



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:07 AM UTC

PDB ID : 7K19 / pdb_00007k19
EMDB ID : EMD-22622
Title : CryoEM structure of DNA-PK catalytic subunit complexed with DNA (Complex I)
Authors : Chen, X.; Gellert, M.; Yang, W.
Deposited on : 2020-09-07
Resolution : 4.30 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

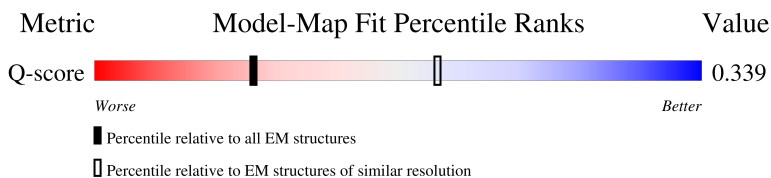
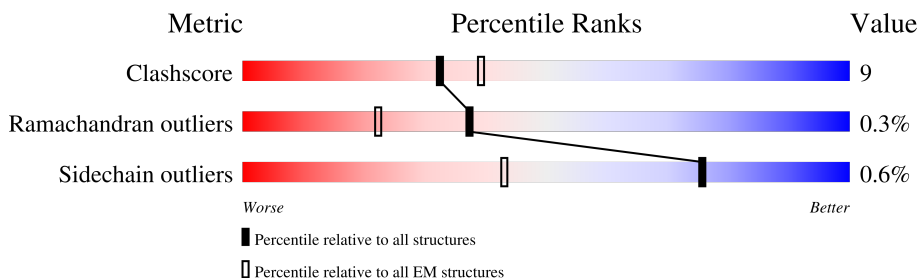
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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	4585 (3.80 - 4.80)

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	4128	
2	D	24	
2	F	24	
3	G	16	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29158 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3569	Total	C	N	O	S	0	0
			28180	18091	4776	5128	185		

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*CP*AP*TP*GP*CP*TP*CP*TP*AP*CP*TP*GP*CP*TP*TP*CP*GP*AP*TP*AP*TP*CP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	24	Total	C	N	O	P	0	0
			484	233	82	146	23		
2	F	8	Total	C	N	O	P	0	0
			164	78	30	48	8		

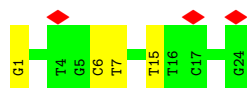
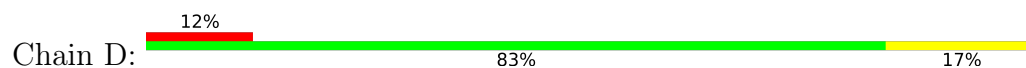
- Molecule 3 is a DNA chain called DNA (5'-D(*AP*AP*GP*CP*AP*GP*TP*AP*GP*AP*GP*CP*AP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	16	Total	C	N	O	P	0	0
			330	157	68	90	15		

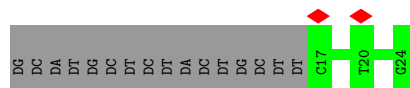
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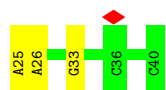
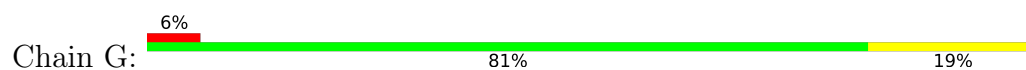
- Molecule 2: DNA (5'-D(*GP*CP*AP*TP*GP*CP*TP*CP*TP*AP*CP*TP*GP*CP*TP*TP*CP*GP*AP*TP*AP*TP*CP*G)-3')



- Molecule 2: DNA (5'-D(*GP*CP*AP*TP*GP*CP*TP*CP*TP*AP*CP*TP*GP*CP*TP*TP*CP*GP*AP*TP*AP*TP*CP*G)-3')



- Molecule 3: DNA (5'-D(*AP*AP*GP*CP*AP*GP*TP*AP*GP*AP*GP*CP*AP*TP*GP*C)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62117	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 ($e^-/\text{\AA}^2$)	45	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	0.059	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	408.31998, 408.31998, 408.31998	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality

