



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 09:31 AM UTC

PDB ID : 7ELB / pdb_00007elb
EMDB ID : EMD-31179
Title : Structure of Machupo virus L polymerase in complex with Z protein (dimeric form)
Authors : Peng, R.; Xu, X.; Peng, Q.; Shi, Y.
Deposited on : 2021-04-09
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.dev132
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) : 2.49

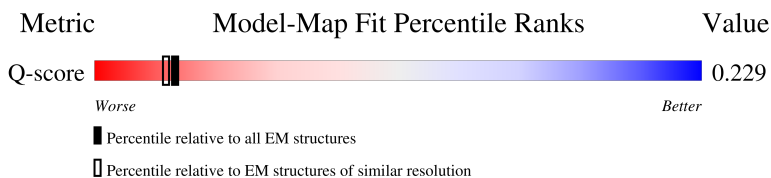
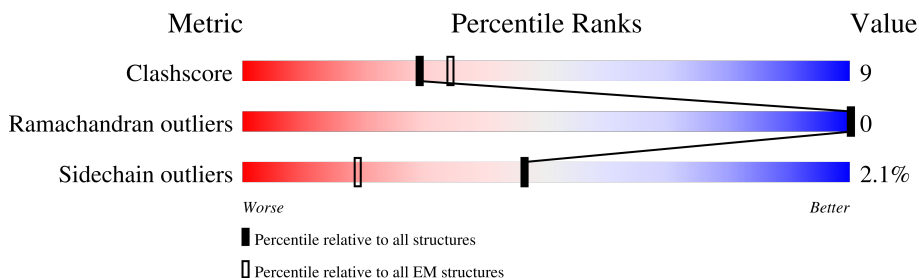
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	A	2209	13% 67% 20% 12%
1	C	2209	13% 67% 20% 12%
2	B	94	45% 7% 48%
2	D	94	45% 7% 48%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 31012 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
1	A	1937	Total	C	N	O	S	0	0
			15094	9621	2518	2861	94		
1	C	1937	Total	C	N	O	S	0	0
			15094	9621	2518	2861	94		

- Molecule 2 is a protein called RING finger protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	49	Total	C	N	O	S	0	0
			407	257	73	68	9		
2	D	49	Total	C	N	O	S	0	0
			407	257	73	68	9		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mn	0
			1	1	
3	C	1	Total	Mn	0
			1	1	

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Zn	0
			2	2	
4	B	2	Total	Zn	0
			2	2	
4	C	2	Total	Zn	0
			2	2	

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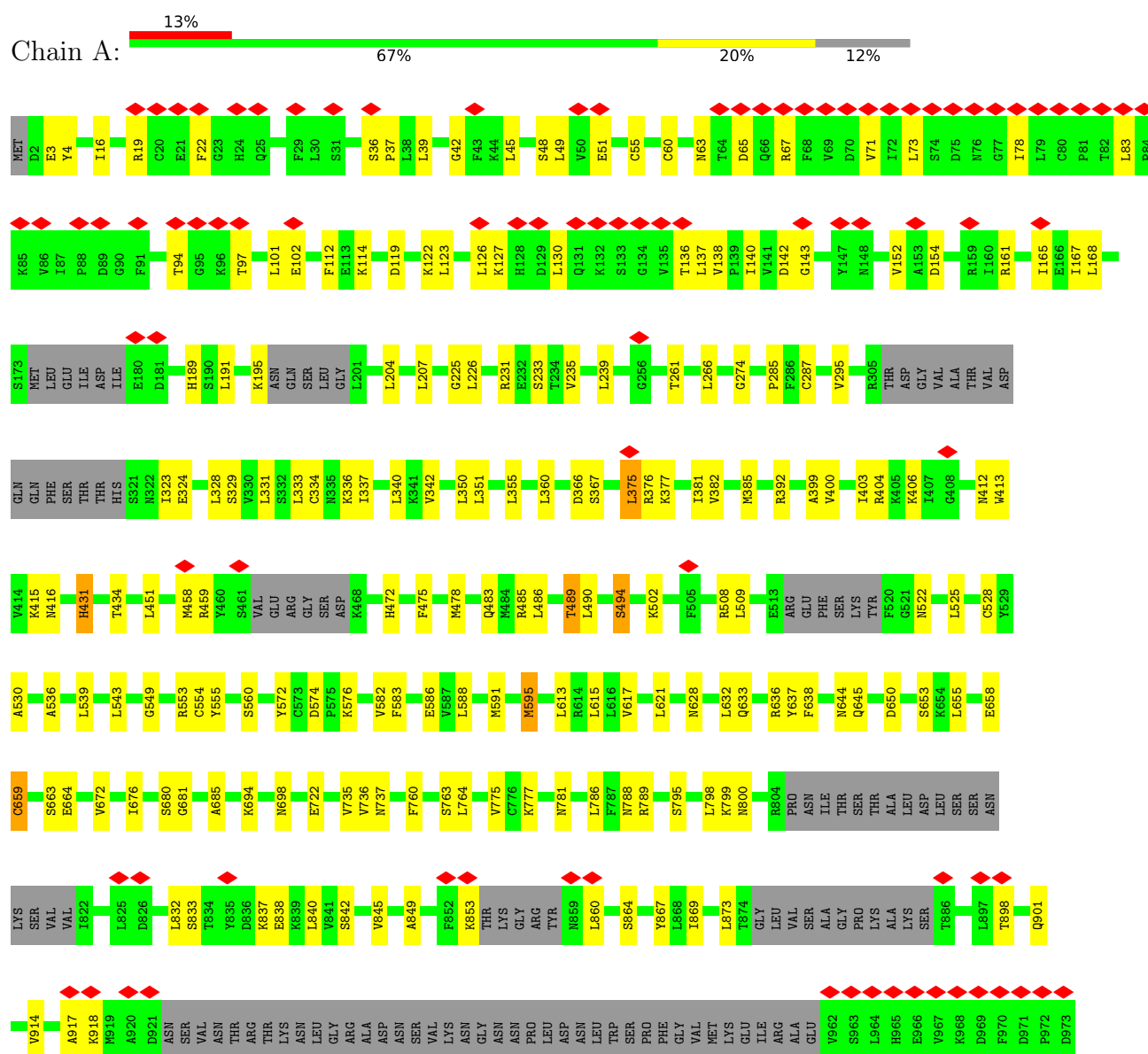
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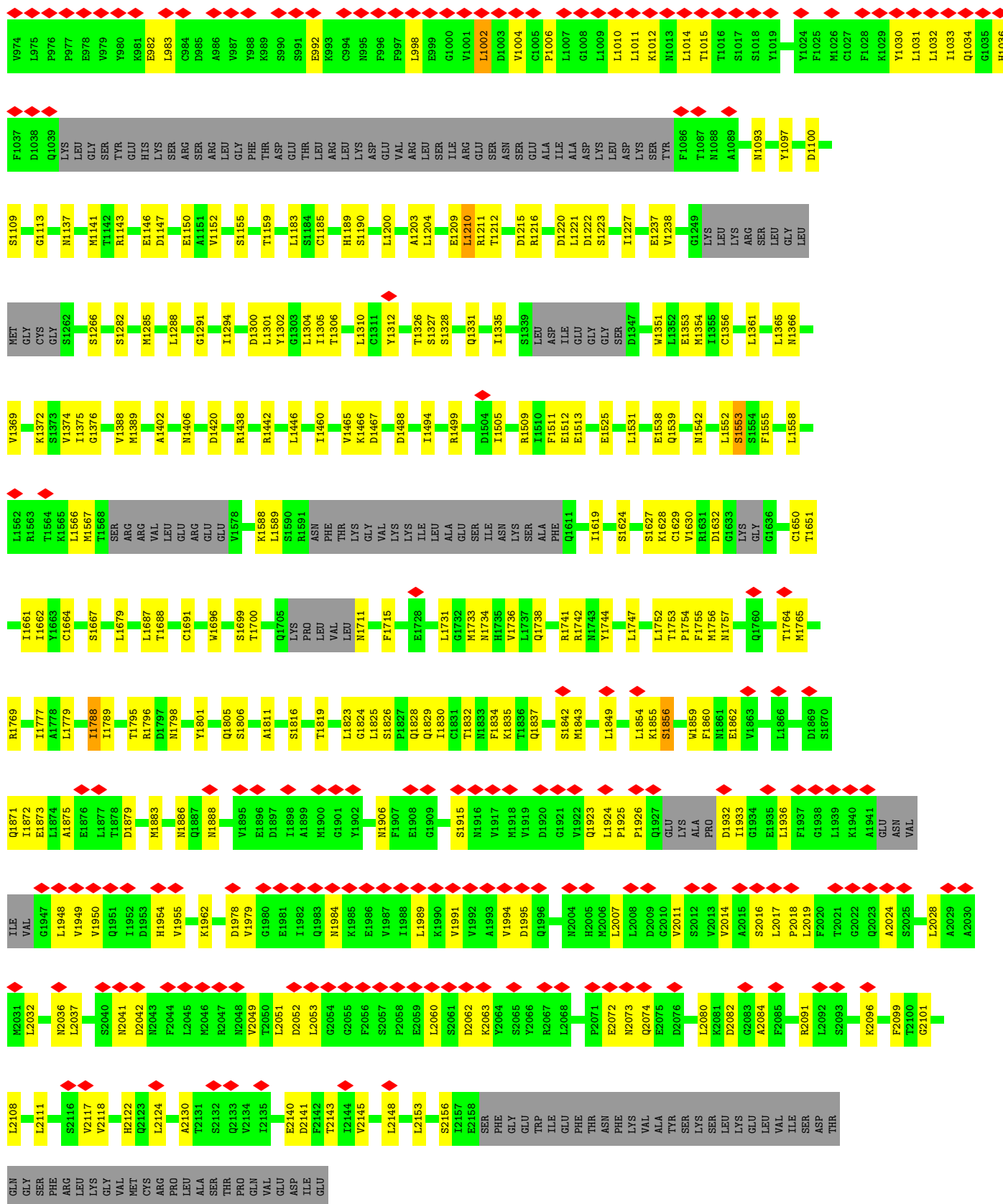
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
4	D	2	2	2	0

3 Residue-property plots

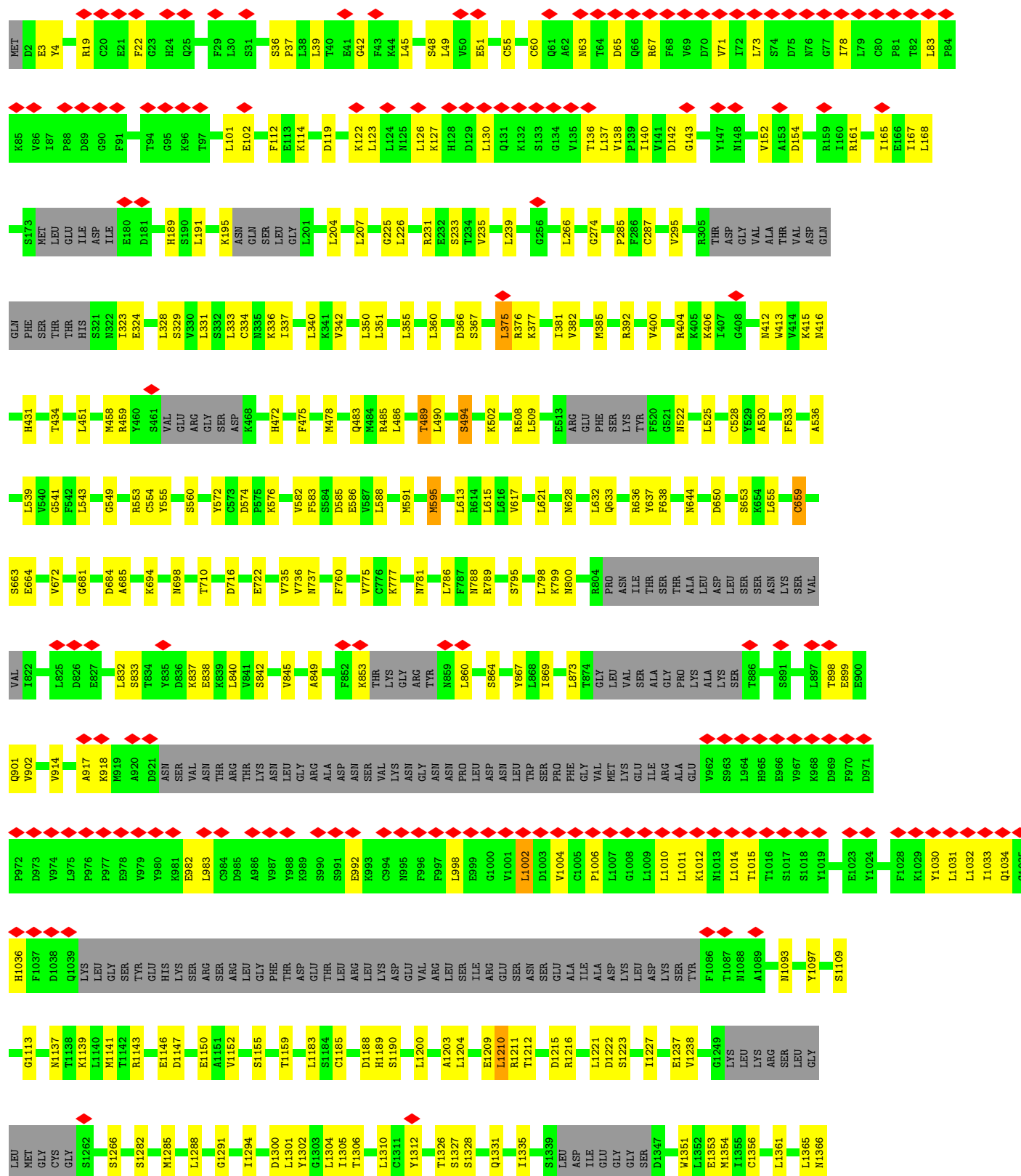
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

