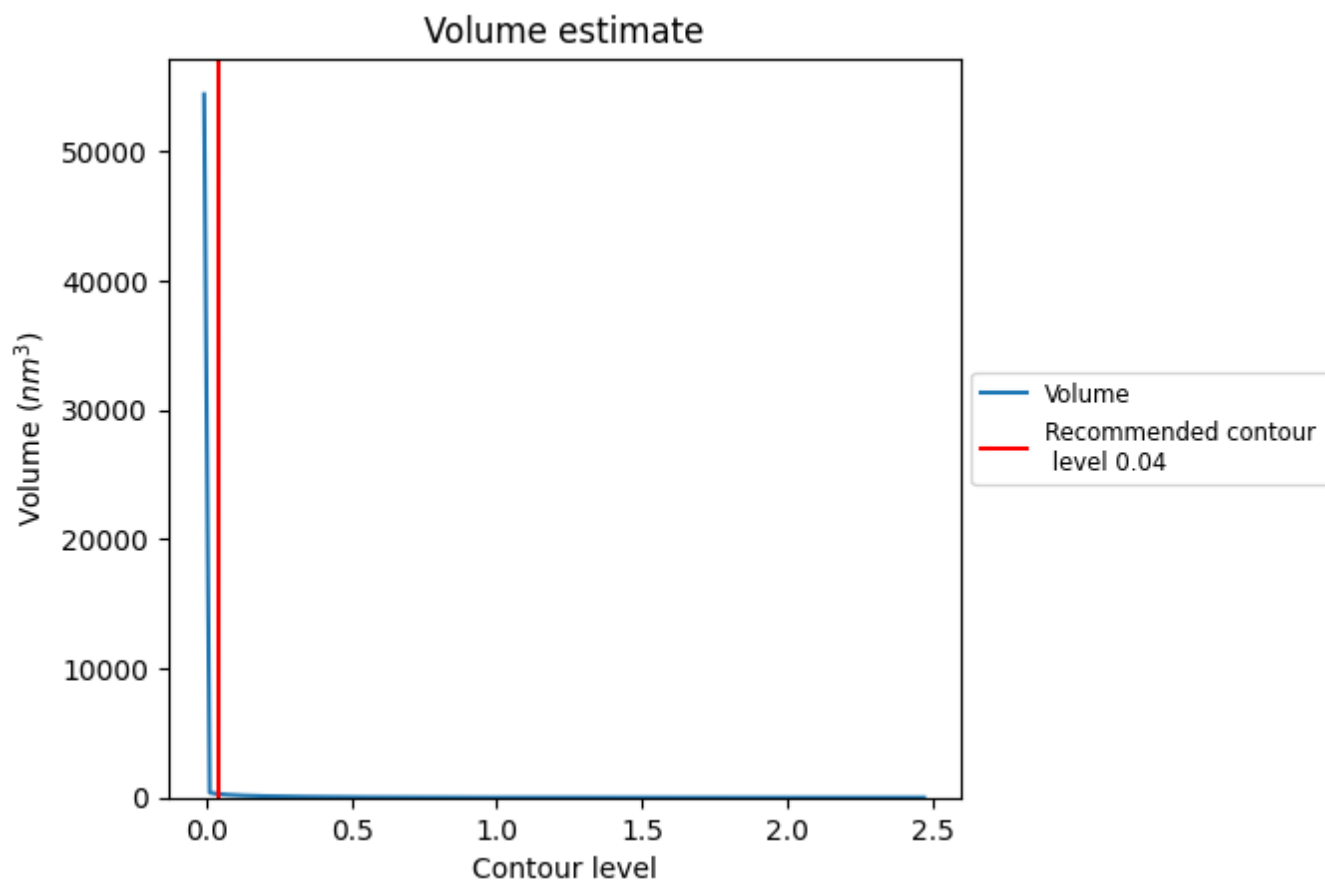
This section contains the results of statistical analysis of the map.

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.