5.1 Standard geometry

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	0.29	0/28742	0.65	20/38884 (0.1%)
2	D	0.30	0/540	0.58	0/831
2	F	0.28	0/183	0.49	0/280
3	G	0.31	0/372	0.58	0/573
All	All	0.29	0/29837	0.65	20/40568 (0.0%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3311	ASN	N-CA-C	-22.78	82.19	112.03
1	A	1469	PRO	N-CA-C	-11.82	88.12	112.47
1	A	4033	VAL	N-CA-C	-7.62	105.88	113.20
1	A	1019	ASP	CA-C-N	7.41	129.10	119.84
1	A	1019	ASP	C-N-CA	7.41	129.10	119.84
1	A	1468	LEU	CA-C-N	6.96	128.53	119.84
1	A	1468	LEU	C-N-CA	6.96	128.53	119.84
1	A	24	ARG	CA-C-N	6.12	133.23	121.54
1	A	24	ARG	C-N-CA	6.12	133.23	121.54
1	A	2034	SER	CA-C-N	6.05	133.10	121.54
1	A	2034	SER	C-N-CA	6.05	133.10	121.54
1	A	3267	LYS	N-CA-C	-5.34	106.64	114.39
1	A	2253	TYR	CA-C-N	5.20	131.47	121.54
1	A	2253	TYR	C-N-CA	5.20	131.47	121.54
1	A	3122	HIS	CA-C-N	5.19	131.45	121.54
1	A	3122	HIS	C-N-CA	5.19	131.45	121.54
1	A	4012	ASP	CA-C-N	5.13	131.34	121.54
1	A	4012	ASP	C-N-CA	5.13	131.34	121.54
1	A	1659	VAL	N-CA-C	-5.10	108.86	113.71
1	A	397	LEU	CA-CB-CG	5.03	133.90	116.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	28180	0	28380	493	0
2	D	484	0	274	3	0
2	F	164	0	91	0	0
3	G	330	0	180	2	0
All	All	29158	0	28925	495	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 (495) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1687:HIS:CE1	1:A:1688:LEU:HD12	1.75	1.22
1:A:1687:HIS:CE1	1:A:1688:LEU:CD1	2.33	1.11
1:A:1687:HIS:ND1	1:A:1688:LEU:HD12	1.73	1.02
1:A:3647:GLY:O	1:A:3651:LEU:HB2	1.70	0.92
1:A:2467:THR:O	1:A:2471:GLU:HB2	1.77	0.84
1:A:4078:VAL:O	1:A:4082:ARG:HB2	1.78	0.84
1:A:1687:HIS:CE1	1:A:1688:LEU:HD11	2.18	0.79
1:A:1992:VAL:HG12	1:A:2183:HIS:HB2	1.66	0.76
1:A:1687:HIS:HE1	1:A:1688:LEU:CD1	1.96	0.76
1:A:2493:ASN:O	1:A:2497:GLU:HB2	1.88	0.74
1:A:1687:HIS:HE1	1:A:1688:LEU:HD11	1.49	0.73
1:A:3636:PHE:O	1:A:3640:PHE:HB2	1.93	0.67
1:A:2290:PRO:HB3	1:A:2295:GLN:HA	1.77	0.67
1:A:1205:ASN:HA	1:A:1275:THR:HA	1.78	0.66
1:A:2527:HIS:HB3	1:A:2530:ARG:HD3	1.77	0.66
1:A:1825:LEU:O	1:A:1829:TRP:HB2	1.95	0.65
1:A:35:ILE:HG21	1:A:85:ILE:HA	1.79	0.64
1:A:970:LEU:HG	1:A:1025:LEU:HD11	1.80	0.64
1:A:2278:GLY:O	1:A:2282:ALA:HB2	1.98	0.63
1:A:3751:LEU:HB3	1:A:3803:ILE:HB	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2254:ARG:O	1:A:2258:GLU:HB2	1.98	0.62
1:A:4019:LYS:HA	1:A:4022:LYS:HE2	1.82	0.62
1:A:3125:ARG:O	1:A:3129:LEU:HB2	1.98	0.62
1:A:669:LEU:HA	1:A:672:ILE:HD12	1.81	0.62
1:A:3780:ALA:O	1:A:3784:ARG:NH1	2.33	0.61
1:A:3771:MET:SD	1:A:3914:SER:OG	2.58	0.61
1:A:2992:ASP:OD1	1:A:2992:ASP:N	2.33	0.61
1:A:3962:ARG:NH1	1:A:4125:GLU:O	2.34	0.61
1:A:2254:ARG:HH11	1:A:2293:GLY:HA2	1.66	0.61
1:A:349:ILE:O	1:A:391:ARG:NH1	2.35	0.60
1:A:3013:TYR:O	1:A:3017:ALA:HB3	2.01	0.60
1:A:3472:ILE:HG13	1:A:3483:MET:HE3	1.84	0.60
1:A:1020:PRO:O	1:A:1026:ARG:NH2	2.35	0.60
1:A:1683:LYS:HG3	1:A:1684:LEU:HG	1.82	0.60
1:A:1971:PRO:HA	1:A:1975:LEU:H	1.65	0.60
1:A:4012:ASP:N	1:A:4012:ASP:OD1	2.35	0.60
1:A:355:ASN:HA	1:A:1733:THR:HG23	1.84	0.59
1:A:2458:VAL:HG11	1:A:2476:ILE:HD11	1.84	0.59
1:A:1687:HIS:ND1	1:A:1688:LEU:CD1	2.55	0.59
1:A:3502:MET:HE2	1:A:3514:VAL:HG21	1.84	0.59
1:A:719:LYS:HG2	1:A:720:GLN:HG2	1.84	0.59
1:A:997:ASN:OD1	1:A:1043:GLN:NE2	2.36	0.59
1:A:3630:ARG:HG3	1:A:3633:ILE:H	1.67	0.58
1:A:2403:CYS:SG	1:A:2404:ARG:N	2.76	0.58
1:A:2548:PRO:HG3	1:A:2846:THR:HB	1.84	0.58
1:A:1724:MET:SD	1:A:1768:ARG:NH2	2.76	0.58
1:A:708:VAL:O	1:A:712:LYS:NZ	2.34	0.58
1:A:1817:GLN:NE2	1:A:1871:MET:SD	2.77	0.58
1:A:2319:ALA:O	1:A:2323:LEU:HB3	2.04	0.58
1:A:3176:MET:HA	1:A:3179:TRP:HB2	1.85	0.58
1:A:3954:PRO:HG2	1:A:4026:SER:HB3	1.85	0.57
1:A:4041:ARG:O	1:A:4045:CYS:HB2	2.03	0.57
1:A:241:ASP:OD1	1:A:243:GLN:NE2	2.38	0.57
1:A:529:ASP:OD1	1:A:529:ASP:N	2.35	0.57
1:A:3028:ASN:HD22	1:A:3031:TRP:HB2	1.68	0.57
1:A:489:ARG:NH2	1:A:2040:MET:SD	2.78	0.56
1:A:1493:PRO:O	1:A:1498:GLN:N	2.38	0.56
1:A:672:ILE:O	1:A:676:ASN:ND2	2.35	0.56
1:A:3810:VAL:HG23	1:A:3930:VAL:HG13	1.86	0.56
1:A:1456:LYS:NZ	1:A:1516:GLU:OE1	2.38	0.56
1:A:1082:PHE:HA	1:A:1085:ILE:HG12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4071:ALA:HB3	1:A:4074:PHE:HB2	1.88	0.56
1:A:70:ARG:NH2	1:A:109:ASN:OD1	2.39	0.56
1:A:787:PRO:O	1:A:790:LYS:NZ	2.36	0.56
1:A:203:GLU:OE1	1:A:207:GLN:NE2	2.38	0.56
1:A:1467:ILE:HG22	1:A:1468:LEU:HG	1.86	0.56
1:A:3175:PRO:HD2	1:A:3178:ILE:HD12	1.87	0.56
1:A:3292:GLY:O	1:A:3296:GLN:NE2	2.39	0.56
1:A:3522:THR:HG22	1:A:3529:ILE:HG21	1.88	0.56
1:A:3646:LYS:HB2	1:A:3650:LYS:HE3	1.88	0.56
1:A:4019:LYS:O	1:A:4023:LYS:NZ	2.39	0.56
1:A:1137:ILE:O	1:A:1141:LYS:NZ	2.38	0.56
1:A:2837:LEU:O	1:A:2841:ASN:ND2	2.34	0.56
1:A:863:GLY:HA2	1:A:3167:ARG:HG3	1.88	0.56
1:A:935:HIS:HB2	1:A:984:TYR:HE1	1.71	0.56
1:A:1089:PHE:HB2	1:A:1096:VAL:HG12	1.88	0.55
1:A:1440:ASP:O	1:A:1445:ARG:NH1	2.39	0.55
1:A:3868:VAL:HG22	1:A:4114:PRO:HB2	1.87	0.55
1:A:1632:TRP:HB3	1:A:1645:VAL:HG21	1.88	0.55
1:A:2856:SER:OG	1:A:2885:GLN:NE2	2.39	0.55
1:A:3140:GLU:OE2	1:A:3164:TRP:NE1	2.39	0.55
1:A:128:LEU:HA	1:A:131:LEU:HD12	1.88	0.55
1:A:306:VAL:O	1:A:310:LYS:NZ	2.39	0.55
1:A:1021:VAL:O	1:A:1021:VAL:HG13	2.06	0.55
1:A:399:GLN:HG2	1:A:400:THR:H	1.72	0.55
1:A:1416:GLU:HG2	1:A:1420:ARG:HH11	1.71	0.55
1:A:1506:SER:HA	1:A:1509:GLN:HB2	1.88	0.55
1:A:3096:VAL:O	1:A:3100:LYS:N	2.39	0.55
1:A:1806:ARG:NH2	1:A:1846:ASP:O	2.40	0.55
1:A:25:CYS:H	1:A:78:PHE:HE1	1.55	0.55
1:A:3820:MET:HG2	1:A:3882:LEU:HD11	1.88	0.55
1:A:1493:PRO:HB3	1:A:1501:PRO:HD3	1.87	0.55
1:A:2471:GLU:OE1	1:A:2475:ASN:ND2	2.39	0.55
1:A:2213:ASN:O	1:A:2217:ASN:ND2	2.35	0.54
1:A:2383:PHE:O	1:A:2418:LYS:NZ	2.40	0.54
1:A:2973:ASP:O	1:A:2977:ASN:ND2	2.40	0.54
1:A:214:GLU:O	1:A:216:LYS:NZ	2.40	0.54
1:A:1420:ARG:NH1	1:A:1466:ASN:O	2.40	0.54
1:A:723:ASP:OD1	1:A:723:ASP:N	2.38	0.54
1:A:1992:VAL:HG12	1:A:2183:HIS:CD2	2.43	0.54
1:A:1560:TYR:O	1:A:1564:SER:OG	2.25	0.54