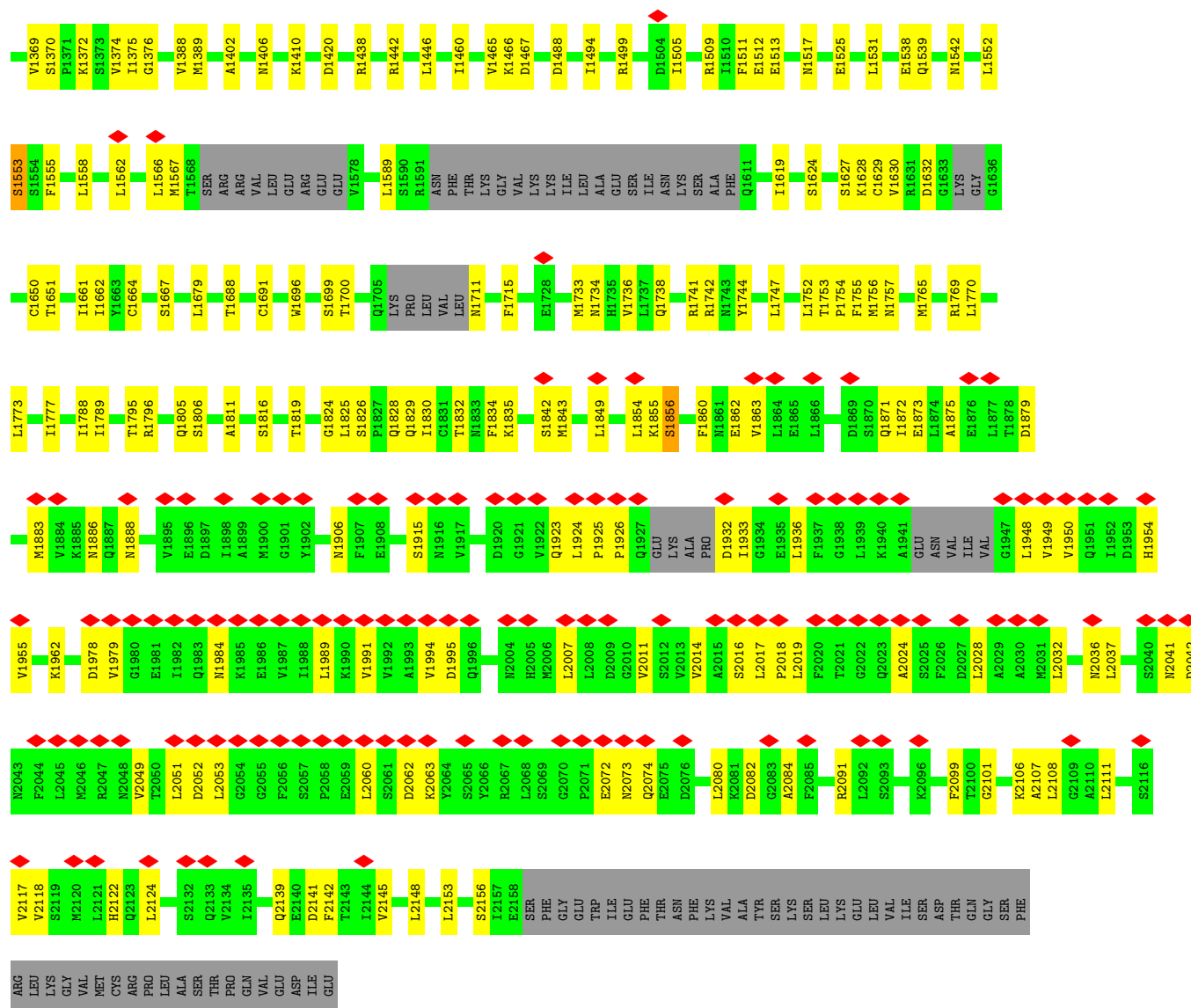
• Molecule 1: RNA-directed RNA polymerase L





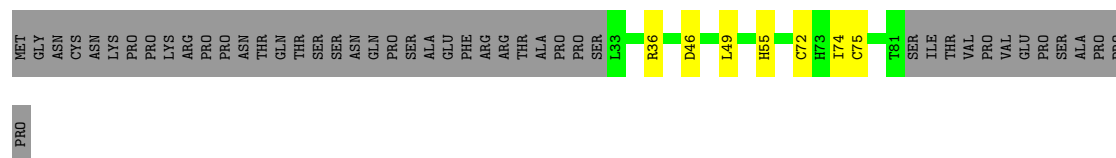
• Molecule 1: RNA-directed RNA polymerase L





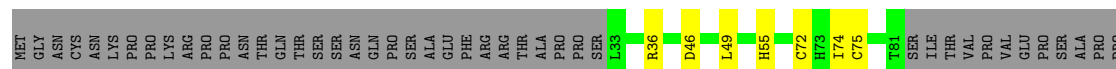
• Molecule 2: RING finger protein Z

Chain B: 45% 7% 48%



• Molecule 2: RING finger protein Z

Chain D: 45% 7% 48%



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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36056	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: MN, 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	A	0.12	0/15349	0.34	2/20744 (0.0%)
1	C	0.12	0/15349	0.33	0/20744
2	B	0.11	0/419	0.36	0/569
2	D	0.11	0/419	0.36	0/569
All	All	0.12	0/31536	0.34	2/42626 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1731	LEU	CA-C-N	6.92	130.16	122.55
1	A	1731	LEU	C-N-CA	6.92	130.16	122.55

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	15094	0	14961	285	0
1	C	15094	0	14961	281	0
2	B	407	0	383	6	0
2	D	407	0	383	6	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
All	All	31012	0	30688	571	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 9.