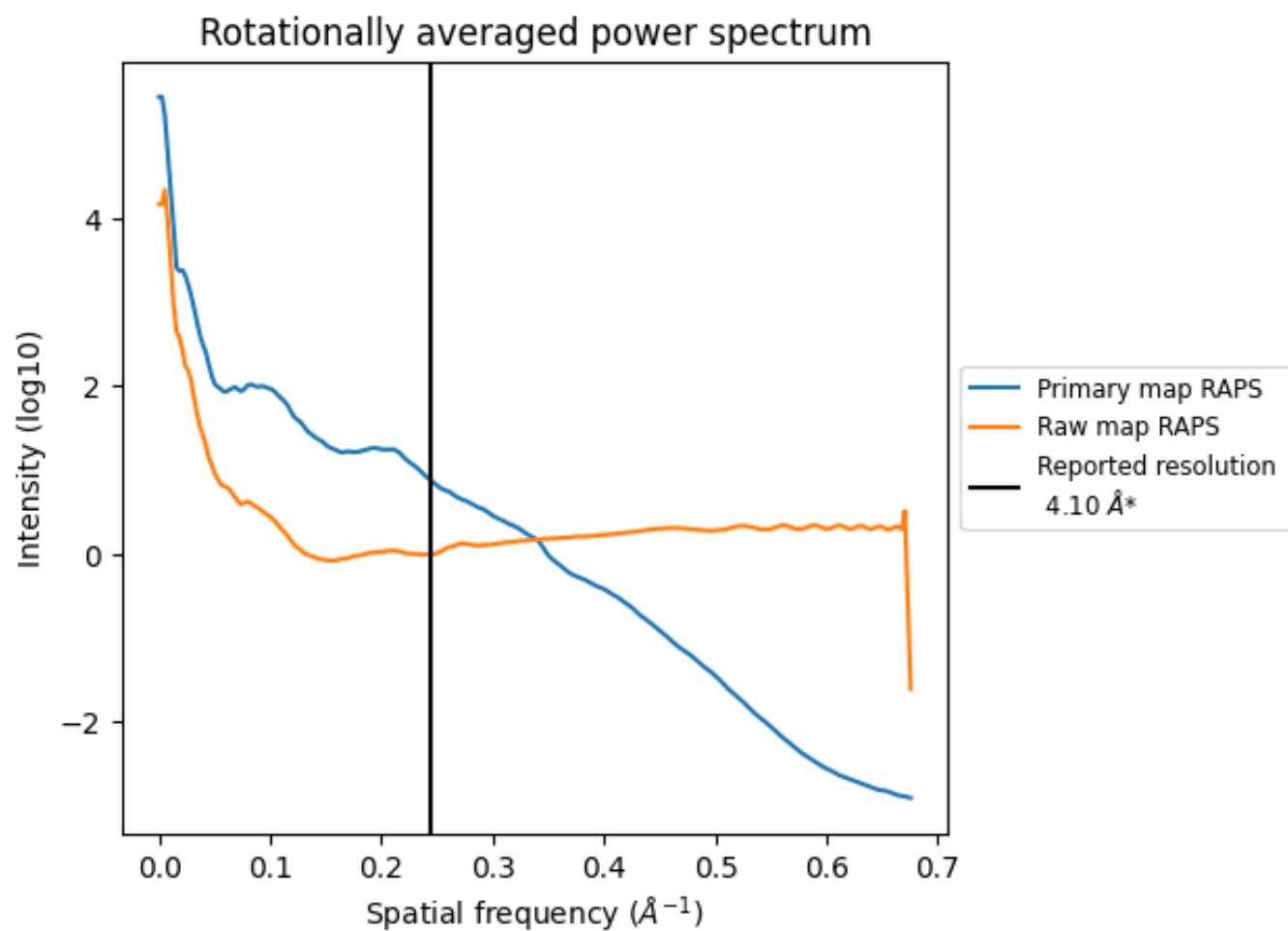
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 285 nm^3 ; this corresponds to an approximate mass of 258 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 ⓘ