1:A:9:ARG:HG3	1:A:57:LEU:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2492:ASP:O	1:A:2496:GLN:NE2	2.41	0.54
1:A:583:LEU:HA	1:A:614:PRO:HA	1.90	0.54
1:A:3792:SER:O	1:A:3804:GLU:HB2	2.06	0.54
1:A:72:SER:O	1:A:72:SER:OG	2.26	0.54
1:A:390:GLN:NE2	1:A:1687:HIS:CE1	2.75	0.54
1:A:390:GLN:HE21	1:A:1687:HIS:CE1	2.26	0.54
1:A:1686:LEU:HD21	1:A:1742:CYS:HB2	1.90	0.54
1:A:66:LEU:HD11	1:A:107:ILE:HD13	1.89	0.54
1:A:1527:ARG:O	1:A:1527:ARG:NH1	2.40	0.53
1:A:959:TYR:O	1:A:963:LYS:NZ	2.40	0.53
1:A:3958:LEU:HD21	1:A:4064:LEU:HD22	1.90	0.53
1:A:4088:ASN:O	1:A:4092:GLN:NE2	2.41	0.53
1:A:2950:LYS:NZ	1:A:2984:GLY:O	2.41	0.53
1:A:3733:ARG:NH1	1:A:3754:GLY:O	2.40	0.53
1:A:3586:LYS:O	1:A:3590:ASN:ND2	2.39	0.53
1:A:3109:SER:O	1:A:3113:ASN:ND2	2.42	0.53
1:A:3731:SER:O	1:A:3734:ARG:NE	2.38	0.53
1:A:3992:ARG:NH1	1:A:4103:GLN:OE1	2.41	0.53
1:A:32:HIS:HB2	1:A:80:GLU:HB3	1.91	0.53
1:A:2103:HIS:HA	1:A:2106:ARG:HG2	1.90	0.53
1:A:3147:LYS:HE3	1:A:3150:ASN:HD21	1.74	0.53
1:A:3362:LEU:HD22	1:A:3380:ARG:HH12	1.73	0.53
1:A:3089:LEU:O	1:A:3093:GLN:NE2	2.42	0.53
1:A:1075:ARG:NH2	1:A:1117:ASP:OD2	2.42	0.52
1:A:1416:GLU:HB3	1:A:1420:ARG:HE	1.74	0.52
1:A:2931:ARG:NH2	1:A:3043:TYR:OH	2.41	0.52
1:A:2962:ARG:NH1	1:A:4101:GLU:OE2	2.41	0.52
1:A:1818:SER:HG	1:A:1822:ARG:HE	1.54	0.52
1:A:3846:MET:HB2	1:A:3858:MET:HE1	1.90	0.52
1:A:463:LYS:O	1:A:463:LYS:NZ	2.42	0.52
1:A:2181:GLY:O	1:A:2183:HIS:N	2.43	0.52
1:A:3172:LYS:HE2	1:A:3248:LYS:HE3	1.91	0.52
1:A:399:GLN:CG	1:A:400:THR:H	2.22	0.52
1:A:321:LYS:HA	1:A:368:LEU:HD21	1.91	0.52
1:A:399:GLN:HG2	1:A:400:THR:N	2.24	0.52
1:A:3450:MET:HE2	1:A:3464:LYS:HD3	1.91	0.52
1:A:3577:GLN:HE21	1:A:3630:ARG:HH22	1.58	0.52
1:A:1693:VAL:HA	1:A:1696:LEU:HD23	1.92	0.52
1:A:2469:CYS:SG	1:A:2470:ARG:N	2.82	0.52
1:A:2425:ARG:NH2	1:A:2460:GLU:OE1	2.41	0.52
1:A:2826:LEU:HA	1:A:2829:LYS:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3796:MET:HB2	1:A:3800:LEU:O	2.10	0.52
1:A:456:VAL:HA	1:A:459:ARG:HD2	1.91	0.52
1:A:3256:MET:HE1	1:A:3280:TYR:HE1	1.75	0.52
1:A:3548:GLY:HA2	1:A:3551:ASN:HD22	1.75	0.52
1:A:28:ALA:HB1	1:A:80:GLU:HB2	1.92	0.51
1:A:69:VAL:O	1:A:73:LEU:N	2.43	0.51
1:A:1055:ASN:O	1:A:1058:SER:OG	2.24	0.51
1:A:3176:MET:O	1:A:3180:ASP:HB2	2.10	0.51
1:A:3474:ARG:O	1:A:3474:ARG:NH2	2.39	0.51
1:A:1603:GLN:NE2	1:A:1607:GLU:OE2	2.41	0.51
1:A:2122:LEU:H	1:A:2126:MET:HB3	1.76	0.51
1:A:3279:SER:HA	1:A:3282:ARG:HD2	1.92	0.51
1:A:2531:LEU:O	1:A:2538:ARG:NH2	2.42	0.51
1:A:3701:ILE:HD12	1:A:3702:PRO:HD2	1.93	0.51
1:A:880:MET:HA	1:A:883:TYR:HB2	1.93	0.51
1:A:86:LEU:HD22	1:A:130:LEU:HD22	1.92	0.51
1:A:1981:LEU:HD12	1:A:1982:ILE:HG13	1.93	0.51
1:A:646:VAL:O	1:A:650:SER:OG	2.27	0.50
1:A:3797:THR:OG1	1:A:3798:SER:N	2.44	0.50
1:A:346:TYR:HA	1:A:349:ILE:HG22	1.93	0.50
1:A:1983:ASP:OD2	1:A:1986:ARG:N	2.41	0.50
1:A:1212:LEU:HD22	1:A:1220:LEU:HD22	1.93	0.50
1:A:3329:LEU:O	1:A:3333:THR:OG1	2.28	0.50
1:A:2205:VAL:HG12	1:A:2208:ASP:H	1.75	0.50
1:A:1406:LEU:HD13	1:A:1415:LEU:HD11	1.92	0.50
1:A:436:GLU:HG3	1:A:478:CYS:HB3	1.93	0.50
1:A:1854:ARG:NH1	1:A:1855:PHE:O	2.42	0.50
1:A:3121:LEU:O	1:A:3124:SER:OG	2.30	0.50
1:A:385:TYR:H	1:A:388:LEU:HD13	1.77	0.50
1:A:1256:TRP:HA	1:A:1259:LEU:HD12	1.93	0.50
1:A:1992:VAL:CG1	1:A:2183:HIS:HB2	2.38	0.50
1:A:3247:ARG:HD3	1:A:3283:LEU:HD12	1.93	0.50
1:A:1190:LEU:O	1:A:1194:PHE:HB2	2.12	0.49
1:A:3629:ARG:NH2	1:A:3630:ARG:O	2.45	0.49
1:A:327:VAL:HA	1:A:330:ASN:HB3	1.94	0.49
1:A:1849:ASP:OD1	1:A:1849:ASP:N	2.43	0.49
1:A:1806:ARG:NH2	1:A:1846:ASP:OD1	2.42	0.49
1:A:1926:ASN:ND2	1:A:1974:ASN:O	2.44	0.49
1:A:121:ALA:N	2:D:15:DT:OP1	2.45	0.49
1:A:4033:VAL:O	1:A:4037:ASN:ND2	2.45	0.49
1:A:24:ARG:NH1	1:A:77:GLU:OE1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:SER:OG	1:A:142:ARG:N	2.46	0.49
1:A:889:GLU:OE1	1:A:891:ARG:NH2	2.45	0.49
1:A:1833:LEU:HG	1:A:1835:ALA:H	1.77	0.49
1:A:1927:MET:HG2	1:A:1934:LEU:HD22	1.94	0.49
1:A:2447:LYS:HD3	1:A:2448:PRO:HD2	1.92	0.49
1:A:324:SER:HA	1:A:327:VAL:HG12	1.95	0.49
1:A:1288:SER:OG	1:A:1289:SER:N	2.44	0.49
1:A:1566:THR:HA	1:A:1569:THR:HG22	1.95	0.49
1:A:1611:GLN:O	1:A:1613:HIS:ND1	2.43	0.49
1:A:993:HIS:O	1:A:997:ASN:ND2	2.45	0.49
1:A:2464:HIS:O	1:A:2470:ARG:NE	2.46	0.49
1:A:3640:PHE:HA	1:A:3643:HIS:HD2	1.76	0.49
1:A:108:LYS:HD3	1:A:152:LEU:HD21	1.94	0.49
1:A:377:ASN:HB3	1:A:380:ASP:H	1.78	0.49
1:A:1265:GLU:OE1	1:A:1340:ARG:NH1	2.46	0.49
1:A:1459:HIS:NE2	1:A:1520:ALA:O	2.44	0.49
1:A:3640:PHE:HA	1:A:3643:HIS:CD2	2.48	0.49
1:A:2428:ASP:O	1:A:2432:GLN:NE2	2.46	0.48
1:A:3641:ASP:OD1	1:A:3641:ASP:N	2.42	0.48
1:A:538:ASP:OD1	1:A:561:ASN:ND2	2.46	0.48
1:A:1896:ILE:HD11	1:A:1911:LEU:H	1.78	0.48
1:A:1071:ASN:HB3	1:A:1074:LYS:HB2	1.94	0.48
1:A:1558:TYR:O	1:A:1561:SER:OG	2.30	0.48
1:A:1680:ALA:O	1:A:1683:LYS:NZ	2.32	0.48
1:A:1709:GLU:OE1	1:A:1712:ARG:NH1	2.46	0.48
1:A:3689:ASP:OD1	1:A:3689:ASP:N	2.46	0.48
1:A:2148:LYS:NZ	1:A:2152:ASN:OD1	2.43	0.48
1:A:3249:GLN:HG3	1:A:3779:SER:HB2	1.96	0.48
1:A:1855:PHE:HB3	1:A:1857:LYS:HG3	1.95	0.48
1:A:1992:VAL:HG12	1:A:2183:HIS:CB	2.41	0.48
1:A:3878:VAL:O	1:A:3965:ARG:NH1	2.46	0.48
1:A:105:VAL:HG12	1:A:147:PHE:HB3	1.96	0.48
1:A:406:ARG:HA	2:D:1:DG:H5'	1.95	0.48
1:A:866:ILE:O	1:A:869:ASN:ND2	2.39	0.48
1:A:2234:ASN:HA	1:A:2237:ILE:HD12	1.95	0.48
1:A:2825:THR:O	1:A:2829:LYS:N	2.39	0.48
1:A:3916:TRP:CD1	1:A:3960:PRO:HB3	2.49	0.48
1:A:178:LEU:HD21	1:A:196:LEU:HD11	1.96	0.48
1:A:474:VAL:HG12	1:A:1558:TYR:HB2	1.96	0.48
1:A:1483:LEU:HD22	1:A:1514:LEU:HD11	1.96	0.48
1:A:2821:ASP:OD1	1:A:2829:LYS:NZ	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LEU:HD22	1:A:110:THR:HG21	1.96	0.47
1:A:176:GLU:OE2	1:A:225:LYS:NZ	2.39	0.47
1:A:2415:LEU:HB3	1:A:2420:PHE:HB2	1.96	0.47
1:A:2528:GLU:HG3	1:A:2529:THR:HG23	1.96	0.47
1:A:3291:GLN:HB3	1:A:3296:GLN:HG2	1.95	0.47
1:A:447:PRO:HG3	1:A:522:PRO:HG3	1.95	0.47
1:A:3352:GLU:HA	1:A:3355:LYS:HE2	1.96	0.47
1:A:1366:THR:O	1:A:1370:ARG:HB2	2.14	0.47
1:A:3163:THR:OG1	1:A:3167:ARG:NH1	2.48	0.47