All (571) 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:C:1011:LEU:HD12	1:C:1034:GLN:HG2	1.60	0.83
1:A:1011:LEU:HD12	1:A:1034:GLN:HG2	1.60	0.81
1:A:1835:LYS:HD3	1:A:1872:ILE:HD12	1.67	0.76
1:C:287:CYS:HB3	1:C:472:HIS:HE1	1.51	0.75
1:A:287:CYS:HB3	1:A:472:HIS:HE1	1.51	0.74
1:C:1835:LYS:HD3	1:C:1872:ILE:HD12	1.67	0.74
1:C:1002:LEU:HD21	1:C:1006:PRO:HD2	1.71	0.73
1:A:412:ASN:O	1:A:416:ASN:ND2	2.23	0.72
1:A:1002:LEU:HD21	1:A:1006:PRO:HD2	1.71	0.72
1:C:412:ASN:O	1:C:416:ASN:ND2	2.23	0.71
1:C:873:LEU:HD22	1:C:1566:LEU:HD11	1.72	0.71
1:C:1886:ASN:HD22	1:C:1888:ASN:H	1.39	0.71
1:A:1886:ASN:HD22	1:A:1888:ASN:H	1.39	0.70
1:A:136:THR:HG21	1:A:918:LYS:HE3	1.74	0.70
1:A:873:LEU:HD22	1:A:1566:LEU:HD11	1.72	0.70
1:C:1552:LEU:HD12	1:C:1630:VAL:HG11	1.75	0.69
1:A:1552:LEU:HD12	1:A:1630:VAL:HG11	1.75	0.68
1:C:136:THR:HG21	1:C:918:LYS:HE3	1.74	0.68
1:C:638:PHE:HB2	1:C:655:LEU:HD21	1.76	0.68
1:A:832:LEU:HG	1:A:837:LYS:HE2	1.76	0.67
1:C:502:LYS:HG2	1:C:1619:ILE:HD12	1.76	0.67
1:A:638:PHE:HB2	1:A:655:LEU:HD21	1.76	0.67
1:C:1738:GLN:NE2	1:C:1765:MET:SD	2.68	0.67
1:A:1004:VAL:HG23	1:A:1006:PRO:HD3	1.77	0.67
1:A:2122:HIS:HB2	1:A:2153:LEU:HD22	1.77	0.67
1:C:832:LEU:HG	1:C:837:LYS:HE2	1.76	0.66
1:C:2111:LEU:HD12	1:C:2117:VAL:HG22	1.77	0.66
1:A:1738:GLN:NE2	1:A:1765:MET:SD	2.68	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1420:ASP:HB2	1:C:1460:ILE:HD11	1.77	0.66
1:A:2111:LEU:HD12	1:A:2117:VAL:HG22	1.76	0.66
1:C:2084:ALA:HB1	1:C:2091:ARG:HG3	1.78	0.66
1:C:2122:HIS:HB2	1:C:2153:LEU:HD22	1.77	0.66
1:A:1420:ASP:HB2	1:A:1460:ILE:HD11	1.77	0.66
1:C:901:GLN:HE22	1:C:1566:LEU:HD13	1.61	0.66
1:A:502:LYS:HG2	1:A:1619:ILE:HD12	1.76	0.65
1:C:323:ILE:HD13	1:C:375:LEU:HD13	1.78	0.65
1:A:2084:ALA:HB1	1:A:2091:ARG:HG3	1.78	0.65
1:C:1979:VAL:HG22	1:C:1994:VAL:HG23	1.79	0.65
1:A:323:ILE:HD13	1:A:375:LEU:HD13	1.78	0.65
1:C:1004:VAL:HG23	1:C:1006:PRO:HD3	1.77	0.65
1:C:1994:VAL:HB	1:C:2053:LEU:HD11	1.78	0.64
1:A:901:GLN:HE22	1:A:1566:LEU:HD13	1.62	0.64
1:C:860:LEU:HA	1:C:1006:PRO:HA	1.79	0.64
1:A:1979:VAL:HG22	1:A:1994:VAL:HG23	1.79	0.64
1:A:231:ARG:HD2	1:A:789:ARG:HH12	1.63	0.64
1:A:1948:LEU:HG	1:A:1950:VAL:HG22	1.80	0.64
1:A:287:CYS:HB3	1:A:472:HIS:CE1	2.32	0.64
1:A:694:LYS:O	1:A:698:ASN:ND2	2.30	0.63
1:C:1948:LEU:HG	1:C:1950:VAL:HG22	1.80	0.63
1:A:1994:VAL:HB	1:A:2053:LEU:HD11	1.78	0.63
1:C:138:VAL:HG11	1:C:845:VAL:HG11	1.79	0.63
1:A:351:LEU:HD13	1:A:406:LYS:HD3	1.80	0.63
1:A:860:LEU:HA	1:A:1006:PRO:HA	1.79	0.63
1:A:138:VAL:HG11	1:A:845:VAL:HG11	1.79	0.63
1:C:1553:SER:O	1:C:1553:SER:OG	2.17	0.63
1:A:65:ASP:HB3	1:A:67:ARG:HD3	1.81	0.63
1:A:998:LEU:HD22	1:A:1012:LYS:HB3	1.80	0.63
1:C:231:ARG:HD2	1:C:789:ARG:HH12	1.63	0.63
1:C:287:CYS:HB3	1:C:472:HIS:CE1	2.32	0.63
1:C:998:LEU:HD22	1:C:1012:LYS:HB3	1.80	0.63
1:C:788:ASN:ND2	1:C:1209:GLU:OE1	2.32	0.62
1:C:1200:LEU:HD22	1:C:1366:ASN:HD22	1.63	0.62
1:C:549:GLY:O	1:C:553:ARG:NH2	2.33	0.62
1:A:788:ASN:ND2	1:A:1209:GLU:OE1	2.32	0.62
1:A:1200:LEU:HD22	1:A:1366:ASN:HD22	1.63	0.61
1:C:351:LEU:HD13	1:C:406:LYS:HD3	1.80	0.61
1:A:1711:ASN:N	1:A:1806:SER:HG	1.99	0.61
1:A:1936:LEU:HD13	1:A:2037:LEU:HD13	1.82	0.61
1:C:65:ASP:HB3	1:C:67:ARG:HD3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:737:ASN:HD21	1:C:1282:SER:H	1.48	0.61
1:A:1566:LEU:HD23	1:A:1567:MET:HE2	1.83	0.61
1:A:1465:VAL:HG22	1:A:1466:LYS:H	1.66	0.61
1:A:549:GLY:O	1:A:553:ARG:NH2	2.33	0.61
1:A:1553:SER:O	1:A:1553:SER:OG	2.17	0.60
1:C:1936:LEU:HD13	1:C:2037:LEU:HD13	1.82	0.60
1:A:1538:GLU:O	1:A:1542:ASN:ND2	2.35	0.60
1:A:832:LEU:HD12	1:A:837:LYS:HG2	1.84	0.60
1:C:1538:GLU:O	1:C:1542:ASN:ND2	2.35	0.60
1:C:1711:ASN:N	1:C:1806:SER:HG	2.00	0.60
1:C:1465:VAL:HG22	1:C:1466:LYS:H	1.66	0.60
1:A:1825:LEU:HG	1:A:1830:ILE:HD11	1.84	0.59
1:A:737:ASN:HD21	1:A:1282:SER:H	1.48	0.59
1:C:694:LYS:O	1:C:698:ASN:ND2	2.30	0.59
1:C:1566:LEU:HD23	1:C:1567:MET:HE2	1.83	0.59
1:C:1494:ILE:HG13	1:C:1679:LEU:HD12	1.85	0.59
1:A:114:LYS:HZ3	1:A:1137:ASN:HB2	1.68	0.59
1:C:1825:LEU:HG	1:C:1830:ILE:HD11	1.84	0.59
1:A:1512:GLU:HB3	1:C:1769:ARG:HD3	1.84	0.58
1:C:485:ARG:O	1:C:489:THR:OG1	2.22	0.58
1:A:1923:GLN:NE2	1:A:2036:ASN:O	2.36	0.58
1:C:83:LEU:HD21	1:C:126:LEU:HD21	1.85	0.58
1:A:1494:ILE:HG13	1:A:1679:LEU:HD12	1.85	0.58
1:A:1764:THR:O	1:C:1517:ASN:ND2	2.36	0.58
1:C:274:GLY:HA3	1:C:672:VAL:HG21	1.86	0.58
1:A:1159:THR:HB	1:A:1304:LEU:HD22	1.85	0.58
1:C:2051:LEU:HD21	1:C:2053:LEU:HD13	1.86	0.58
1:A:539:LEU:HA	1:A:560:SER:O	2.04	0.58
1:A:1210:LEU:HG	1:A:1221:LEU:HD11	1.85	0.58
1:C:1923:GLN:NE2	1:C:2036:ASN:O	2.36	0.57
1:A:1984:ASN:HB3	1:A:1989:LEU:HA	1.87	0.57
1:C:595:MET:HE3	1:C:613:LEU:HD21	1.87	0.57
1:A:595:MET:HE3	1:A:613:LEU:HD21	1.86	0.57
1:C:1210:LEU:HG	1:C:1221:LEU:HD11	1.85	0.57
1:A:83:LEU:HD21	1:A:126:LEU:HD21	1.85	0.57
1:A:225:GLY:O	1:A:781:ASN:ND2	2.37	0.57
1:A:274:GLY:HA3	1:A:672:VAL:HG21	1.86	0.57
1:C:539:LEU:HA	1:C:560:SER:O	2.04	0.57
1:C:832:LEU:HD12	1:C:837:LYS:HG2	1.84	0.57
1:C:1159:THR:HB	1:C:1304:LEU:HD22	1.85	0.57
1:A:485:ARG:O	1:A:489:THR:OG1	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1769:ARG:HD3	1:C:1512:GLU:HB3	1.87	0.57
1:C:1984:ASN:HB3	1:C:1989:LEU:HA	1.87	0.57
1:A:1505:ILE:HG13	1:A:1511:PHE:HB2	1.86	0.57
1:A:1994:VAL:HG21	1:A:2053:LEU:HD21	1.87	0.57
1:A:2141:ASP:O	1:A:2145:VAL:HG23	2.05	0.57
1:A:840:LEU:HD22	1:A:873:LEU:HD21	1.86	0.56
1:C:840:LEU:HD22	1:C:873:LEU:HD21	1.86	0.56
1:A:1465:VAL:HG21	1:A:1811:ALA:HA	1.87	0.56
1:A:1872:ILE:HG13	1:A:1873:GLU:H	1.70	0.56
1:C:1994:VAL:HG21	1:C:2053:LEU:HD21	1.87	0.56
1:A:2051:LEU:HD21	1:A:2053:LEU:HD13	1.86	0.56
1:C:1505:ILE:HG13	1:C:1511:PHE:HB2	1.86	0.56
1:C:2141:ASP:O	1:C:2145:VAL:HG23	2.05	0.56
1:A:508:ARG:HE	1:A:509:LEU:H	1.54	0.56
1:C:225:GLY:O	1:C:781:ASN:ND2	2.37	0.56
1:C:1465:VAL:HG21	1:C:1811:ALA:HA	1.87	0.56
1:C:1152:VAL:O	1:C:1155:SER:OG	2.22	0.56
1:A:1856:SER:O	1:A:1856:SER:OG	2.23	0.55
1:A:1849:LEU:HD11	1:A:2080:LEU:HB2	1.87	0.55
1:A:1402:ALA:O	1:A:1406:ASN:ND2	2.39	0.55
1:A:1650:CYS:SG	1:A:1667:SER:OG	2.65	0.55
1:C:633:GLN:HG2	1:C:636:ARG:HH12	1.71	0.55
1:C:917:ALA:HB2	1:C:1010:LEU:HD22	1.89	0.55
2:D:55:HIS:HE1	2:D:75:CYS:HB3	1.72	0.55
1:A:633:GLN:HG2	1:A:636:ARG:HH12	1.71	0.55
1:A:1555:PHE:HD2	1:A:1632:ASP:HA	1.72	0.55
1:C:508:ARG:HE	1:C:509:LEU:H	1.54	0.55
1:C:650:ASP:OD1	1:C:653:SER:OG	2.21	0.55
1:C:736:VAL:HG22	1:C:737:ASN:H	1.71	0.55
1:C:1650:CYS:SG	1:C:1667:SER:OG	2.65	0.54
1:C:1849:LEU:HD11	1:C:2080:LEU:HB2	1.87	0.54
1:C:1872:ILE:HG13	1:C:1873:GLU:H	1.70	0.54
1:A:644:ASN:HD22	1:A:1374:VAL:HG12	1.72	0.54
1:C:101:LEU:HD11	1:C:142:ASP:HB2	1.90	0.54
1:C:140:ILE:HG12	1:C:842:SER:HB2	1.88	0.54
1:A:1756:MET:HE3	1:A:1757:ASN:H	1.73	0.54
1:C:1555:PHE:HD2	1:C:1632:ASP:HA	1.72	0.54
2:B:55:HIS:HE1	2:B:75:CYS:HB3	1.72	0.54
1:A:736:VAL:HG22	1:A:737:ASN:H	1.71	0.54
1:A:1093:ASN:HA	1:A:1097:TYR:HB3	1.90	0.54
1:A:1661:ILE:HG22	1:A:1662:ILE:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1211:ARG:HD3	1:A:1216:ARG:HD2	1.90	0.54
1:C:664:GLU:N	1:C:664:GLU:OE1	2.41	0.54
1:A:152:VAL:HG13	1:A:154:ASP:H	1.73	0.54
1:C:152:VAL:HG13	1:C:154:ASP:H	1.73	0.54
1:A:628:ASN:O	1:A:632:LEU:HG	2.08	0.54
1:A:917:ALA:HB2	1:A:1010:LEU:HD22	1.89	0.54
1:A:650:ASP:OD1	1:A:653:SER:OG	2.21	0.53
1:A:1829:GLN:HA	1:A:1832:THR:HG22	1.90	0.53
1:A:140:ILE:HG12	1:A:842:SER:HB2	1.88	0.53
1:C:1211:ARG:HD3	1:C:1216:ARG:HD2	1.90	0.53
1:C:1756:MET:HE3	1:C:1757:ASN:H	1.73	0.53
1:A:664:GLU:N	1:A:664:GLU:OE1	2.41	0.53
1:C:588:LEU:HA	1:C:591:MET:HG2	1.91	0.53
1:C:1777:ILE:HG13	1:C:1789:ILE:HG13	1.89	0.53
1:A:101:LEU:HD11	1:A:142:ASP:HB2	1.90	0.53
1:A:1777:ILE:HG13	1:A:1789:ILE:HG13	1.89	0.53
1:C:1402:ALA:O	1:C:1406:ASN:ND2	2.39	0.53
1:A:588:LEU:HA	1:A:591:MET:HG2	1.91	0.53
1:C:628:ASN:O	1:C:632:LEU:HG	2.09	0.53
1:C:1465:VAL:HG13	1:C:1467:ASP:H	1.74	0.53
1:C:644:ASN:HD22	1:C:1374:VAL:HG12	1.72	0.53
1:A:849:ALA:O	1:A:853:LYS:NZ	2.42	0.53
1:C:849:ALA:O	1:C:853:LYS:NZ	2.42	0.53
1:A:1388:VAL:HG12	1:A:1389:MET:H	1.73	0.53
1:C:1664:CYS:SG	1:C:1667:SER:OG	2.64	0.52
1:A:1465:VAL:HG13	1:A:1467:ASP:H	1.74	0.52
1:C:1661:ILE:HG22	1:C:1662:ILE:HG12	1.90	0.52
1:C:1093:ASN:HA	1:C:1097:TYR:HB3	1.90	0.52
1:A:1223:SER:O	1:A:1227:ILE:HG12	2.10	0.52
1:A:1389:MET:HE2	2:B:36:ARG:HE	1.75	0.52
1:C:681:GLY:HA3	1:C:685:ALA:HB2	1.92	0.52
1:C:1011:LEU:O	1:C:1015:THR:HG23	2.10	0.52
1:C:2062:ASP:O	1:C:2063:LYS:HD3	2.10	0.52
1:A:1011:LEU:O	1:A:1015:THR:HG23	2.10	0.52
1:C:1389:MET:HE2	2:D:36:ARG:HE	1.73	0.52
1:C:1738:GLN:HG3	1:C:1741:ARG:HH21	1.75	0.52
1:C:1829:GLN:HA	1:C:1832:THR:HG22	1.90	0.52
1:A:2062:ASP:O	1:A:2063:LYS:HD3	2.10	0.52
1:C:1030:TYR:HD1	1:C:1033:ILE:HD11	1.75	0.52
1:A:1738:GLN:HG3	1:A:1741:ARG:HH21	1.75	0.52
1:C:1388:VAL:HG12	1:C:1389:MET:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:ASP:HA	2:D:49:LEU:HD11	1.91	0.51
1:A:1664:CYS:SG	1:A:1667:SER:OG	2.64	0.51
1:A:681:GLY:HA3	1:A:685:ALA:HB2	1.92	0.51
1:C:1856:SER:O	1:C:1856:SER:OG	2.23	0.51
1:C:1925:PRO:HG2	1:C:1926:PRO:HD3	1.93	0.51
1:C:2099:PHE:HD2	1:C:2101:GLY:H	1.58	0.51
1:A:1030:TYR:HD1	1:A:1033:ILE:HD11	1.75	0.51
1:A:2099:PHE:HD2	1:A:2101:GLY:H	1.59	0.51
2:B:46:ASP:HA	2:B:49:LEU:HD11	1.91	0.51
1:C:36:SER:OG	1:C:37:PRO:HD3	2.11	0.51
1:C:165:ILE:HG23	1:C:191:LEU:HD23	1.93	0.51
1:A:360:LEU:HD13	1:A:434:THR:HG21	1.93	0.51
1:A:2028:LEU:HD12	1:A:2032:LEU:HD21	1.92	0.51
1:C:39:LEU:HD13	1:C:168:LEU:HD11	1.93	0.51
1:C:799:LYS:HG3	1:C:800:ASN:ND2	2.26	0.51
1:C:898:THR:H	1:C:901:GLN:HB2	1.76	0.51
1:C:2028:LEU:HD12	1:C:2032:LEU:HD21	1.92	0.51
1:A:36:SER:OG	1:A:37:PRO:HD3	2.11	0.51
1:A:39:LEU:HD13	1:A:168:LEU:HD11	1.93	0.51
1:A:617:VAL:O	1:A:621:LEU:HG	2.11	0.51
1:C:864:SER:O	1:C:867:TYR:HB3	2.11	0.51
1:C:1855:LYS:HA	1:C:1860:PHE:HD1	1.76	0.51
1:A:400:VAL:O	1:A:404:ARG:HG2	2.11	0.50
1:C:400:VAL:O	1:C:404:ARG:HG2	2.11	0.50
1:A:1925:PRO:HG2	1:A:1926:PRO:HD3	1.93	0.50
1:C:360:LEU:HD13	1:C:434:THR:HG21	1.93	0.50
1:C:722:GLU:CD	1:C:1266:SER:HB3	2.36	0.50
1:A:864:SER:O	1:A:867:TYR:HB3	2.11	0.50
1:A:340:LEU:HB3	1:A:342:VAL:HG13	1.93	0.50
1:C:1699:SER:OG	1:C:1700:THR:N	2.45	0.50
1:A:204:LEU:HD23	1:A:204:LEU:H	1.77	0.50
1:C:1223:SER:O	1:C:1227:ILE:HG12	2.10	0.50
1:A:1855:LYS:HA	1:A:1860:PHE:HD1	1.76	0.50
1:C:617:VAL:O	1:C:621:LEU:HG	2.11	0.50
1:A:334:CYS:HA	1:A:337:ILE:HG22	1.94	0.50
1:A:554:CYS:HB3	1:A:572:TYR:HD1	1.76	0.50
1:A:914:VAL:O	1:A:918:LYS:HE2	2.12	0.50
1:A:1924:LEU:N	1:A:1925:PRO:HD2	2.27	0.50
1:A:1991:VAL:HG21	1:A:2053:LEU:HD12	1.94	0.50
1:A:722:GLU:CD	1:A:1266:SER:HB3	2.36	0.50
1:A:799:LYS:HG3	1:A:800:ASN:ND2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:THR:H	1:A:901:GLN:HB2	1.76	0.50
1:A:1699:SER:OG	1:A:1700:THR:N	2.45	0.50
1:C:1991:VAL:HG21	1:C:2053:LEU:HD12	1.94	0.50
1:A:165:ILE:HG23	1:A:191:LEU:HD23	1.93	0.49
1:C:1924:LEU:N	1:C:1925:PRO:HD2	2.27	0.49
1:A:1826:SER:O	1:A:1829:GLN:N	2.42	0.49
1:C:554:CYS:HB3	1:C:572:TYR:HD1	1.76	0.49
1:C:340:LEU:HB3	1:C:342:VAL:HG13	1.93	0.49
1:A:1152:VAL:O	1:A:1155:SER:OG	2.23	0.49
1:C:114:LYS:HZ3	1:C:1137:ASN:HB2	1.77	0.49
1:C:914:VAL:O	1:C:918:LYS:HE2	2.12	0.49
1:C:334:CYS:HA	1:C:337:ILE:HG22	1.94	0.49
1:C:1109:SER:OG	1:C:1113:GLY:O	2.28	0.48
1:A:285:PRO:HG2	1:A:615:LEU:HD21	1.95	0.48
1:A:1014:LEU:HD13	1:A:1030:TYR:CZ	2.48	0.48
1:C:1715:PHE:HD2	1:C:1805:GLN:HB2	1.78	0.48
1:C:1915:SER:HB2	1:C:1954:HIS:CG	2.48	0.48
1:A:659:CYS:HB2	1:A:664:GLU:HB2	1.96	0.48
1:C:48:SER:HA	1:C:51:GLU:HG2	1.96	0.48
1:C:659:CYS:HB2	1:C:664:GLU:HB2	1.96	0.48
1:C:1014:LEU:HD13	1:C:1030:TYR:CZ	2.48	0.48
1:C:204:LEU:HD23	1:C:204:LEU:H	1.77	0.48
1:A:1627:SER:OG	1:A:1628:LYS:N	2.47	0.48
1:C:1627:SER:OG	1:C:1628:LYS:N	2.47	0.48
1:A:102:GLU:HG3	1:A:123:LEU:HD21	1.95	0.48
1:A:1650:CYS:SG	1:A:1651:THR:N	2.86	0.48
1:A:1915:SER:HB2	1:A:1954:HIS:CG	2.48	0.48
1:A:1948:LEU:HD11	1:A:1950:VAL:HG13	1.94	0.48
1:C:1948:LEU:HD11	1:C:1950:VAL:HG13	1.94	0.48
1:A:2017:LEU:HG	1:A:2018:PRO:HD2	1.96	0.48
1:A:860:LEU:HD11	1:A:1004:VAL:HB	1.96	0.48
1:A:127:LYS:NZ	1:A:137:LEU:O	2.47	0.48
1:A:737:ASN:ND2	1:A:1282:SER:OG	2.47	0.48
1:C:127:LYS:NZ	1:C:137:LEU:O	2.47	0.48
2:D:46:ASP:OD1	2:D:46:ASP:N	2.46	0.48
1:A:1855:LYS:HA	1:A:1860:PHE:CD1	2.49	0.47
1:C:1826:SER:O	1:C:1826:SER:OG	2.32	0.47
1:C:1855:LYS:HA	1:C:1860:PHE:CD1	2.49	0.47
1:A:329:SER:O	1:A:333:LEU:HG	2.14	0.47
1:A:1915:SER:H	1:A:1954:HIS:HB2	1.79	0.47
1:C:336:LYS:O	1:C:336:LYS:NZ	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1711:ASN:N	1:C:1806:SER:OG	2.46	0.47
1:A:1711:ASN:N	1:A:1806:SER:OG	2.46	0.47
2:B:46:ASP:OD1	2:B:46:ASP:N	2.46	0.47
1:C:1915:SER:H	1:C:1954:HIS:HB2	1.79	0.47
1:A:786:LEU:HD21	1:A:1312:TYR:CD2	2.50	0.47
1:C:329:SER:O	1:C:333:LEU:HG	2.14	0.47
1:C:285:PRO:HG2	1:C:615:LEU:HD21	1.95	0.47
1:C:737:ASN:ND2	1:C:1282:SER:OG	2.47	0.47
1:C:1650:CYS:SG	1:C:1651:THR:N	2.86	0.47
1:C:2017:LEU:HG	1:C:2018:PRO:HD2	1.96	0.47
1:A:48:SER:HA	1:A:51:GLU:HG2	1.96	0.47
1:A:1204:LEU:HD22	1:A:1302:TYR:HD1	1.79	0.47
1:A:1512:GLU:HG3	1:A:1513:GLU:HG3	1.97	0.47
1:A:1871:GLN:HA	1:A:1871:GLN:OE1	2.15	0.47
1:C:860:LEU:HD11	1:C:1004:VAL:HB	1.96	0.47
1:C:1189:HIS:NE2	1:C:1331:GLN:OE1	2.48	0.47