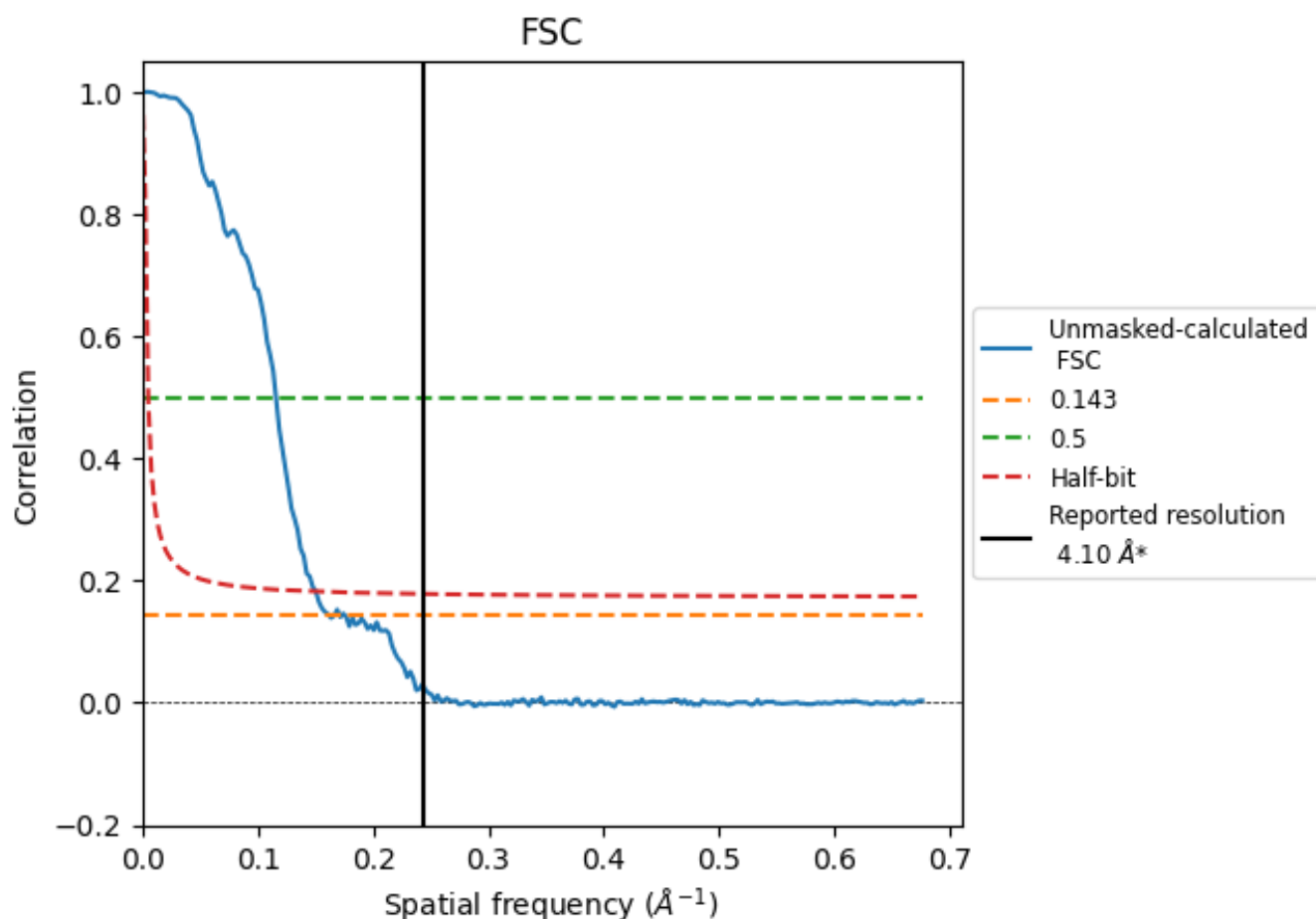


*Reported resolution corresponds to spatial frequency of 0.244 $\text{\AA}^{-1}$

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 0.244 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