1:A:721:TYR:HB2	1:A:726:LEU:HG	1.95	0.47
1:A:2872:ASP:OD1	1:A:2875:ALA:N	2.47	0.47
1:A:3283:LEU:O	1:A:3287:ARG:HB2	2.14	0.47
1:A:3735:PRO:HB3	1:A:3753:LYS:HG2	1.96	0.47
1:A:3872:ARG:HH12	1:A:4114:PRO:HB3	1.79	0.47
1:A:1169:VAL:HA	1:A:1172:LEU:HD12	1.95	0.47
1:A:2191:ALA:O	1:A:2195:SER:OG	2.30	0.47
1:A:449:TYR:HB3	1:A:454:GLN:HG2	1.97	0.47
1:A:1328:GLU:HA	1:A:1331:ASN:HB3	1.97	0.47
1:A:1859:ASN:HD21	1:A:1861:SER:HB3	1.79	0.47
1:A:3048:LYS:HB3	1:A:3061:LEU:HD22	1.96	0.47
1:A:336:ASN:OD1	1:A:336:ASN:N	2.47	0.47
1:A:1413:ASP:OD1	1:A:1413:ASP:N	2.45	0.47
1:A:3875:GLU:HG3	1:A:3965:ARG:HE	1.80	0.47
1:A:3026:ASP:N	1:A:3026:ASP:OD1	2.48	0.46
1:A:2165:LEU:HD11	1:A:2193:ILE:HG23	1.97	0.46
1:A:569:VAL:HA	1:A:572:VAL:HG12	1.97	0.46
1:A:2254:ARG:HA	1:A:2257:PHE:HB3	1.97	0.46
1:A:2477:LEU:HA	1:A:2480:ILE:HG22	1.98	0.46
1:A:2264:ASP:OD1	1:A:2266:ASN:ND2	2.49	0.46
1:A:559:SER:OG	1:A:560:LEU:N	2.49	0.46
1:A:2210:VAL:HG23	1:A:2214:ARG:HH22	1.80	0.46
1:A:3466:PRO:HB2	1:A:4004:VAL:HG11	1.96	0.46
1:A:1596:VAL:HG22	1:A:1600:MET:HE3	1.98	0.46
1:A:2465:PRO:HA	1:A:2470:ARG:HH21	1.81	0.46
1:A:1759:LEU:HD23	1:A:1797:LEU:HB3	1.97	0.46
1:A:2955:SER:O	1:A:2971:GLN:NE2	2.48	0.46
1:A:1323:SER:O	1:A:1323:SER:OG	2.32	0.46
1:A:3352:GLU:HB3	1:A:3356:ALA:HB2	1.98	0.46
1:A:3519:GLU:OE1	1:A:3557:ARG:NH1	2.48	0.46
1:A:3951:GLN:O	1:A:4068:HIS:NE2	2.49	0.46
1:A:205:LYS:NZ	1:A:247:GLU:OE2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3857:LEU:HA	1:A:3860:LYS:HE3	1.97	0.45
1:A:124:LYS:HB2	1:A:124:LYS:HE3	1.80	0.45
1:A:984:TYR:HA	1:A:987:LEU:HB3	1.97	0.45
1:A:1747:LEU:HD21	1:A:1781:SER:HB3	1.97	0.45
1:A:1969:GLU:HB3	1:A:1977:ILE:HG13	1.97	0.45
1:A:3089:LEU:HA	1:A:3092:LEU:HD12	1.99	0.45
1:A:3800:LEU:HD12	1:A:3800:LEU:HA	1.80	0.45
1:A:65:LEU:HA	1:A:68:PHE:HB3	1.99	0.45
1:A:848:LEU:O	1:A:852:ARG:HB2	2.16	0.45
1:A:1264:LEU:HD13	1:A:1341:ILE:HD13	1.99	0.45
1:A:1988:TYR:HD2	1:A:2144:LEU:HD22	1.82	0.45
1:A:2140:LEU:HA	1:A:2143:ARG:HH11	1.82	0.45
1:A:2167:PRO:HA	1:A:2170:GLN:HB2	1.98	0.45
1:A:3262:LEU:HD23	1:A:3265:GLU:HB3	1.99	0.45
1:A:3422:GLN:NE2	1:A:3423:GLN:OE1	2.46	0.45
1:A:3589:SER:OG	1:A:3593:ARG:NH2	2.39	0.45
1:A:616:LYS:HD2	1:A:2034:SER:HA	1.98	0.45
1:A:1668:PHE:HA	1:A:1671:VAL:HG12	1.99	0.45
1:A:290:TYR:HA	1:A:293:LEU:HD12	1.99	0.45
1:A:2257:PHE:O	1:A:2261:SER:OG	2.29	0.45
1:A:667:TYR:HA	1:A:670:LEU:HD12	1.98	0.45
1:A:2442:MET:HE2	1:A:2446:LEU:HD11	1.98	0.45
1:A:1992:VAL:HG13	1:A:2183:HIS:H	1.82	0.45
1:A:2182:ILE:O	1:A:2186:VAL:N	2.39	0.45
1:A:2826:LEU:O	1:A:2830:ASN:ND2	2.49	0.45
1:A:2424:MET:HE3	1:A:2424:MET:HB2	1.72	0.45
1:A:3259:LEU:HA	1:A:3262:LEU:HB2	1.98	0.45
1:A:3591:ASP:HB3	1:A:3609:MET:HE1	1.98	0.45
1:A:3917:ILE:HD12	1:A:4051:LEU:HD13	1.99	0.45
1:A:178:LEU:HA	1:A:181:LEU:HD12	1.99	0.44
1:A:1934:LEU:HA	1:A:1937:ARG:HB2	1.98	0.44
1:A:1976:LEU:HD12	1:A:1979:GLU:HG2	1.99	0.44
1:A:1538:LEU:HG	1:A:1556:GLY:HA2	1.99	0.44
1:A:1871:MET:HE1	1:A:1936:ARG:HE	1.83	0.44
1:A:2980:ASP:OD1	1:A:2980:ASP:N	2.49	0.44
1:A:246:ARG:O	1:A:250:ASN:ND2	2.41	0.44
1:A:1204:PRO:HB2	1:A:1275:THR:HG22	1.98	0.44
1:A:1868:THR:HG23	1:A:1936:ARG:HH22	1.82	0.44
1:A:2180:GLU:OE2	1:A:2183:HIS:NE2	2.44	0.44
1:A:3069:MET:O	1:A:3070:HIS:ND1	2.51	0.44
1:A:3382:PHE:HE2	1:A:3442:TYR:HE1	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1359:LEU:HD11	1:A:1363:LEU:HD23	2.00	0.44
1:A:2327:LEU:HA	1:A:2330:VAL:HG12	1.99	0.44
1:A:1131:ILE:HA	1:A:1134:LEU:HD12	1.98	0.44
1:A:1218:SER:HA	1:A:1221:ILE:HG22	1.99	0.44
1:A:3723:ASP:HA	1:A:3741:ARG:HH12	1.83	0.44
1:A:179:GLY:HA3	1:A:226:GLY:HA2	1.99	0.44
1:A:1368:LEU:HA	1:A:1371:VAL:HG12	1.99	0.44
1:A:1717:LEU:HD12	1:A:1717:LEU:HA	1.88	0.44
1:A:1726:SER:OG	1:A:1727:ARG:NH2	2.51	0.44
1:A:3631:LYS:HG2	1:A:3683:CYS:HA	2.00	0.44
1:A:4075:ARG:HA	1:A:4078:VAL:HG12	1.99	0.44
1:A:4089:ILE:N	1:A:4109:ASP:OD2	2.48	0.44
3:G:25:DA:H2''	3:G:26:DA:C8	2.52	0.44
1:A:263:LYS:HB3	3:G:33:DG:H4'	1.99	0.44
1:A:400:THR:OG1	1:A:401:ASP:OD1	2.28	0.44
1:A:1790:SER:O	1:A:1793:THR:OG1	2.32	0.44
1:A:3963:LEU:HD12	1:A:3963:LEU:HA	1.90	0.44
1:A:148:LYS:HD3	1:A:148:LYS:HA	1.82	0.44
1:A:862:LEU:HD22	1:A:867:ASN:HB3	1.98	0.44
1:A:3547:THR:HA	1:A:3550:LYS:HZ3	1.83	0.44
1:A:39:GLY:HA2	1:A:88:PHE:CE1	2.53	0.43
1:A:3419:PHE:O	1:A:3422:GLN:NE2	2.41	0.43
1:A:1424:THR:O	1:A:1427:SER:OG	2.32	0.43
1:A:2211:LEU:HD23	1:A:2214:ARG:HH21	1.84	0.43
2:D:6:DC:H1'	2:D:7:DT:H5'	2.00	0.43
1:A:261:ASP:N	1:A:261:ASP:OD1	2.40	0.43
1:A:889:GLU:O	1:A:891:ARG:NH1	2.51	0.43
1:A:1392:MET:HE3	1:A:1392:MET:HB3	1.92	0.43
1:A:2493:ASN:O	1:A:2497:GLU:CB	2.63	0.43
1:A:55:THR:HG22	1:A:92:PHE:HZ	1.83	0.43
1:A:637:LYS:HA	1:A:637:LYS:HD3	1.81	0.43
1:A:1436:LEU:O	1:A:1445:ARG:NH2	2.50	0.43
1:A:1938:ARG:NH1	1:A:2092:GLU:OE2	2.51	0.43
1:A:2507:ILE:HG21	1:A:2547:SER:HB3	2.01	0.43
1:A:3181:ASP:O	1:A:3185:ASN:HB2	2.18	0.43
1:A:3873:LYS:HD2	1:A:3873:LYS:HA	1.83	0.43
1:A:3468:LEU:HA	1:A:3471:ILE:HG22	2.00	0.43
1:A:2957:LEU:HD23	1:A:2957:LEU:HA	1.89	0.43
1:A:3581:PRO:HB2	1:A:3617:LEU:HD22	1.99	0.43
1:A:3838:GLU:OE1	1:A:3874:ARG:NE	2.47	0.43
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:HD22	1:A:178:LEU:HD22	2.01	0.43
1:A:264:ARG:H	1:A:264:ARG:HG2	1.44	0.43
1:A:1949:ILE:HG21	1:A:2100:LEU:HD22	2.00	0.43
1:A:2257:PHE:O	1:A:2261:SER:CB	2.67	0.43
1:A:269:SER:OG	1:A:273:ARG:NH2	2.52	0.43
1:A:3932:MET:HE3	1:A:3932:MET:HB2	1.85	0.43
1:A:2173:ALA:HB3	1:A:2211:LEU:HD22	2.01	0.43
1:A:3049:LEU:HD23	1:A:3085:GLU:HB2	1.99	0.43
1:A:3227:ILE:HA	1:A:3230:LEU:HB2	2.00	0.43
1:A:4078:VAL:O	1:A:4082:ARG:CB	2.59	0.43
1:A:972:LEU:HD23	1:A:972:LEU:HA	1.81	0.43
1:A:1376:LEU:HD23	1:A:1376:LEU:HA	1.84	0.43
1:A:1949:ILE:HA	1:A:1952:ILE:HG22	2.01	0.43
1:A:2097:LEU:HD13	1:A:2100:LEU:HD21	2.00	0.43
1:A:2219:LEU:HD13	1:A:2238:ILE:HG12	2.01	0.43
1:A:3678:GLY:HA3	1:A:3683:CYS:HB2	2.00	0.43
1:A:155:LYS:NZ	1:A:159:GLU:OE2	2.50	0.42
1:A:3090:TYR:O	1:A:3094:ASP:N	2.52	0.42