1:C:1204:LEU:HD22	1:C:1302:TYR:HD1	1.79	0.47
1:A:490:LEU:O	1:A:494:SER:OG	2.33	0.47
1:A:1220:ASP:OD1	1:A:1220:ASP:N	2.44	0.47
1:A:1715:PHE:HD2	1:A:1805:GLN:HB2	1.78	0.47
1:A:1688:THR:HA	1:A:1691:CYS:SG	2.55	0.47
1:C:483:GLN:HA	1:C:486:LEU:HD12	1.97	0.47
1:C:833:SER:O	1:C:837:LYS:HG3	2.16	0.47
1:C:1211:ARG:HG3	1:C:1216:ARG:HA	1.97	0.47
1:C:1512:GLU:HG3	1:C:1513:GLU:HG3	1.97	0.47
1:C:1688:THR:HA	1:C:1691:CYS:SG	2.55	0.47
1:C:102:GLU:HG3	1:C:123:LEU:HD21	1.95	0.46
1:C:490:LEU:O	1:C:494:SER:OG	2.33	0.46
1:C:2019:LEU:C	1:C:2024:ALA:HA	2.39	0.46
1:A:1189:HIS:NE2	1:A:1331:GLN:OE1	2.48	0.46
1:C:350:LEU:HD22	1:C:392:ARG:HH12	1.80	0.46
1:C:1752:LEU:HG	1:C:1753:THR:HG23	1.97	0.46
1:A:350:LEU:HD22	1:A:392:ARG:HH12	1.80	0.46
1:C:189:HIS:CD2	1:C:195:LYS:HD3	2.51	0.46
1:A:189:HIS:CD2	1:A:195:LYS:HD3	2.51	0.46
1:A:226:LEU:HD21	1:A:1203:ALA:HB1	1.98	0.46
1:C:1310:LEU:HD11	1:C:1361:LEU:HB3	1.97	0.46
1:A:833:SER:O	1:A:837:LYS:HG3	2.16	0.46
1:A:2019:LEU:C	1:A:2024:ALA:HA	2.39	0.46
1:C:324:GLU:O	1:C:328:LEU:HG	2.15	0.46
1:C:355:LEU:HD13	1:C:413:TRP:HZ3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:VAL:O	1:A:239:LEU:HG	2.15	0.46
1:A:355:LEU:HD13	1:A:413:TRP:HZ3	1.81	0.46
1:A:2073:ASN:O	1:A:2074:GLN:HG3	2.16	0.46
1:C:235:VAL:O	1:C:239:LEU:HG	2.15	0.46
1:A:1752:LEU:HG	1:A:1753:THR:HG23	1.97	0.46
1:A:582:VAL:HG22	1:A:583:PHE:CD2	2.51	0.46
1:A:1310:LEU:HD11	1:A:1361:LEU:HB3	1.98	0.46
1:A:1499:ARG:HD3	1:A:1819:THR:HB	1.98	0.46
1:C:582:VAL:HG22	1:C:583:PHE:CD2	2.51	0.46
1:C:684:ASP:OD1	1:C:684:ASP:N	2.44	0.46
1:C:786:LEU:HD21	1:C:1312:TYR:CD2	2.50	0.46
1:A:586:GLU:HG3	1:A:1438:ARG:HD3	1.98	0.45
1:A:1211:ARG:HG3	1:A:1216:ARG:HA	1.97	0.45
1:A:1872:ILE:HD11	1:A:1875:ALA:HB3	1.98	0.45
1:C:543:LEU:HD11	1:C:555:TYR:HB3	1.98	0.45
1:C:1871:GLN:HA	1:C:1871:GLN:OE1	2.15	0.45
1:A:458:MET:HB2	1:A:525:LEU:HD13	1.98	0.45
1:C:586:GLU:HG3	1:C:1438:ARG:HD3	1.98	0.45
1:C:1872:ILE:HD11	1:C:1875:ALA:HB3	1.98	0.45
1:A:323:ILE:HD12	1:A:323:ILE:H	1.80	0.45
1:A:415:LYS:H	1:A:415:LYS:HD2	1.82	0.45
1:A:459:ARG:HD3	1:A:522:ASN:HD21	1.82	0.45
1:A:1109:SER:OG	1:A:1113:GLY:O	2.28	0.45
1:C:458:MET:HB2	1:C:525:LEU:HD13	1.99	0.45
1:C:585:ASP:OD1	1:C:585:ASP:N	2.45	0.45
1:A:324:GLU:O	1:A:328:LEU:HG	2.15	0.45
1:A:775:VAL:HG23	1:A:1365:LEU:HA	1.97	0.45
1:C:459:ARG:HD3	1:C:522:ASN:HD21	1.82	0.45
1:C:1558:LEU:HD12	1:C:1629:CYS:HB2	1.98	0.45
1:C:2073:ASN:O	1:C:2074:GLN:HG3	2.16	0.45
1:A:55:CYS:C	1:A:60:CYS:HB2	2.42	0.45
1:A:483:GLN:HA	1:A:486:LEU:HD12	1.97	0.45
1:C:525:LEU:HD23	1:C:528:CYS:SG	2.56	0.45
1:A:663:SER:OG	1:A:664:GLU:OE1	2.34	0.45
1:C:1499:ARG:HD3	1:C:1819:THR:HB	1.98	0.45
2:B:55:HIS:CE1	2:B:75:CYS:HB3	2.52	0.45
1:C:55:CYS:C	1:C:60:CYS:HB2	2.42	0.45
1:C:1488:ASP:OD1	1:C:1488:ASP:N	2.50	0.45
1:A:543:LEU:HD11	1:A:555:TYR:HB3	1.98	0.45
1:A:63:ASN:OD1	1:A:67:ARG:NH1	2.50	0.45
1:A:1566:LEU:HG	1:A:1567:MET:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1742:ARG:HH22	1:A:1769:ARG:H	1.64	0.45
1:A:2096:LYS:NZ	1:A:2130:ALA:O	2.38	0.45
1:C:1742:ARG:HH22	1:C:1769:ARG:H	1.64	0.45
1:C:1826:SER:O	1:C:1829:GLN:N	2.42	0.45
1:C:415:LYS:H	1:C:415:LYS:HD2	1.82	0.44
2:D:55:HIS:CE1	2:D:75:CYS:HB3	2.52	0.44
1:A:2118:VAL:HA	1:A:2153:LEU:HD11	1.99	0.44
1:C:204:LEU:HB2	1:C:207:LEU:HD23	1.99	0.44
1:C:226:LEU:HD21	1:C:1203:ALA:HB1	1.98	0.44
1:C:2060:LEU:HD23	1:C:2060:LEU:H	1.82	0.44
1:C:2108:LEU:HD22	1:C:2117:VAL:HG13	1.99	0.44
1:C:2118:VAL:HA	1:C:2153:LEU:HD11	1.99	0.44
1:A:2060:LEU:H	1:A:2060:LEU:HD23	1.82	0.44
1:C:63:ASN:OD1	1:C:67:ARG:NH1	2.50	0.44
1:C:323:ILE:HD12	1:C:323:ILE:H	1.80	0.44
1:C:1955:VAL:HB	1:C:1979:VAL:HB	2.00	0.44
1:A:377:LYS:HE2	1:A:451:LEU:HD22	1.99	0.44
1:A:525:LEU:HD23	1:A:528:CYS:SG	2.56	0.44
1:C:586:GLU:O	1:C:1438:ARG:NH2	2.43	0.44
1:C:775:VAL:HG23	1:C:1365:LEU:HA	1.97	0.44
1:C:1353:GLU:HA	1:C:1356:CYS:SG	2.58	0.44
1:C:1842:SER:HB2	1:C:2080:LEU:HG	1.99	0.44
1:C:42:GLY:O	1:C:45:LEU:HG	2.18	0.44
1:C:475:PHE:HA	1:C:478:MET:HG3	1.99	0.44
1:C:1291:GLY:HA3	1:C:1294:ILE:HD12	2.00	0.44
1:A:1488:ASP:OD1	1:A:1488:ASP:N	2.50	0.44
1:A:1842:SER:HB2	1:A:2080:LEU:HG	1.99	0.44
1:C:1843:MET:HG2	1:C:2082:ASP:HA	2.00	0.44
1:A:204:LEU:HB2	1:A:207:LEU:HD23	1.98	0.44
1:A:1742:ARG:NH2	1:A:1769:ARG:H	2.16	0.44
1:A:2028:LEU:HD22	1:A:2049:VAL:HG22	1.99	0.44
1:C:663:SER:OG	1:C:664:GLU:OE1	2.34	0.44
1:C:1862:GLU:HG2	1:C:1871:GLN:HE22	1.83	0.44
1:A:1291:GLY:HA3	1:A:1294:ILE:HD12	2.00	0.44
1:C:119:ASP:HA	1:C:122:LYS:HE3	2.00	0.44
1:C:377:LYS:HE2	1:C:451:LEU:HD22	1.99	0.44
1:C:536:ALA:HB3	1:C:539:LEU:HG	1.99	0.44
1:C:1326:THR:HA	1:C:1331:GLN:HG3	1.99	0.44
1:C:1742:ARG:NH2	1:C:1769:ARG:H	2.16	0.44
1:A:1212:THR:OG1	1:A:1216:ARG:N	2.50	0.44
1:A:2108:LEU:HD22	1:A:2117:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2117:VAL:HG11	1:A:2148:LEU:HD13	2.00	0.44
1:C:1948:LEU:HD12	1:C:1949:VAL:H	1.83	0.44
1:C:2011:VAL:HA	1:C:2014:VAL:HG12	2.00	0.44
1:A:1843:MET:HG2	1:A:2082:ASP:HA	2.00	0.43
1:A:1955:VAL:HB	1:A:1979:VAL:HB	2.00	0.43
1:C:4:TYR:HB2	1:C:167:ILE:HD11	1.99	0.43
1:A:4:TYR:HB2	1:A:167:ILE:HD11	1.99	0.43
1:A:1288:LEU:H	1:A:1288:LEU:HD23	1.83	0.43
1:A:1305:ILE:HG13	1:A:1306:THR:N	2.33	0.43
1:A:2011:VAL:HA	1:A:2014:VAL:HG12	2.00	0.43
1:A:2017:LEU:HB3	1:A:2019:LEU:HG	2.01	0.43
1:A:42:GLY:O	1:A:45:LEU:HG	2.18	0.43
1:A:536:ALA:HB3	1:A:539:LEU:HG	1.99	0.43
1:A:1558:LEU:HD12	1:A:1629:CYS:HB2	1.99	0.43
1:A:1906:ASN:HD21	1:A:1962:LYS:HB2	1.83	0.43
1:C:1212:THR:OG1	1:C:1216:ARG:N	2.51	0.43
1:C:1505:ILE:O	1:C:1509:ARG:NH1	2.51	0.43
1:C:1824:GLY:C	1:C:1825:LEU:HD22	2.43	0.43
1:A:295:VAL:HG23	1:A:489:THR:HB	2.00	0.43
1:A:1143:ARG:O	1:A:1146:GLU:HG2	2.19	0.43
1:A:1826:SER:O	1:A:1828:GLN:N	2.51	0.43
1:A:1862:GLU:HG2	1:A:1871:GLN:HE22	1.83	0.43
1:C:295:VAL:HG23	1:C:489:THR:HB	2.00	0.43
1:C:1566:LEU:HG	1:C:1567:MET:HG3	1.99	0.43
1:C:67:ARG:HB2	1:C:71:VAL:HG11	2.01	0.43
1:C:1327:SER:O	1:C:1328:SER:OG	2.37	0.43
1:C:1351:TRP:HB3	1:C:1354:MET:HE2	2.00	0.43
1:C:1826:SER:O	1:C:1828:GLN:N	2.51	0.43
1:C:2028:LEU:HD22	1:C:2049:VAL:HG22	1.99	0.43
1:A:676:ILE:O	1:A:680:SER:OG	2.36	0.43
1:A:1238:VAL:HG22	1:A:1282:SER:HA	2.01	0.43
1:A:1326:THR:HA	1:A:1331:GLN:HG3	1.99	0.43
1:A:1824:GLY:C	1:A:1825:LEU:HD22	2.43	0.43
1:A:1835:LYS:HA	1:A:1835:LYS:HD2	1.81	0.43
1:C:1143:ARG:O	1:C:1146:GLU:HG2	2.19	0.43
1:A:266:LEU:HD12	1:A:638:PHE:CE1	2.54	0.43
1:A:475:PHE:HA	1:A:478:MET:HG3	2.00	0.43
1:A:1505:ILE:O	1:A:1509:ARG:NH1	2.51	0.43
1:C:1300:ASP:OD1	1:C:1328:SER:HB3	2.19	0.43
1:C:1566:LEU:HG	1:C:1567:MET:N	2.34	0.43
1:A:119:ASP:HA	1:A:122:LYS:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1353:GLU:HA	1:A:1356:CYS:SG	2.58	0.43
1:A:1879:ASP:O	1:A:1883:MET:HG2	2.19	0.43
1:C:530:ALA:HA	1:C:543:LEU:O	2.19	0.43
1:C:366:ASP:OD1	1:C:367:SER:N	2.52	0.42
1:C:982:GLU:HG2	1:C:983:LEU:HD22	2.00	0.42
1:C:1185:CYS:HB3	1:C:1375:ILE:HG13	2.01	0.42
1:C:1305:ILE:HG13	1:C:1306:THR:N	2.33	0.42
1:C:2017:LEU:HB3	1:C:2019:LEU:HG	2.01	0.42
1:A:735:VAL:HG22	1:A:1285:MET:O	2.18	0.42
1:C:2117:VAL:HG11	1:C:2148:LEU:HD13	2.00	0.42
1:A:530:ALA:HA	1:A:543:LEU:O	2.19	0.42
1:A:1300:ASP:OD1	1:A:1328:SER:HB3	2.19	0.42
1:A:2140:GLU:O	1:A:2143:THR:OG1	2.30	0.42
1:C:735:VAL:HG22	1:C:1285:MET:O	2.18	0.42
1:C:1183:LEU:HB3	1:C:1335:ILE:HB	2.01	0.42
1:C:1733:MET:HG3	1:C:1734:ASN:H	1.83	0.42
1:C:1835:LYS:HA	1:C:1835:LYS:HD2	1.81	0.42
1:A:982:GLU:HG2	1:A:983:LEU:HD22	2.00	0.42
1:A:1147:ASP:O	1:A:1150:GLU:HG2	2.20	0.42
1:A:1798:ASN:ND2	1:A:1801:TYR:OH	2.44	0.42
1:A:1834:PHE:HZ	1:A:1854:LEU:HD12	1.84	0.42
2:B:72:CYS:SG	2:B:74:ILE:HG22	2.60	0.42
1:C:1237:GLU:N	1:C:1237:GLU:OE1	2.52	0.42
1:C:1906:ASN:HD21	1:C:1962:LYS:HB2	1.83	0.42
2:D:72:CYS:SG	2:D:74:ILE:HG22	2.60	0.42
1:A:366:ASP:OD1	1:A:367:SER:N	2.52	0.42
1:A:406:LYS:HE2	1:A:406:LYS:HB2	1.90	0.42
1:A:1100:ASP:OD1	1:A:1100:ASP:N	2.50	0.42
1:A:1948:LEU:HD12	1:A:1949:VAL:H	1.83	0.42
1:C:83:LEU:HD22	1:C:130:LEU:HD13	2.02	0.42
1:C:1879:ASP:O	1:C:1883:MET:HG2	2.19	0.42
1:C:1978:ASP:OD2	1:C:1995:ASP:HB3	2.20	0.42
1:A:67:ARG:HB2	1:A:71:VAL:HG11	2.01	0.42
1:A:637:TYR:CZ	1:A:1372:LYS:HD2	2.55	0.42
1:A:1442:ARG:O	1:A:1446:LEU:HD23	2.19	0.42
1:A:1566:LEU:HG	1:A:1567:MET:N	2.34	0.42
1:A:1237:GLU:N	1:A:1237:GLU:OE1	2.52	0.42
1:C:161:ARG:O	1:C:165:ILE:HG12	2.20	0.42
1:A:1795:THR:HG22	1:A:1796:ARG:H	1.85	0.42
1:A:2032:LEU:HD23	1:A:2032:LEU:H	1.85	0.42
1:C:266:LEU:HD12	1:C:638:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:644:ASN:CG	1:C:1376:GLY:HA3	2.45	0.42
1:C:1139:LYS:HE3	1:C:1139:LYS:HB2	1.90	0.42
1:C:1238:VAL:HG22	1:C:1282:SER:HA	2.01	0.42
1:C:1834:PHE:HZ	1:C:1854:LEU:HD12	1.84	0.42
1:A:336:LYS:O	1:A:336:LYS:NZ	2.43	0.42
1:A:1183:LEU:HB3	1:A:1335:ILE:HB	2.01	0.42
1:A:1539:GLN:HA	1:A:1542:ASN:HD21	1.85	0.42
1:C:376:ARG:O	1:C:381:ILE:HG22	2.20	0.42
1:C:1011:LEU:HG	1:C:1034:GLN:HE21	1.85	0.42
1:C:1288:LEU:HD23	1:C:1288:LEU:H	1.83	0.42
1:C:1539:GLN:HA	1:C:1542:ASN:HD21	1.85	0.42
1:C:1795:THR:HG22	1:C:1796:ARG:H	1.85	0.42
1:A:1200:LEU:HD21	1:A:1302:TYR:CZ	2.55	0.42
1:C:574:ASP:OD2	1:C:576:LYS:HG2	2.20	0.42
1:C:1147:ASP:O	1:C:1150:GLU:HG2	2.20	0.42
1:A:119:ASP:HA	1:A:122:LYS:HG2	2.02	0.41
1:A:376:ARG:O	1:A:381:ILE:HG22	2.20	0.41
1:A:1351:TRP:HB3	1:A:1354:MET:HE2	2.00	0.41
1:C:710:THR:OG1	1:C:716:ASP:OD2	2.31	0.41
1:C:1200:LEU:HD21	1:C:1302:TYR:CZ	2.55	0.41
1:C:1442:ARG:O	1:C:1446:LEU:HD23	2.19	0.41
1:C:2032:LEU:HD23	1:C:2032:LEU:H	1.84	0.41
1:A:1978:ASP:OD2	1:A:1995:ASP:HB3	2.20	0.41
1:A:2017:LEU:C	1:A:2019:LEU:H	2.28	0.41
1:C:112:PHE:HE1	1:C:143:GLY:HA3	1.85	0.41
1:C:382:VAL:HG23	1:C:385:MET:HB2	2.01	0.41
1:A:382:VAL:HG23	1:A:385:MET:HB2	2.01	0.41
1:A:1011:LEU:HG	1:A:1034:GLN:HE21	1.85	0.41
1:A:1185:CYS:HB3	1:A:1375:ILE:HG13	2.01	0.41
1:A:1588:LYS:HE3	1:A:1588:LYS:HB3	1.96	0.41
1:C:1420:ASP:CB	1:C:1460:ILE:HD11	2.49	0.41
1:C:637:TYR:CZ	1:C:1372:LYS:HD2	2.55	0.41
1:C:1410:LYS:HD2	1:C:1562:LEU:HD12	2.03	0.41
1:A:83:LEU:HD22	1:A:130:LEU:HD13	2.02	0.41
1:A:644:ASN:CG	1:A:1376:GLY:HA3	2.45	0.41
1:C:1738:GLN:NE2	1:C:1765:MET:HA	2.36	0.41
1:C:1744:TYR:HB3	1:C:1747:LEU:HB3	2.02	0.41
1:A:161:ARG:O	1:A:165:ILE:HG12	2.20	0.41
1:A:1744:TYR:HB3	1:A:1747:LEU:HB3	2.02	0.41
1:A:1823:LEU:HD21	1:C:2107:ALA:HB2	2.03	0.41
1:A:2041:ASN:OD1	1:A:2042:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:760:PHE:HB3	1:C:777:LYS:HE3	2.03	0.41
1:C:2017:LEU:HD23	1:C:2019:LEU:HD23	2.02	0.41
1:A:112:PHE:HE1	1:A:143:GLY:HA3	1.85	0.41
1:A:1837:GLN:NE2	1:A:1859:TRP:HB2	2.36	0.41
1:C:73:LEU:HD12	1:C:78:ILE:HG21	2.03	0.41
1:C:899:GLU:O	1:C:902:VAL:HG12	2.21	0.41
1:C:1696:TRP:HA	1:C:1816:SER:OG	2.21	0.41
1:A:19:ARG:H	1:A:22:PHE:HD2	1.68	0.41
1:A:2007:LEU:HD21	1:A:2063:LYS:O	2.21	0.41
1:C:2041:ASN:OD1	1:C:2042:ASP:N	2.53	0.41
1:C:2139:GLN:O	1:C:2142:PHE:N	2.49	0.41
1:A:94:THR:O	1:A:97:THR:OG1	2.36	0.41
1:A:261:THR:HG23	1:A:645:GLN:O	2.21	0.41
1:A:431:HIS:ND1	1:A:431:HIS:N	2.69	0.41
1:A:760:PHE:HB3	1:A:777:LYS:HE3	2.03	0.41
1:A:1137:ASN:O	1:A:1141:MET:HG2	2.21	0.41
1:A:1525:GLU:H	1:A:1525:GLU:CD	2.29	0.41
1:A:1733:MET:HG3	1:A:1734:ASN:H	1.86	0.41
1:C:1589:LEU:HB2	1:C:1755:PHE:HE2	1.85	0.41
1:C:2017:LEU:C	1:C:2019:LEU:H	2.28	0.41
1:A:1420:ASP:CB	1:A:1460:ILE:HD11	2.49	0.41
1:A:1696:TRP:HA	1:A:1816:SER:OG	2.21	0.41
1:A:1932:ASP:CG	1:A:1933:ILE:H	2.29	0.41
1:C:1860:PHE:CE2	1:C:1862:GLU:HB2	2.56	0.41
1:C:1932:ASP:CG	1:C:1933:ILE:H	2.29	0.41
1:A:1388:VAL:HG12	1:A:1389:MET:N	2.36	0.40
1:A:1589:LEU:HB2	1:A:1755:PHE:HE2	1.86	0.40
1:A:1752:LEU:C	1:A:1754:PRO:HD3	2.46	0.40
1:A:1753:THR:N	1:A:1754:PRO:HD3	2.36	0.40
1:C:1525:GLU:CD	1:C:1525:GLU:H	2.29	0.40
1:A:574:ASP:OD2	1:A:576:LYS:HG2	2.20	0.40
1:A:586:GLU:O	1:A:1438:ARG:NH2	2.43	0.40
1:A:763:SER:OG	1:A:764:LEU:N	2.54	0.40
1:A:1327:SER:O	1:A:1328:SER:OG	2.37	0.40
1:A:1823:LEU:HA	1:C:2106:LYS:HG2	2.03	0.40
1:C:19:ARG:H	1:C:22:PHE:HD2	1.68	0.40
1:C:1752:LEU:C	1:C:1754:PRO:HD3	2.46	0.40
1:A:73:LEU:HD12	1:A:78:ILE:HG21	2.03	0.40
1:A:1688:THR:HG22	1:A:1788:ILE:HD12	2.04	0.40
1:C:119:ASP:HA	1:C:122:LYS:HG2	2.02	0.40
1:C:1188:ASP:O	1:C:1370:SER:OG	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1871:GLN:NE2	1:C:1872:ILE:HG12	2.36	0.40
1:C:2007:LEU:HD21	1:C:2063:LYS:O	2.21	0.40
1:A:399:ALA:O	1:A:403:ILE:HG12	2.21	0.40
1:A:658:GLU:CD	1:A:658:GLU:H	2.30	0.40
1:C:533:PHE:CZ	1:C:541:GLY:HA3	2.57	0.40
1:C:1770:LEU:HB2	1:C:1773:LEU:HB3	2.04	0.40
1:C:1863:VAL:HG12	1:C:1883:MET:HE1	2.03	0.40
1:A:16:ILE:O	1:A:16:ILE:HG13	2.21	0.40
1:A:1687:LEU:HD23	1:A:1779:LEU:HD11	2.03	0.40
1:C:1137:ASN:O	1:C:1141:MET:HG2	2.21	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	1899/2209 (86%)	1744 (92%)	155 (8%)	0	100	100
1	C	1899/2209 (86%)	1744 (92%)	155 (8%)	0	100	100
2	B	47/94 (50%)	34 (72%)	13 (28%)	0	100	100
2	D	47/94 (50%)	34 (72%)	13 (28%)	0	100	100
All	All	3892/4606 (84%)	3556 (91%)	336 (9%)	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	1690/2007 (84%)	1654 (98%)	36 (2%)	47	65
1	C	1690/2007 (84%)	1654 (98%)	36 (2%)	47	65
2	B	47/88 (53%)	47 (100%)	0	100	100
2	D	47/88 (53%)	47 (100%)	0	100	100
All	All	3474/4190 (83%)	3402 (98%)	72 (2%)	46	65