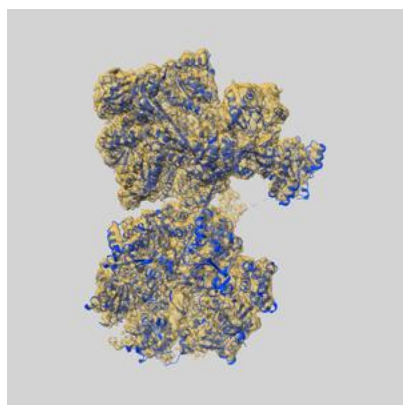
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.18	8.64	6.64

*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 6.18 differs from the reported value 4.1 by more than 10 %

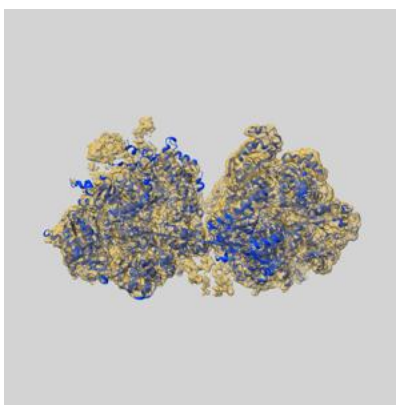
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49747 and PDB model 9NSP. Per-residue inclusion information can be found in section [3](#) on page [6](#).

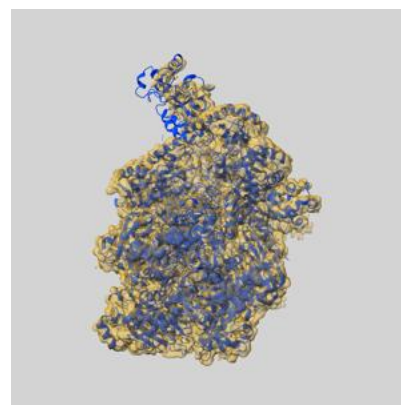
9.1 Map-model overlay [i](#)



X



Y



Z

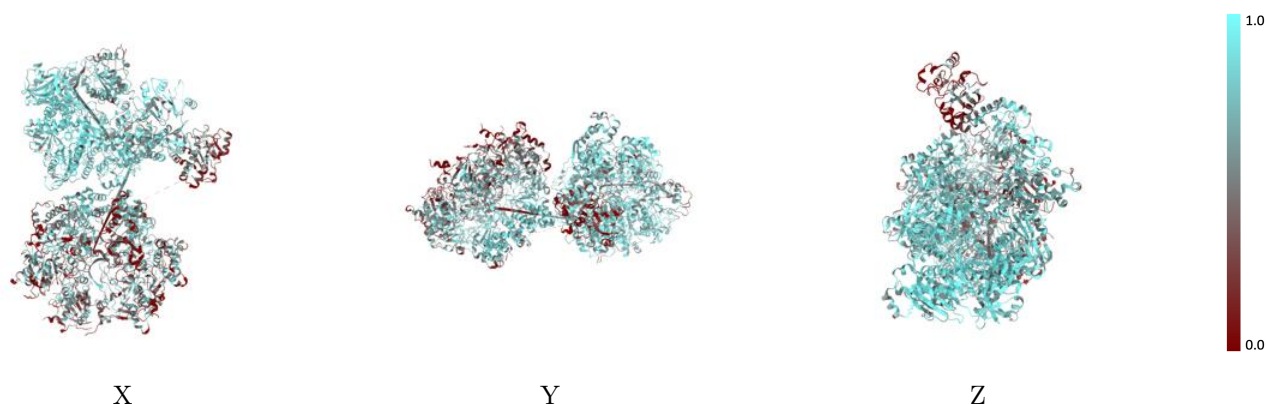
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