1:A:3659:PHE:HE2	1:A:3662:ILE:HG22	1.84	0.42
1:A:15:LEU:HA	1:A:18:THR:HG22	2.01	0.42
1:A:1261:LEU:HD21	1:A:1337:VAL:HA	1.99	0.42
1:A:3269:ARG:HB2	1:A:3272:TRP:HB2	2.01	0.42
1:A:348:ILE:HG21	1:A:362:ALA:HB3	2.01	0.42
1:A:660:LEU:HD23	1:A:660:LEU:HA	1.86	0.42
1:A:3529:ILE:HD12	1:A:3529:ILE:HA	1.93	0.42
1:A:1103:ALA:HA	1:A:1106:ILE:HD12	2.01	0.42
1:A:1178:ARG:HD3	1:A:1179:PRO:HD2	2.01	0.42
1:A:2542:LEU:HD23	1:A:2542:LEU:HA	1.90	0.42
1:A:3885:ARG:HA	1:A:3888:VAL:HG12	2.01	0.42
1:A:671:SER:HA	1:A:674:VAL:HG12	2.01	0.42
1:A:1424:THR:OG1	1:A:1425:ALA:N	2.52	0.42
1:A:3095:ASP:OD1	1:A:3095:ASP:N	2.45	0.42
1:A:3262:LEU:O	1:A:3266:SER:N	2.46	0.42
1:A:3480:LEU:HD11	1:A:3510:GLN:HE22	1.85	0.42
1:A:149:ILE:O	1:A:153:PHE:N	2.47	0.42
1:A:254:LYS:HD3	1:A:254:LYS:HA	1.80	0.42
1:A:1795:VAL:HG23	1:A:1798:LEU:HD23	2.01	0.42
1:A:1992:VAL:CG1	1:A:2183:HIS:CD2	3.02	0.42
1:A:3414:MET:HE3	1:A:3414:MET:HB3	1.85	0.42
1:A:1342:MET:O	1:A:1346:THR:HG23	2.19	0.42
1:A:1744:LYS:HA	1:A:1744:LYS:HD2	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1825:LEU:HD22	1:A:1879:VAL:HG21	2.00	0.42
1:A:2341:LEU:HA	1:A:2344:LEU:HB2	2.01	0.42
1:A:919:LEU:HA	1:A:972:LEU:HD21	2.01	0.42
1:A:3466:PRO:HA	1:A:3469:LEU:HB2	2.01	0.42
1:A:3581:PRO:HA	1:A:3584:LEU:HD12	2.01	0.42
1:A:3677:PRO:HB3	1:A:3728:VAL:HB	2.02	0.42
1:A:108:LYS:HE3	1:A:108:LYS:HB3	1.94	0.42
1:A:1097:GLU:OE1	1:A:1098:GLN:NE2	2.52	0.42
1:A:1737:ASN:HA	1:A:1740:VAL:HG22	2.02	0.42
1:A:2919:ASP:OD1	1:A:2922:ARG:NH1	2.52	0.42
1:A:3476:PRO:HA	1:A:3480:LEU:HD13	2.02	0.42
1:A:3706:ASP:OD1	1:A:3706:ASP:N	2.48	0.42
1:A:1888:ASP:OD1	1:A:1888:ASP:N	2.49	0.42
1:A:2986:PRO:HB2	1:A:2991:LYS:HG2	2.01	0.42
1:A:3011:LEU:HD23	1:A:3047:SER:HB3	2.01	0.42
1:A:3096:VAL:HA	1:A:3099:ALA:HB3	2.01	0.42
1:A:3462:ARG:NH1	1:A:3497:SER:OG	2.53	0.42
1:A:896:VAL:HG23	1:A:903:PRO:HD2	2.02	0.41
1:A:1992:VAL:HG12	1:A:2183:HIS:CG	2.55	0.41
1:A:2158:ARG:HD2	1:A:2158:ARG:HA	1.89	0.41
1:A:2491:THR:OG1	1:A:2495:SER:OG	2.37	0.41
1:A:2492:ASP:HB3	1:A:2495:SER:H	1.84	0.41
1:A:2837:LEU:HD11	1:A:2871:LEU:HA	2.01	0.41
1:A:3650:LYS:HB2	1:A:3654:MET:HE3	2.01	0.41
1:A:1171:TRP:O	1:A:1175:HIS:HB2	2.19	0.41
1:A:3054:GLN:OE1	1:A:3054:GLN:N	2.52	0.41
1:A:3588:TRP:HA	1:A:3609:MET:HE2	2.01	0.41
1:A:3938:ILE:HD12	1:A:3938:ILE:HA	1.83	0.41
1:A:4033:VAL:HG12	1:A:4037:ASN:HD21	1.86	0.41
1:A:1504:ASP:HB3	1:A:1507:CYS:H	1.85	0.41
1:A:1680:ALA:N	1:A:1683:LYS:HD3	2.36	0.41
1:A:966:PHE:O	1:A:969:LEU:N	2.54	0.41
1:A:1526:GLU:HA	1:A:1529:VAL:HG22	2.02	0.41
1:A:3341:LEU:HB3	1:A:3348:LEU:HD11	2.03	0.41
1:A:3679:ASN:O	1:A:3725:ARG:NH1	2.54	0.41
1:A:3988:LEU:O	1:A:3992:ARG:HG2	2.21	0.41
1:A:4076:ASP:N	1:A:4076:ASP:OD1	2.51	0.41
1:A:1727:ARG:NH2	1:A:1771:GLN:O	2.54	0.41
1:A:2130:HIS:HB2	1:A:2164:TRP:HE1	1.85	0.41
1:A:2216:LEU:HD13	1:A:2241:LEU:HD23	2.03	0.41
1:A:3027:LEU:HD23	1:A:3027:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ASP:N	1:A:542:ASP:OD1	2.49	0.41
1:A:865:GLN:HB3	1:A:3170:ASP:HB3	2.03	0.41
1:A:1783:ARG:HG2	1:A:1830:HIS:CG	2.55	0.41
1:A:3441:ALA:HB1	1:A:3444:ALA:HB3	2.02	0.41
1:A:726:LEU:HA	1:A:726:LEU:HD23	1.84	0.41
1:A:1354:GLU:O	1:A:1358:LEU:N	2.53	0.41
1:A:2155:GLU:N	1:A:2155:GLU:OE1	2.52	0.41
1:A:2995:GLU:O	1:A:2999:LEU:HG	2.21	0.41
1:A:3013:TYR:O	1:A:3017:ALA:CB	2.68	0.41
1:A:3443:PRO:HA	1:A:3446:VAL:HG12	2.02	0.41
1:A:3851:ASP:OD1	1:A:3851:ASP:N	2.54	0.41
1:A:3982:SER:O	1:A:3986:HIS:ND1	2.54	0.41
1:A:2211:LEU:HD23	1:A:2214:ARG:HD2	2.02	0.41
1:A:2887:PRO:HA	1:A:2890:ILE:HD12	2.03	0.41
1:A:3271:ASP:HA	1:A:3274:VAL:HG22	2.03	0.41
1:A:3314:SER:O	1:A:3314:SER:OG	2.30	0.41
1:A:3489:SER:O	1:A:3489:SER:OG	2.34	0.41
1:A:83:GLU:HG3	1:A:126:PRO:HG2	2.03	0.41
1:A:351:ASN:N	1:A:391:ARG:HH12	2.19	0.41
1:A:621:SER:HA	1:A:624:ILE:HG12	2.01	0.41
1:A:801:LYS:O	1:A:852:ARG:NH1	2.54	0.41
1:A:937:MET:HE3	1:A:937:MET:HB2	1.91	0.41
1:A:1588:ASP:OD1	1:A:1588:ASP:N	2.53	0.41
1:A:1618:LEU:HA	1:A:1621:THR:HG22	2.03	0.41
1:A:3043:TYR:O	1:A:3047:SER:OG	2.31	0.41
1:A:3162:ASN:O	1:A:3166:ASN:HB2	2.20	0.41
1:A:3189:PHE:HA	1:A:3192:LYS:HB2	2.03	0.41
1:A:3710:LYS:HA	1:A:3711:PRO:HD3	1.91	0.41
1:A:4036:LYS:HE3	1:A:4036:LYS:HB3	1.96	0.41
1:A:1069:HIS:CD2	1:A:1074:LYS:HG2	2.56	0.41
1:A:1469:PRO:HD2	1:A:1469:PRO:O	2.20	0.41
1:A:2540:LEU:HD13	1:A:2540:LEU:HA	1.94	0.41
1:A:3825:LYS:HE2	1:A:3825:LYS:HB3	1.86	0.41
1:A:1063:LEU:HA	1:A:1066:LEU:HD12	2.03	0.40
1:A:1101:PHE:HA	1:A:1104:LEU:HB3	2.03	0.40
1:A:1186:LYS:HD3	1:A:1186:LYS:HA	1.78	0.40
1:A:1976:LEU:HG	1:A:1980:ASN:HB2	2.03	0.40
1:A:3672:LYS:HE3	1:A:3672:LYS:HB3	1.78	0.40
1:A:3830:SER:O	1:A:3830:SER:OG	2.38	0.40
1:A:4054:ALA:H	1:A:4103:GLN:NE2	2.19	0.40
1:A:455:LEU:HD13	1:A:455:LEU:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:907:LEU:HG	1:A:910:PHE:HZ	1.86	0.40
1:A:1726:SER:HA	1:A:1772:HIS:CE1	2.57	0.40
1:A:1946:ASN:HA	1:A:1949:ILE:HG12	2.02	0.40
1:A:2154:GLU:H	1:A:2154:GLU:HG3	1.66	0.40
1:A:3136:THR:HA	1:A:3139:GLN:HB3	2.02	0.40
1:A:3179:TRP:HH2	1:A:3241:LYS:HG2	1.86	0.40
1:A:3310:ASN:HB2	1:A:3313:SER:HB3	2.03	0.40
1:A:3877:LYS:HA	1:A:3877:LYS:HD3	1.84	0.40
1:A:1094:SER:N	1:A:1097:GLU:OE2	2.54	0.40
1:A:1369:MET:N	1:A:1369:MET:SD	2.94	0.40
1:A:2385:LEU:HD12	1:A:2385:LEU:HA	1.88	0.40
1:A:2424:MET:HE2	1:A:2435:CYS:HB2	2.03	0.40
1:A:2484:TYR:HD1	1:A:2484:TYR:HA	1.78	0.40
1:A:3329:LEU:HA	1:A:3332:THR:HG22	2.03	0.40
1:A:3729:MET:HB2	1:A:3735:PRO:HD2	2.02	0.40
1:A:98:GLN:HG3	1:A:138:PHE:HE1	1.86	0.40
1:A:463:LYS:HA	1:A:463:LYS:HD2	1.82	0.40
1:A:1573:LYS:HB3	1:A:1573:LYS:HE2	1.91	0.40
1:A:1876:ILE:HD13	1:A:1876:ILE:HA	1.94	0.40
1:A:2441:LYS:HD2	1:A:2441:LYS:HA	1.72	0.40
1:A:3794:VAL:HA	1:A:3795:PRO:HD3	1.93	0.40
1:A:654:ILE:O	1:A:658:THR:OG1	2.34	0.40
1:A:1400:VAL:HG13	1:A:1461:ALA:HB2	2.02	0.40
1:A:3024:PRO:HA	1:A:3025:PRO:HD3	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3527/4128 (85%)	3067 (87%)	449 (13%)	11 (0%)	36	71