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	49	LEU
1	A	233	SER
1	A	331	LEU
1	A	375	LEU
1	A	431	HIS
1	A	489	THR
1	A	494	SER
1	A	595	MET
1	A	659	CYS
1	A	795	SER
1	A	798	LEU
1	A	838	GLU
1	A	869	ILE
1	A	992	GLU
1	A	1002	LEU
1	A	1031	LEU
1	A	1032	LEU
1	A	1036	HIS
1	A	1190	SER
1	A	1210	LEU
1	A	1215	ASP
1	A	1222	ASP
1	A	1301	LEU
1	A	1369	VAL
1	A	1531	LEU
1	A	1553	SER
1	A	1624	SER
1	A	1736	VAL
1	A	1788	ILE

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Mol	Chain	Res	Type
1	A	1856	SER
1	A	2016	SER
1	A	2052	ASP
1	A	2072	GLU
1	A	2124	LEU
1	A	2156	SER
1	C	3	GLU
1	C	49	LEU
1	C	233	SER
1	C	331	LEU
1	C	375	LEU
1	C	431	HIS
1	C	489	THR
1	C	494	SER
1	C	595	MET
1	C	659	CYS
1	C	795	SER
1	C	798	LEU
1	C	838	GLU
1	C	869	ILE
1	C	992	GLU
1	C	1002	LEU
1	C	1031	LEU
1	C	1032	LEU
1	C	1036	HIS
1	C	1190	SER
1	C	1210	LEU
1	C	1215	ASP
1	C	1222	ASP
1	C	1301	LEU
1	C	1369	VAL
1	C	1531	LEU
1	C	1553	SER
1	C	1624	SER
1	C	1736	VAL
1	C	1788	ILE
1	C	1856	SER
1	C	2016	SER
1	C	2052	ASP
1	C	2072	GLU
1	C	2124	LEU
1	C	2156	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	HIS
1	A	288	ASN
1	A	335	ASN
1	A	431	HIS
1	A	512	ASN
1	A	522	ASN
1	A	568	GLN
1	A	628	ASN
1	A	647	HIS
1	A	737	ASN
1	A	771	GLN
1	A	788	ASN
1	A	872	ASN
1	A	901	GLN
1	A	1124	GLN
1	A	1128	ASN
1	A	1206	GLN
1	A	1272	GLN
1	A	1292	GLN
1	A	1308	GLN
1	A	1414	GLN
1	A	1496	ASN
1	A	1517	ASN
1	A	1539	GLN
1	A	1542	ASN
1	A	1611	GLN
1	A	1669	ASN
1	A	1738	GLN
1	A	1829	GLN
1	A	1837	GLN
1	A	1871	GLN
1	A	1886	ASN
1	A	1888	ASN
1	A	2043	ASN
1	A	2073	ASN
1	A	2146	HIS
2	B	73	HIS
1	C	288	ASN
1	C	335	ASN
1	C	512	ASN
1	C	522	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	568	GLN
1	C	628	ASN
1	C	647	HIS
1	C	737	ASN
1	C	771	GLN
1	C	788	ASN
1	C	872	ASN
1	C	901	GLN
1	C	1039	GLN
1	C	1124	GLN
1	C	1128	ASN
1	C	1154	ASN
1	C	1206	GLN
1	C	1272	GLN
1	C	1292	GLN
1	C	1308	GLN
1	C	1414	GLN
1	C	1496	ASN
1	C	1542	ASN
1	C	1611	GLN
1	C	1669	ASN
1	C	1738	GLN
1	C	1829	GLN
1	C	1837	GLN
1	C	1871	GLN
1	C	1886	ASN
1	C	1888	ASN
1	C	2073	ASN
1	C	2146	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 10 are 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