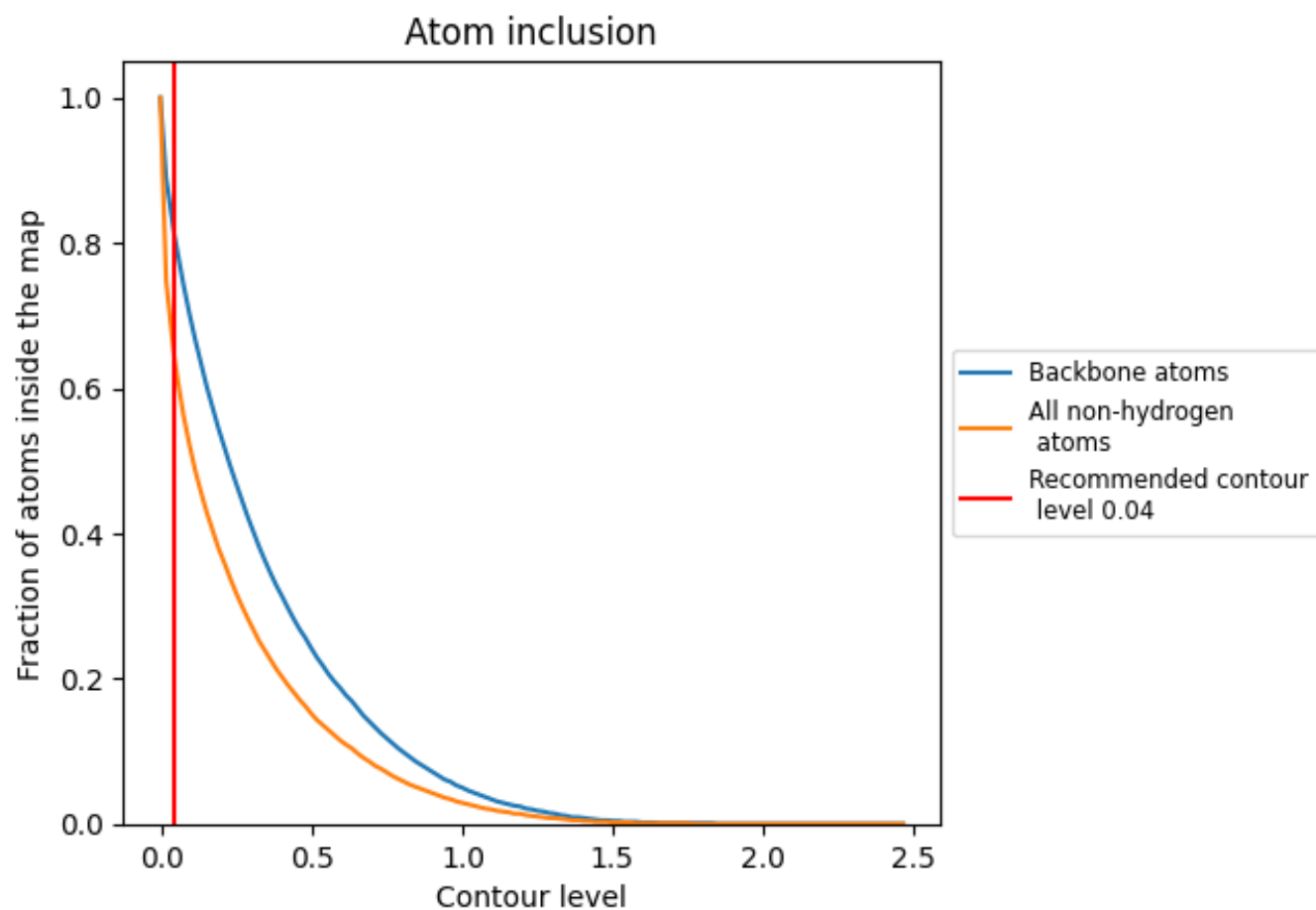
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 64% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6430	0.1520
A	0.8400	0.3470
B	0.6870	0.1980
C	0.7120	0.1090
D	0.6600	0.1590
E	0.4030	0.0360
H	0.5540	0.0640
I	0.5790	0.0700
J	0.5800	0.0640
K	0.5640	0.0560
T	0.5960	0.1200

1.0

0.0

<0.0