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1020	PRO
1	A	399	GLN
1	A	1992	VAL
1	A	2183	HIS
1	A	2467	THR
1	A	167	PRO
1	A	1687	HIS
1	A	1991	PRO
1	A	4032	ASN
1	A	3345	PRO
1	A	1469	PRO

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	3094/3671 (84%)	3074 (99%)	20 (1%)	78 80

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	100	ILE
1	A	162	LEU
1	A	264	ARG
1	A	352	VAL
1	A	521	VAL
1	A	870	LEU
1	A	873	VAL
1	A	874	THR
1	A	1345	THR
1	A	1473	THR
1	A	2142	ILE
1	A	2315	VAL
1	A	2545	LEU

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Mol	Chain	Res	Type
1	A	2944	THR
1	A	3311	ASN
1	A	3505	LEU
1	A	3601	VAL
1	A	3918	LEU
1	A	4033	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	ASN
1	A	303	HIS
1	A	322	GLN
1	A	325	ASN
1	A	339	GLN
1	A	351	ASN
1	A	539	GLN
1	A	562	HIS
1	A	625	ASN
1	A	720	GLN
1	A	739	ASN
1	A	786	GLN
1	A	1049	GLN
1	A	1071	ASN
1	A	1385	ASN
1	A	1589	ASN
1	A	1665	HIS
1	A	1817	GLN
1	A	1859	ASN
1	A	1897	ASN
1	A	1957	ASN
1	A	1989	ASN
1	A	2348	GLN
1	A	2414	GLN
1	A	2432	GLN
1	A	2464	HIS
1	A	2472	GLN
1	A	2475	ASN
1	A	2481	HIS
1	A	2534	ASN
1	A	2553	HIS
1	A	2830	ASN

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Mol	Chain	Res	Type
1	A	2885	GLN
1	A	2977	ASN
1	A	3028	ASN
1	A	3093	GLN
1	A	3113	ASN
1	A	3123	GLN
1	A	3150	ASN
1	A	3154	GLN
1	A	3379	GLN
1	A	3383	GLN
1	A	3422	GLN
1	A	3423	GLN
1	A	3510	GLN
1	A	3524	ASN
1	A	3551	ASN
1	A	3569	GLN
1	A	3577	GLN
1	A	3660	ASN
1	A	3697	ASN
1	A	3783	GLN
1	A	3863	ASN
1	A	3908	HIS
1	A	3924	HIS
1	A	3944	HIS
1	A	4037	ASN
1	A	4088	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.

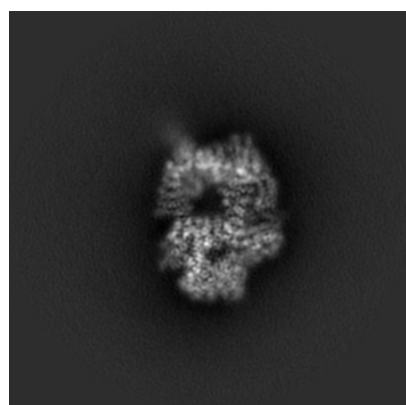
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22622. These allow visual inspection of the internal detail of the map and identification of artifacts.

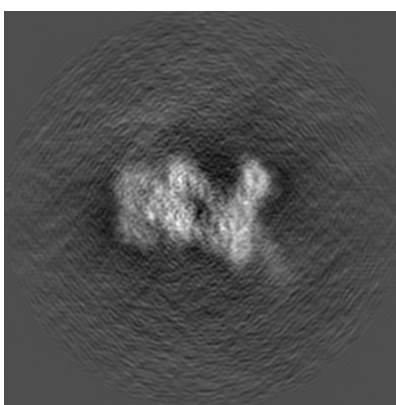
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

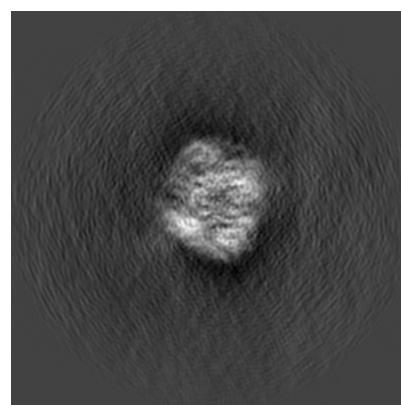
6.1.1 Primary map



X



Y

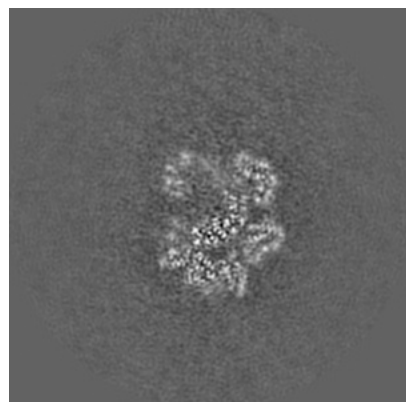


Z

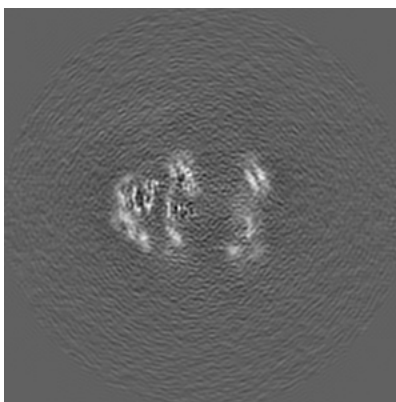
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

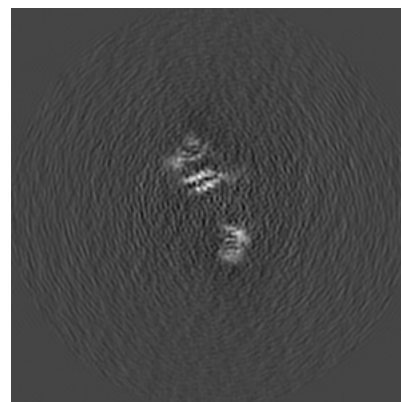
6.2.1 Primary map



X Index: 176



Y Index: 176

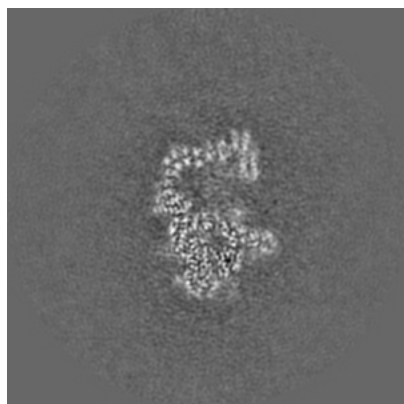


Z Index: 176

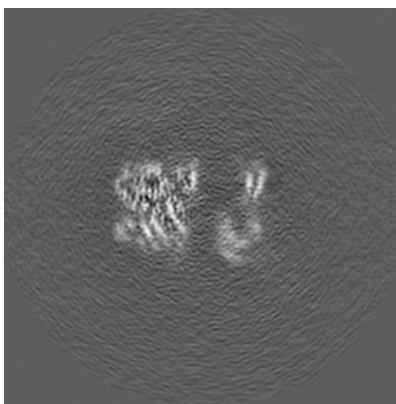
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

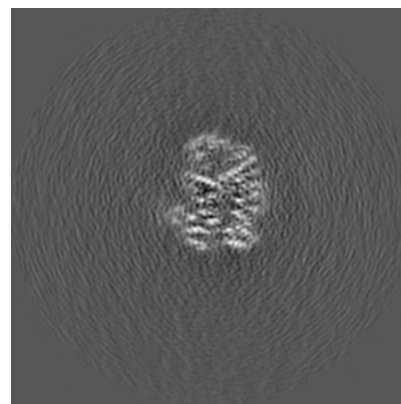
6.3.1 Primary map



X Index: 193



Y Index: 166

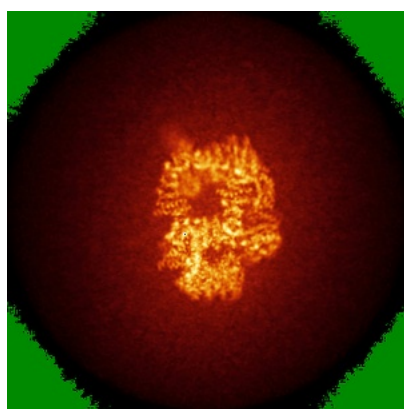


Z Index: 155

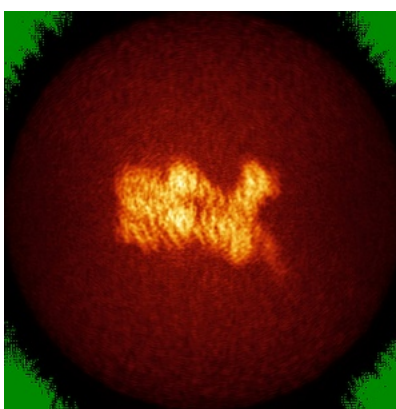
The images above show the largest variance slices of the map in three orthogonal directions.