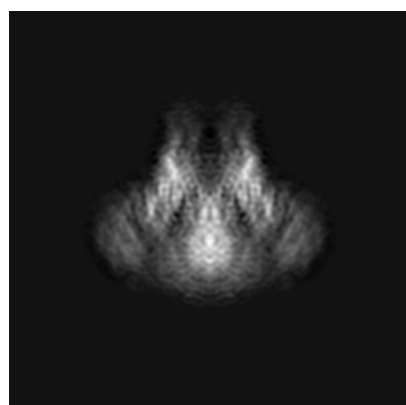
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31179. These allow visual inspection of the internal detail of the map and identification of artifacts.

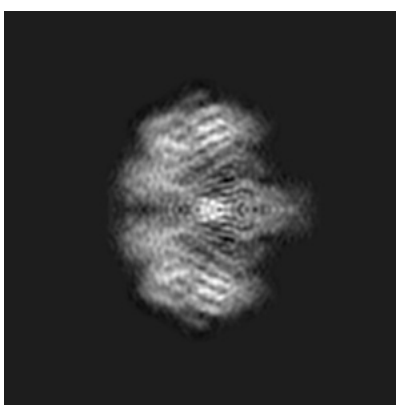
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

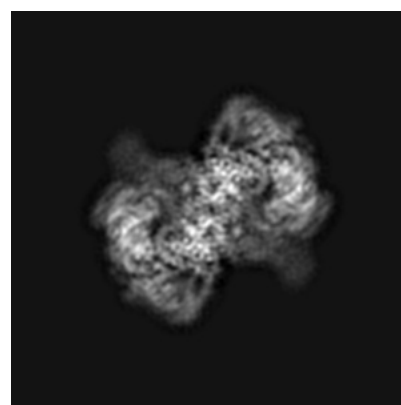
6.1.1 Primary map



X



Y



Z

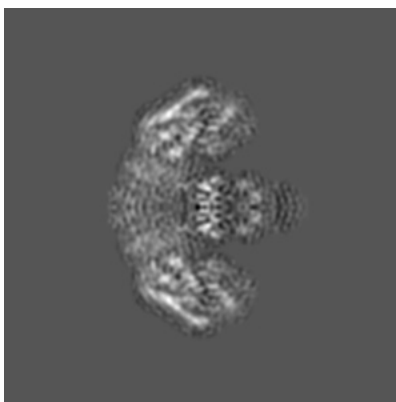
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

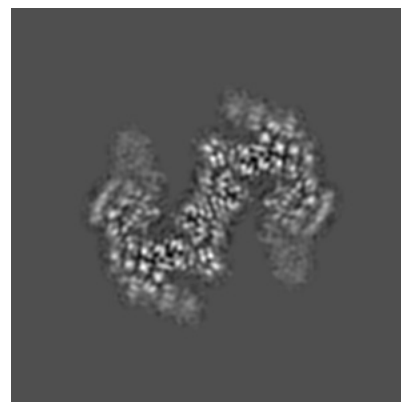
6.2.1 Primary map



X Index: 128



Y Index: 128

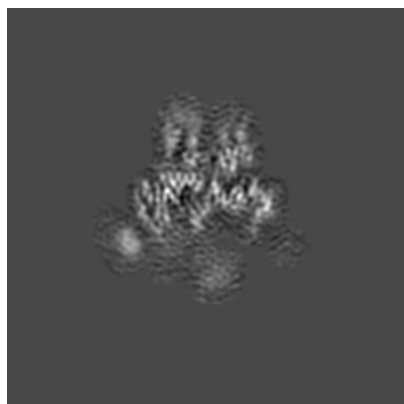


Z Index: 128

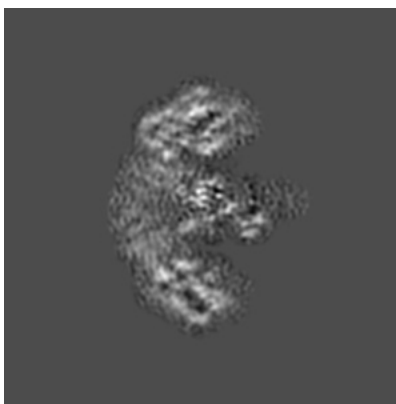
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

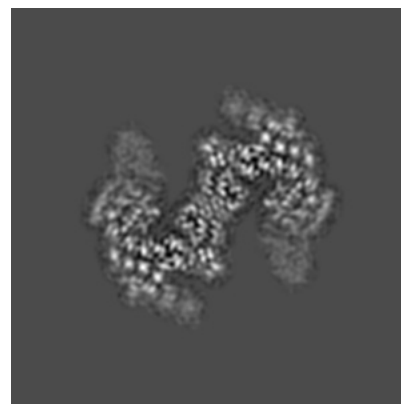
6.3.1 Primary map



X Index: 125



Y Index: 131

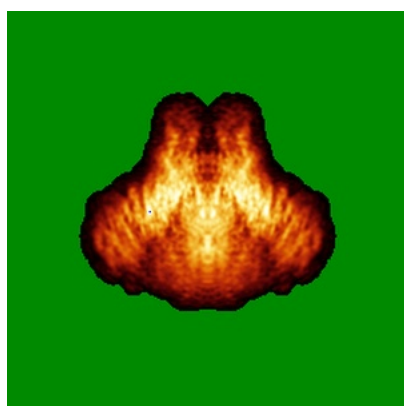


Z Index: 129

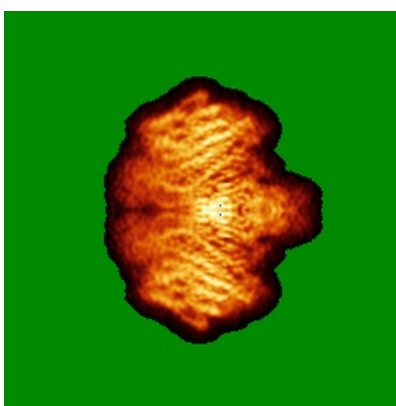
The images above show the largest variance slices of the map in three orthogonal directions.