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

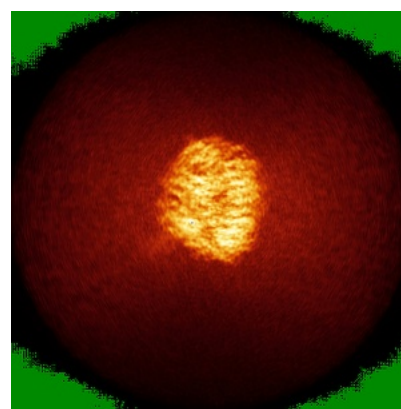
6.4.1 Primary map



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 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

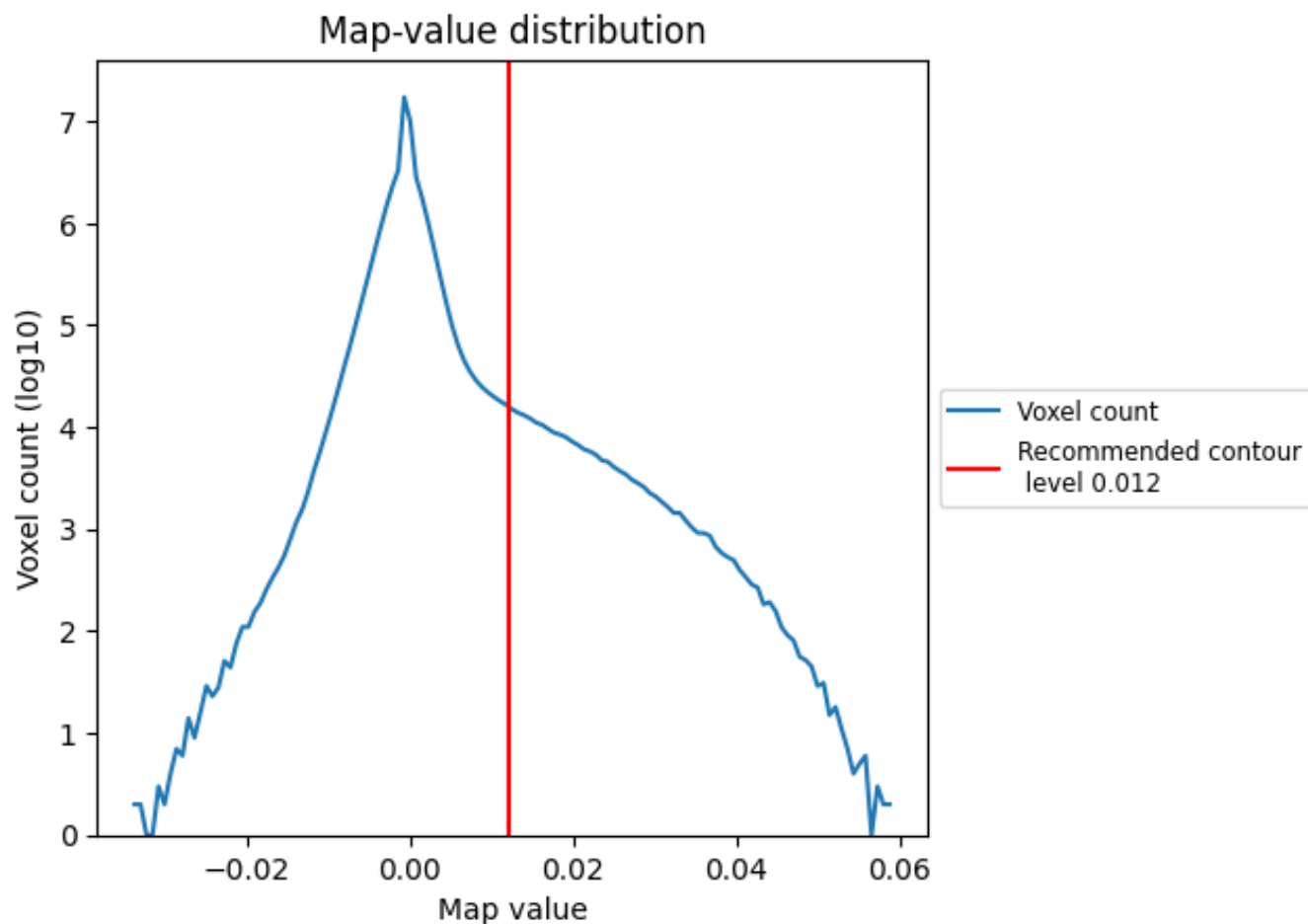
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

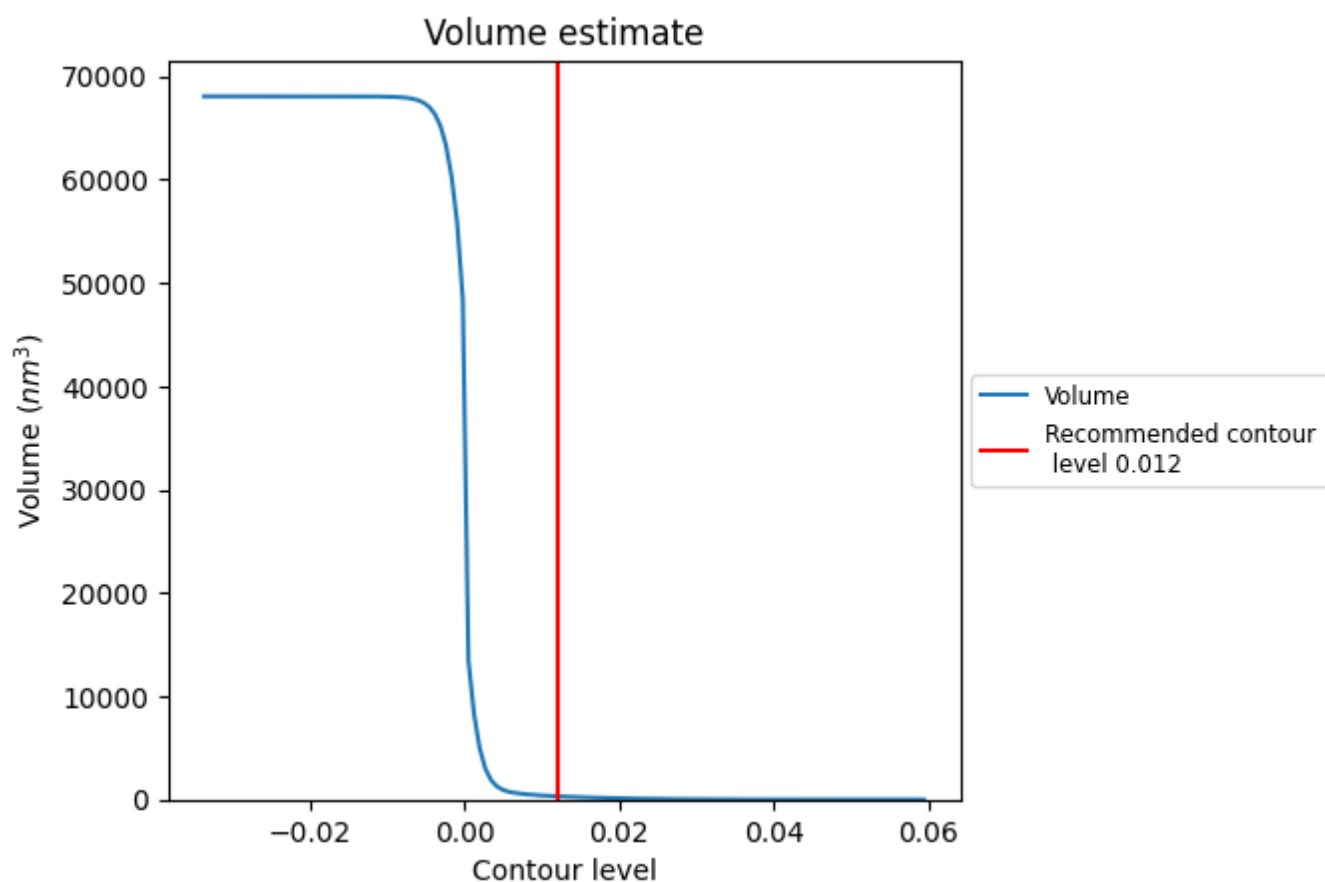
This section contains the results of statistical analysis of the map.

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.

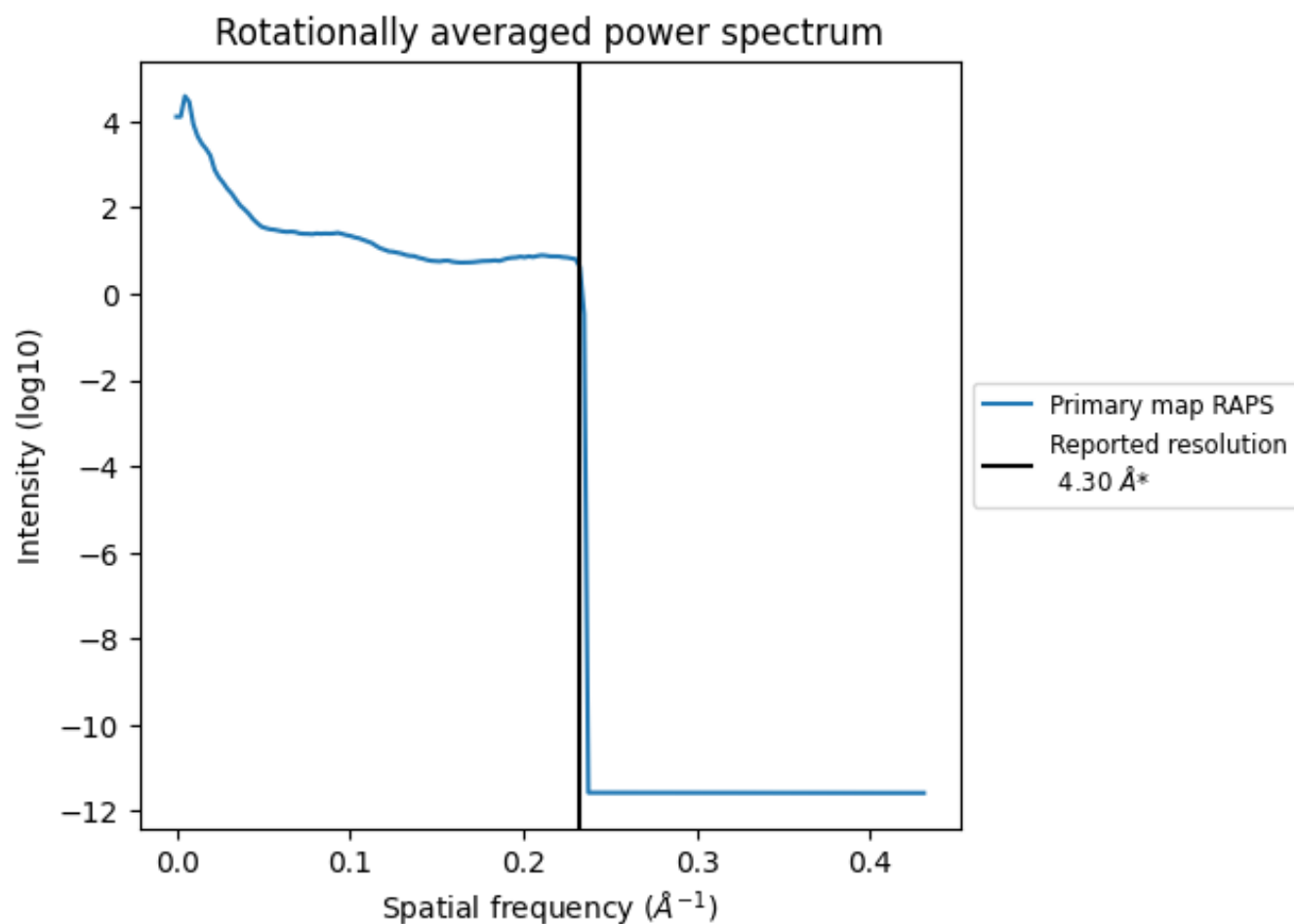
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 317 nm³; this corresponds to an approximate mass of 286 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 0.233 $\text{\AA}^{-1}$

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

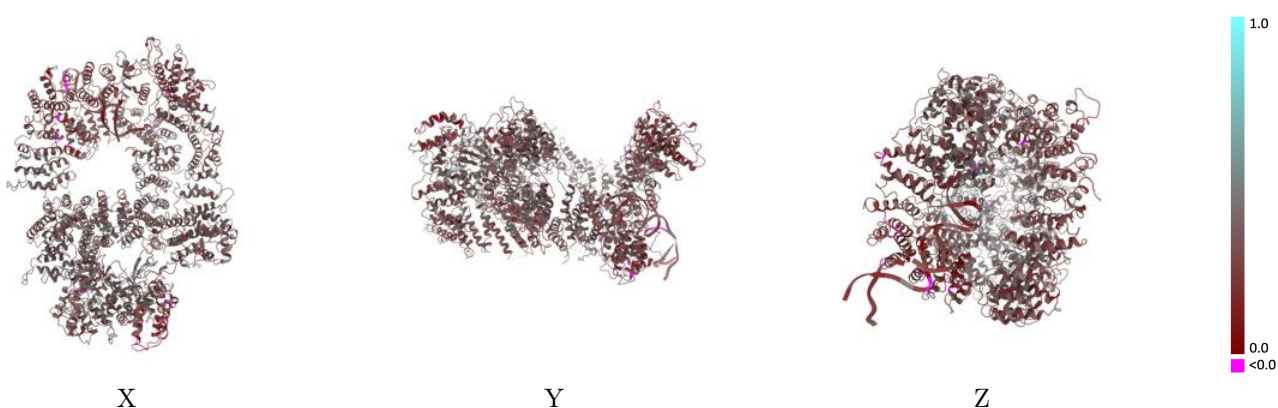
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-22622 and PDB model 7K19. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

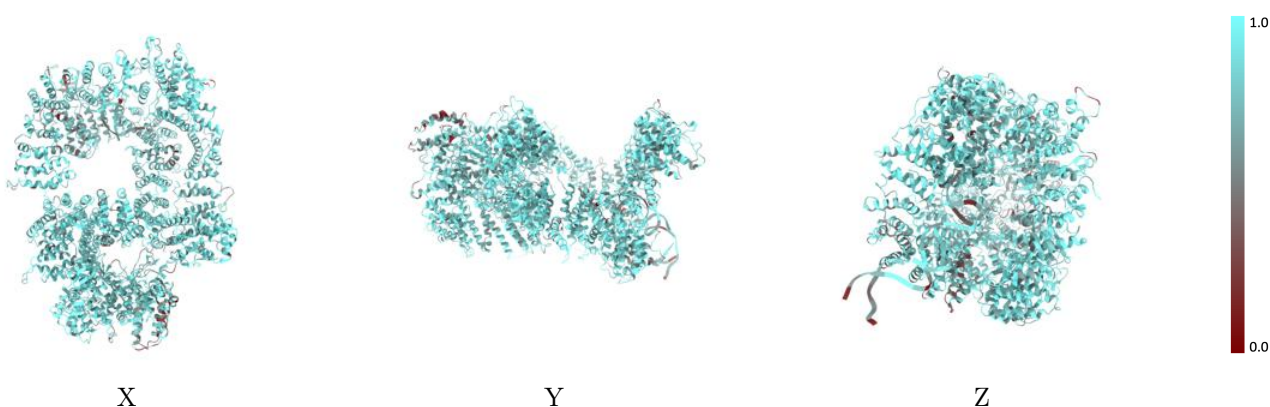
This section was not generated.

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



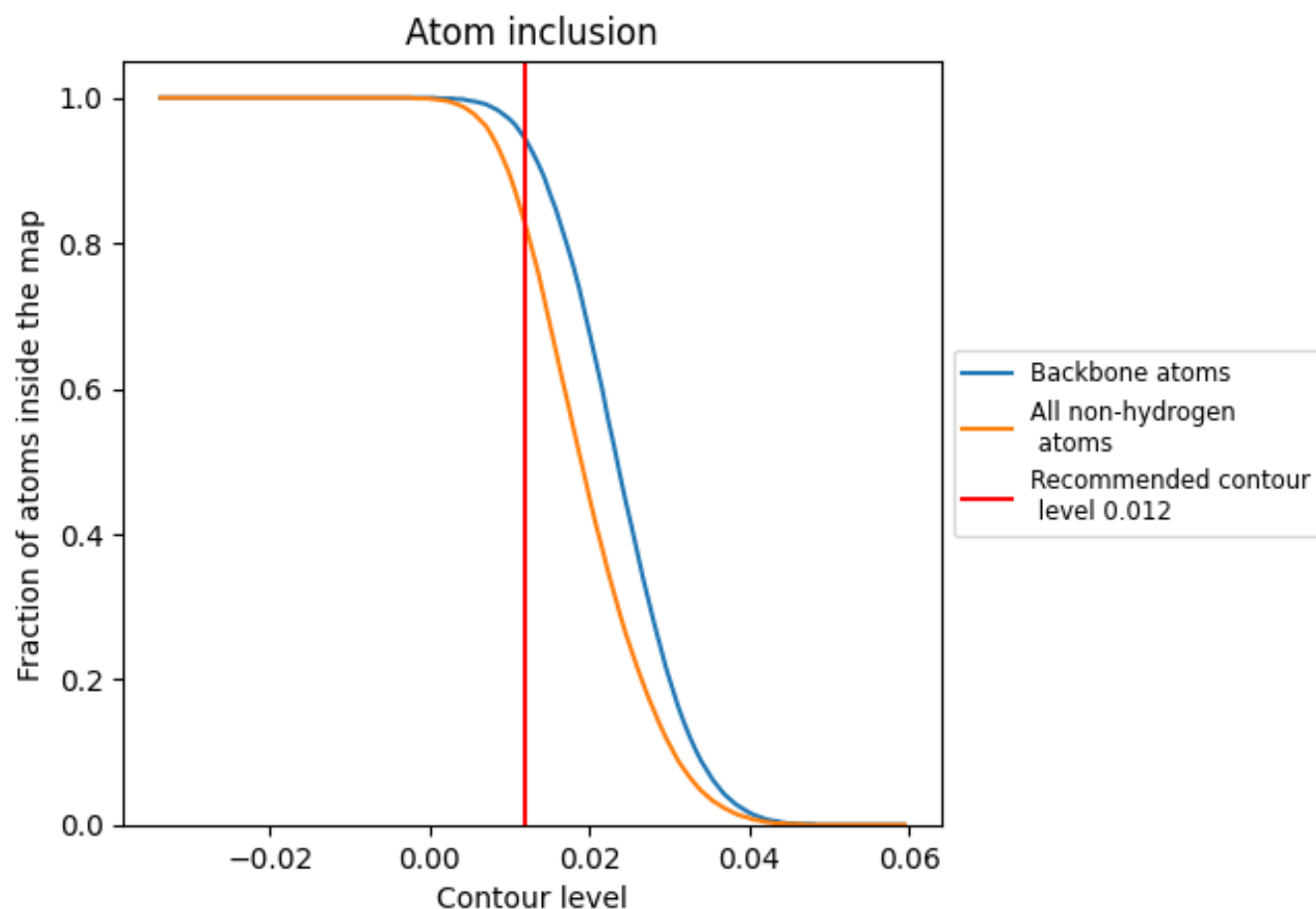
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 82% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8240	0.3390
A	0.8290	0.3430
D	0.6610	0.2000
F	0.5670	0.2560
G	0.7640	0.2420