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

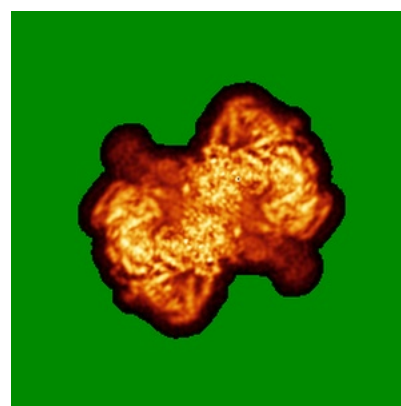
6.4.1 Primary map



X



Y

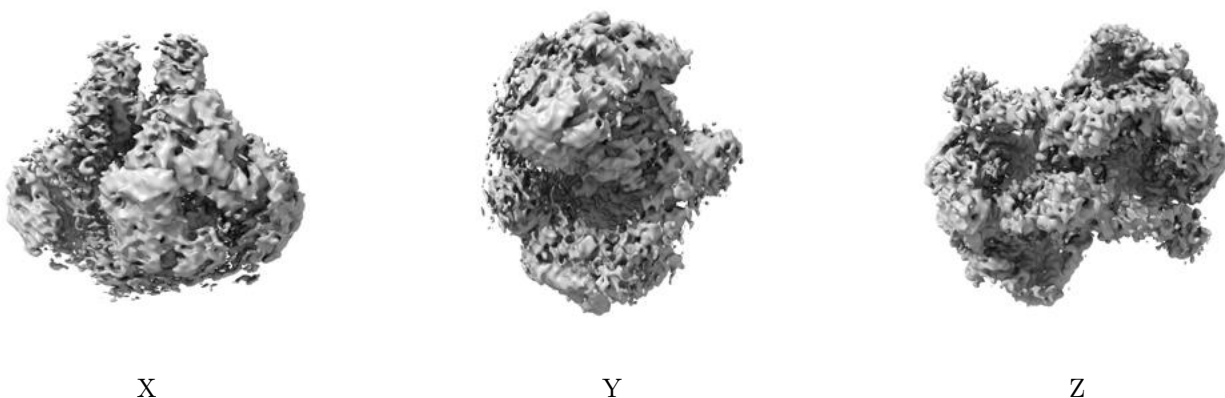


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

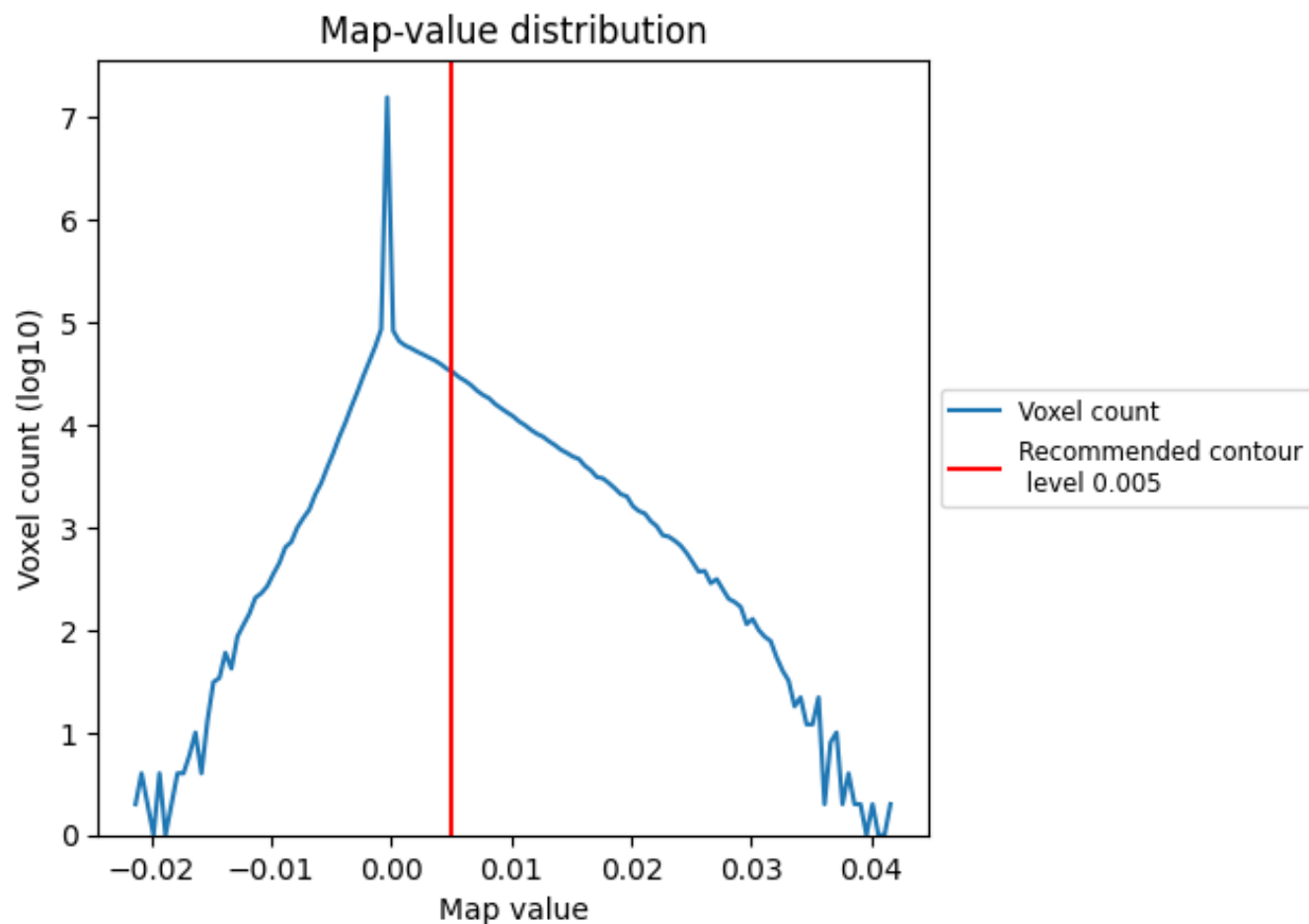
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

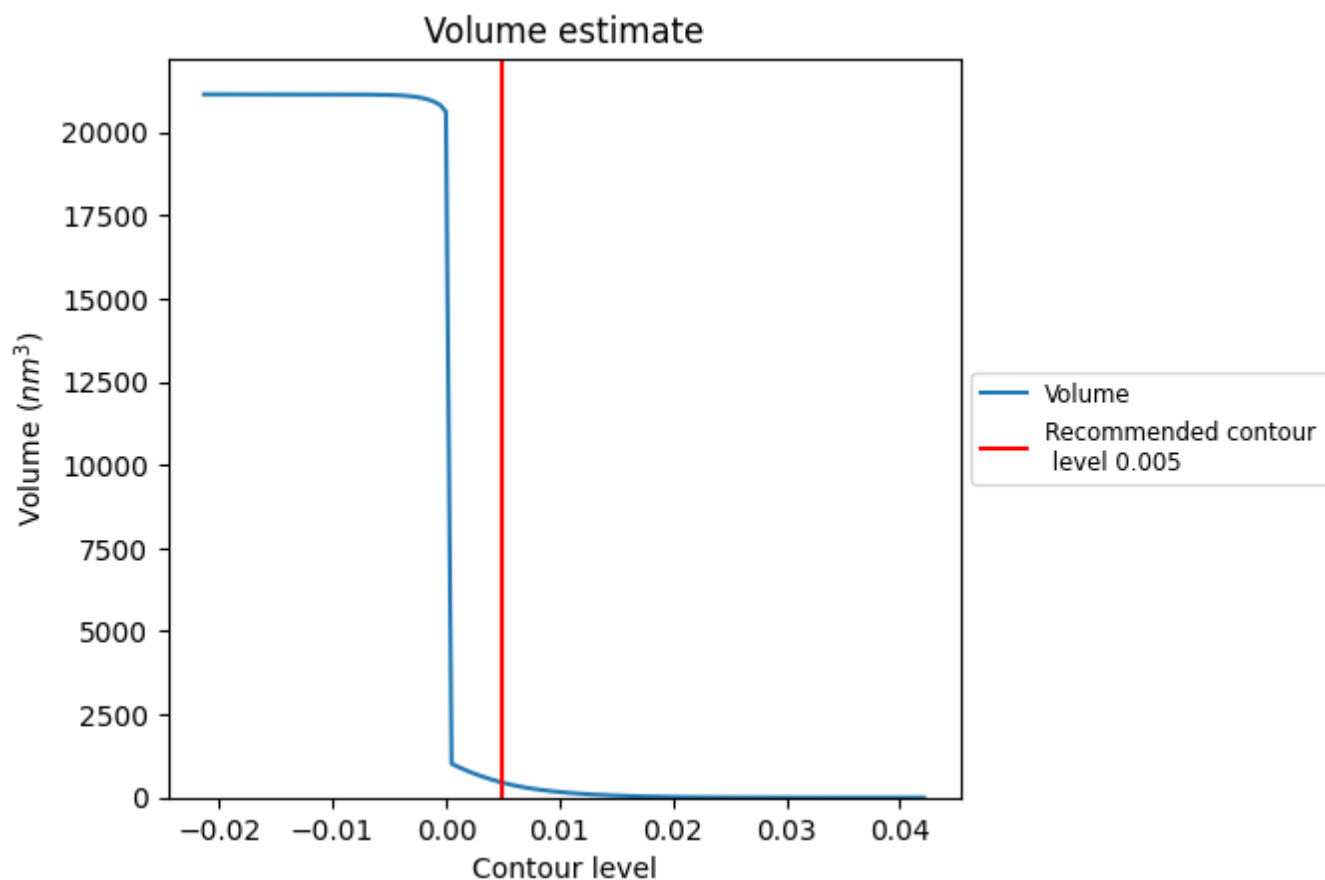
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

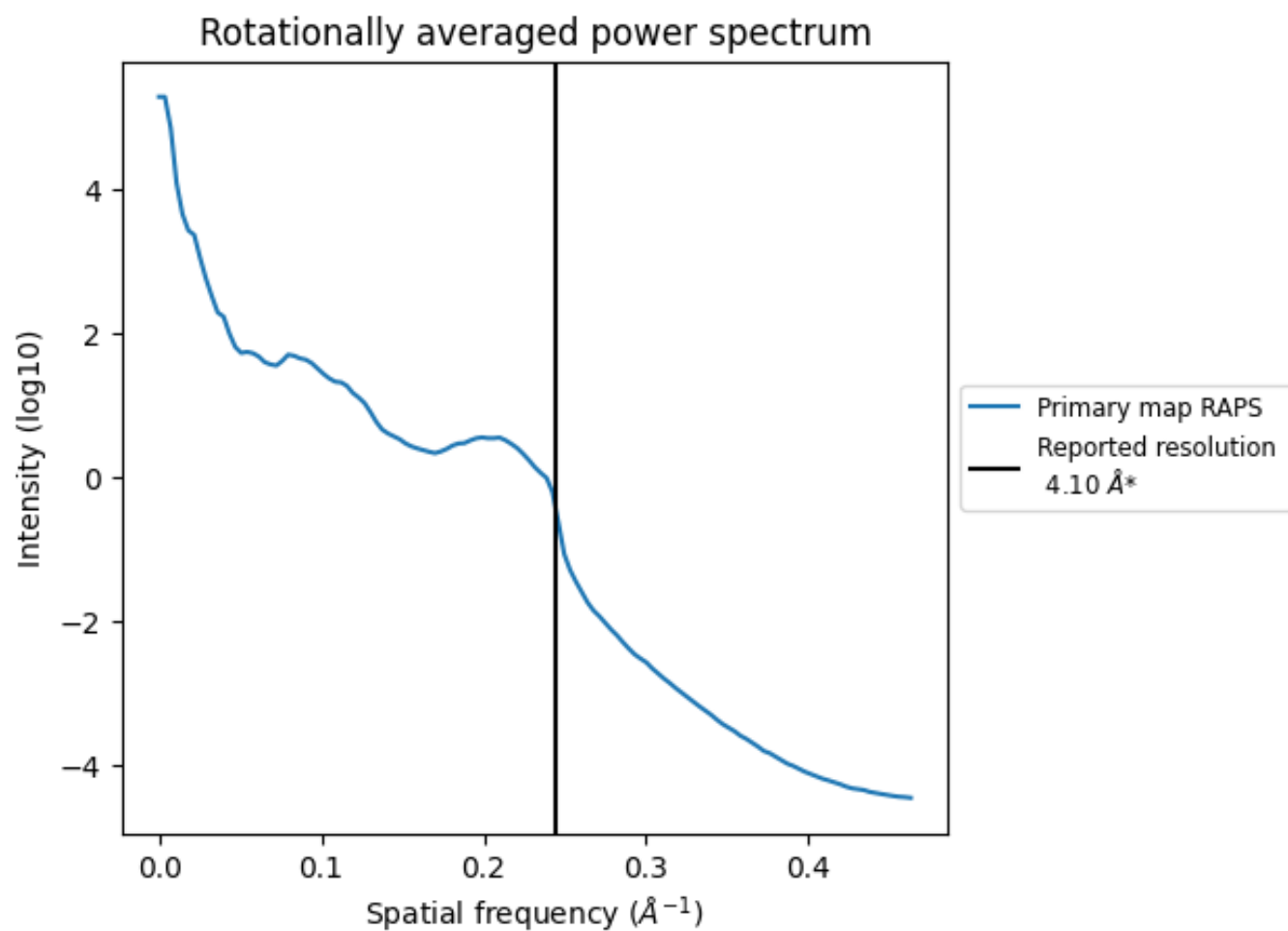
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 447 nm^3 ; this corresponds to an approximate mass of 404 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 ⓘ

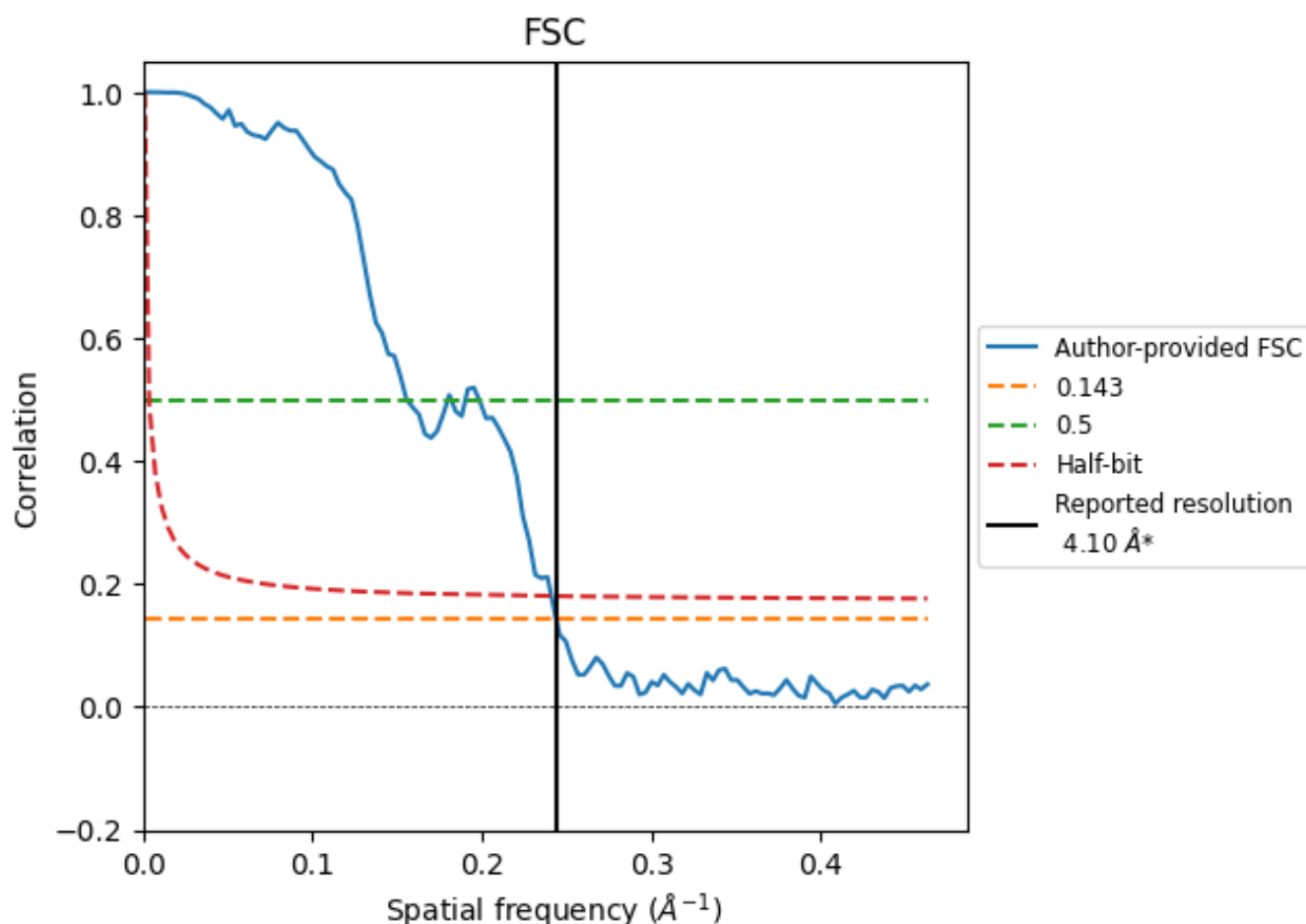


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

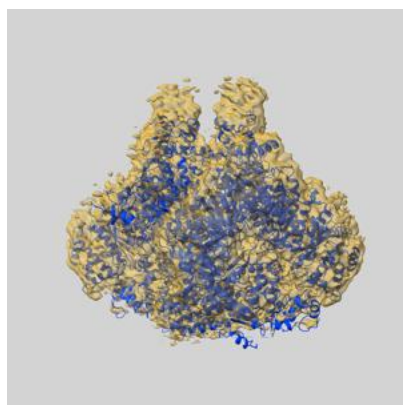
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.10	6.43	4.15
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

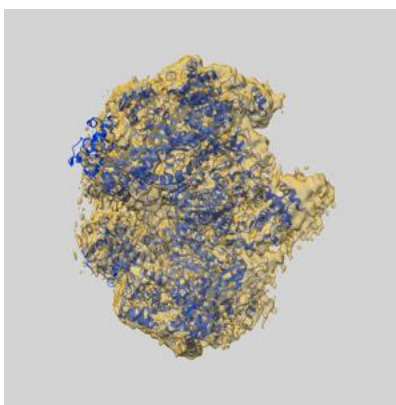
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31179 and PDB model 7ELB. Per-residue inclusion information can be found in section [3](#) on page [5](#).

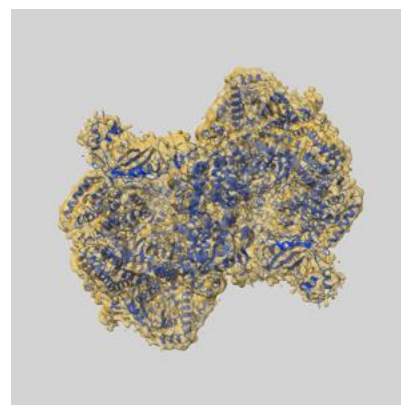
9.1 Map-model overlay [i](#)



X



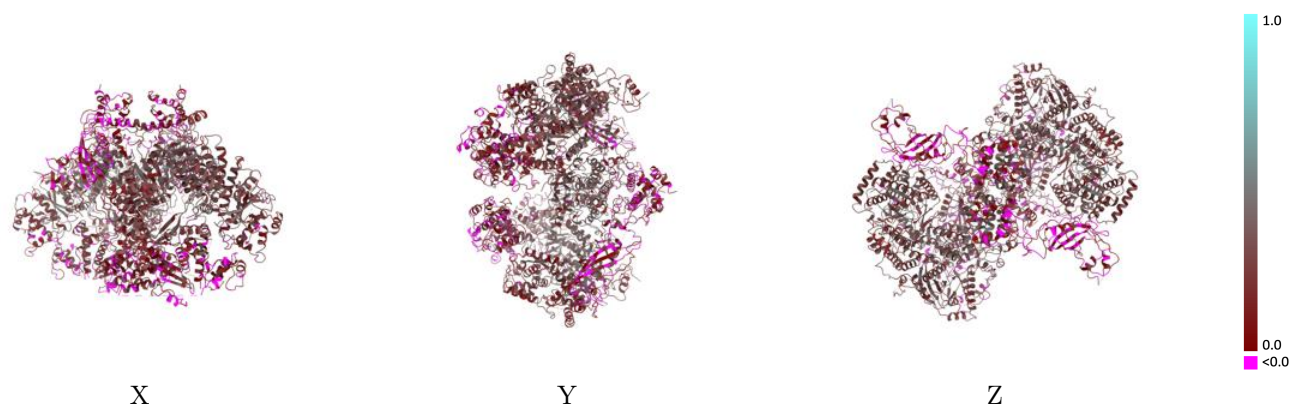
Y



Z

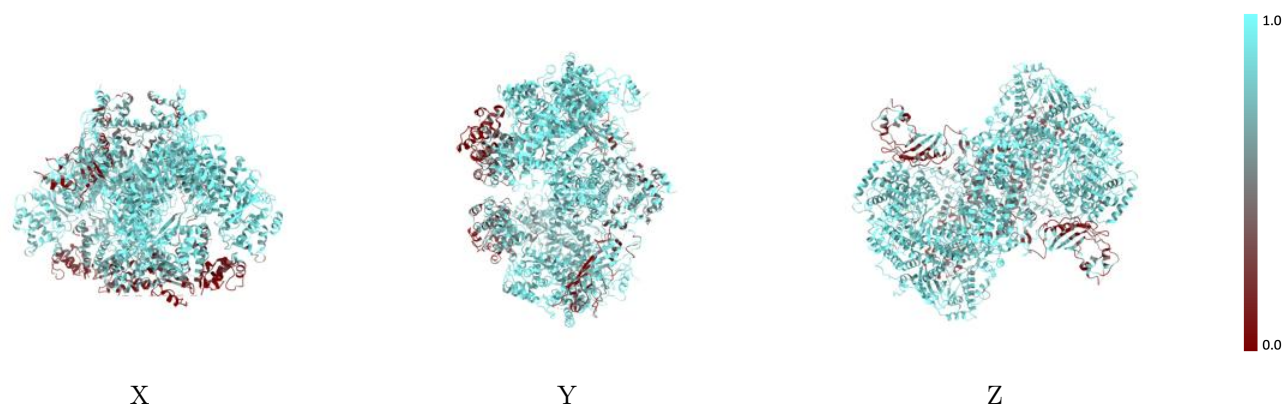
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



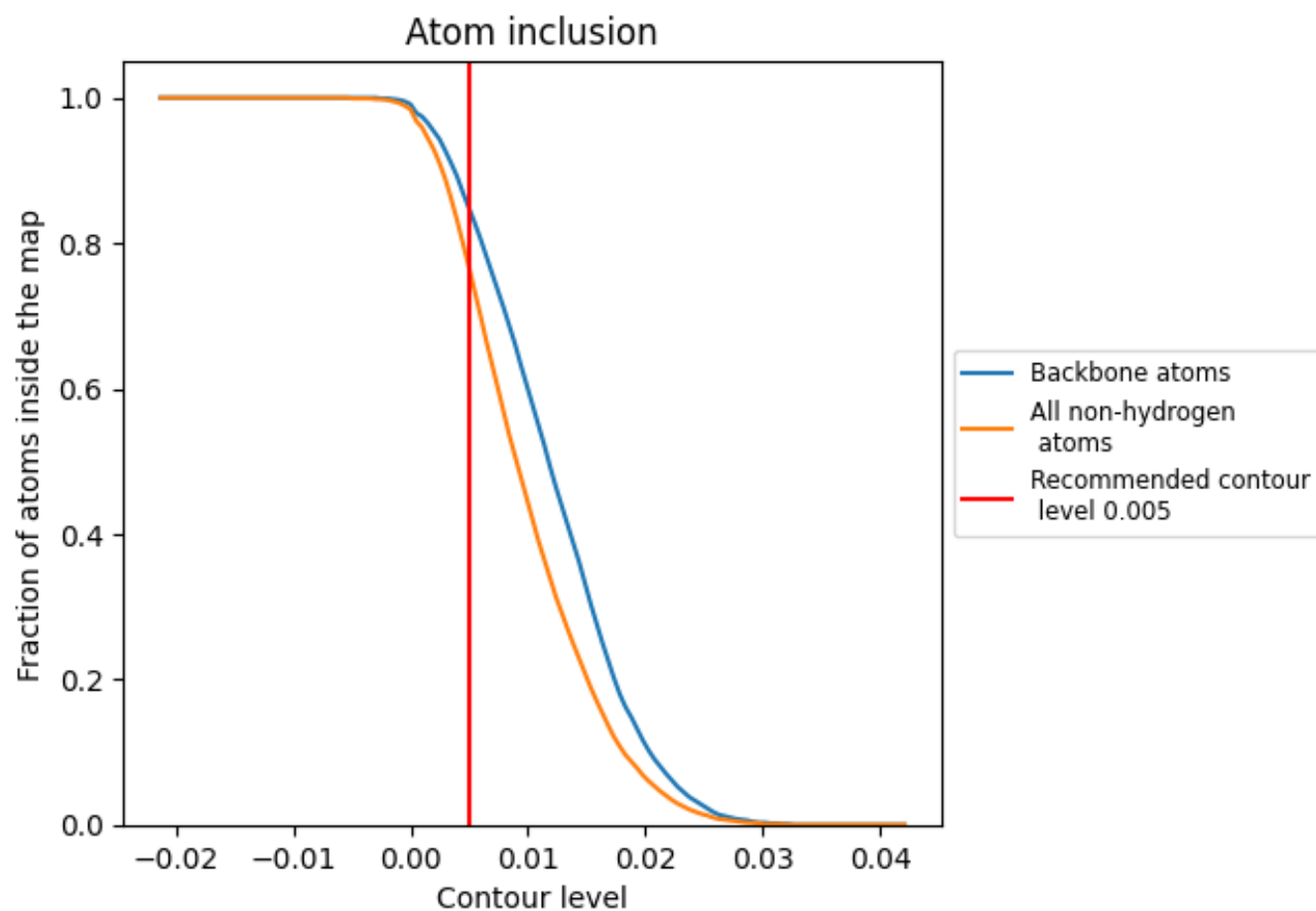
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 77% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7660	0.2290
A	0.7620	0.2290
B	0.9200	0.2180
C	0.7600	0.2300
D	0.9220	0.2270

