



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:25 AM UTC

PDB ID : 7K1N / pdb_00007k1n
EMDB ID : EMD-22626
Title : CryoEM structure of inactivated-form DNA-PK (Complex V)
Authors : Chen, X.; Gellert, M.; Yang, W.
Deposited on : 2020-09-08
Resolution : 3.90 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:

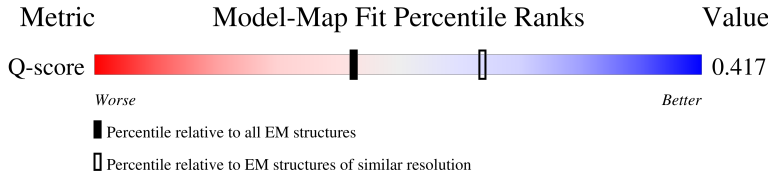
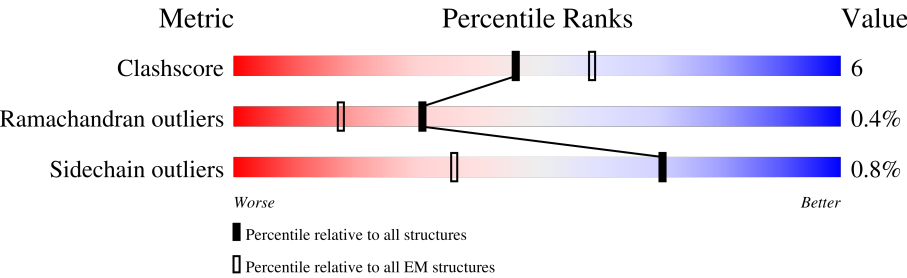
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.90 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.



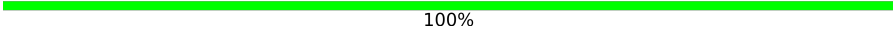
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	B	609	
3	C	732	
4	D	24	

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Mol	Chain	Length	Quality of chain
4	F	24	 8% 88% 12%
5	E	16	 6% 69% 12% 19%
5	G	16	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 39521 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	3634	Total	C	N	O	S	0	0
			28808	18485	4884	5252	187		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	490	Total	C	N	O	S	0	0
			3954	2533	671	733	17		

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	655	Total	C	N	O	S	0	0
			5251	3359	877	989	26		

- Molecule 4 is a DNA chain called DNA (5'-D(P*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
4	D	24	Total	C	N	O	P	0	0
			484	233	82	146	23		
4	F	21	Total	C	N	O	P	0	0
			425	204	69	131	21		

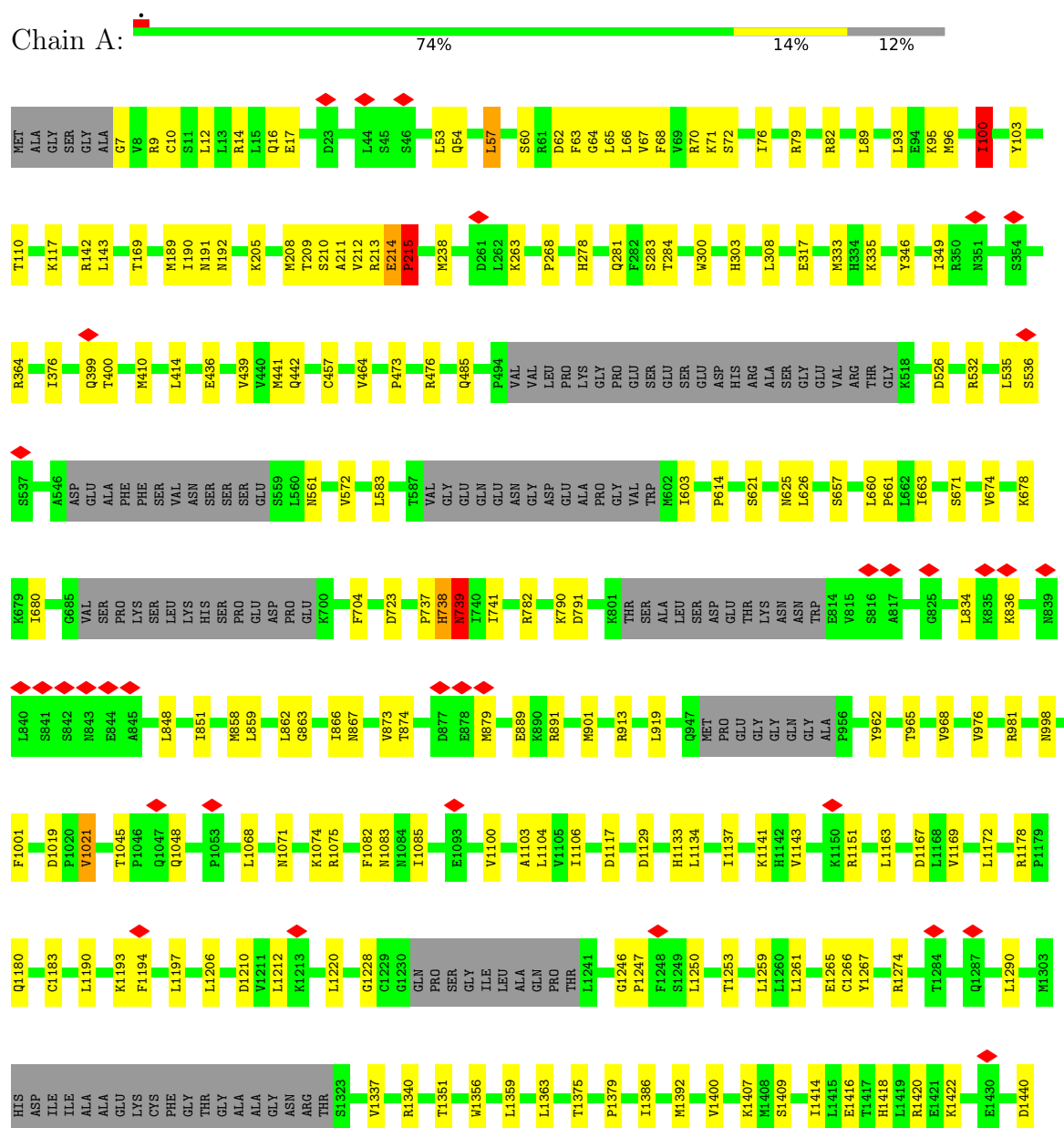
- Molecule 5 is a DNA chain called DNA (5'-D(P*AP*AP*GP*CP*AP*GP*TP*AP*GP*AP*GP*CP*A)-3').

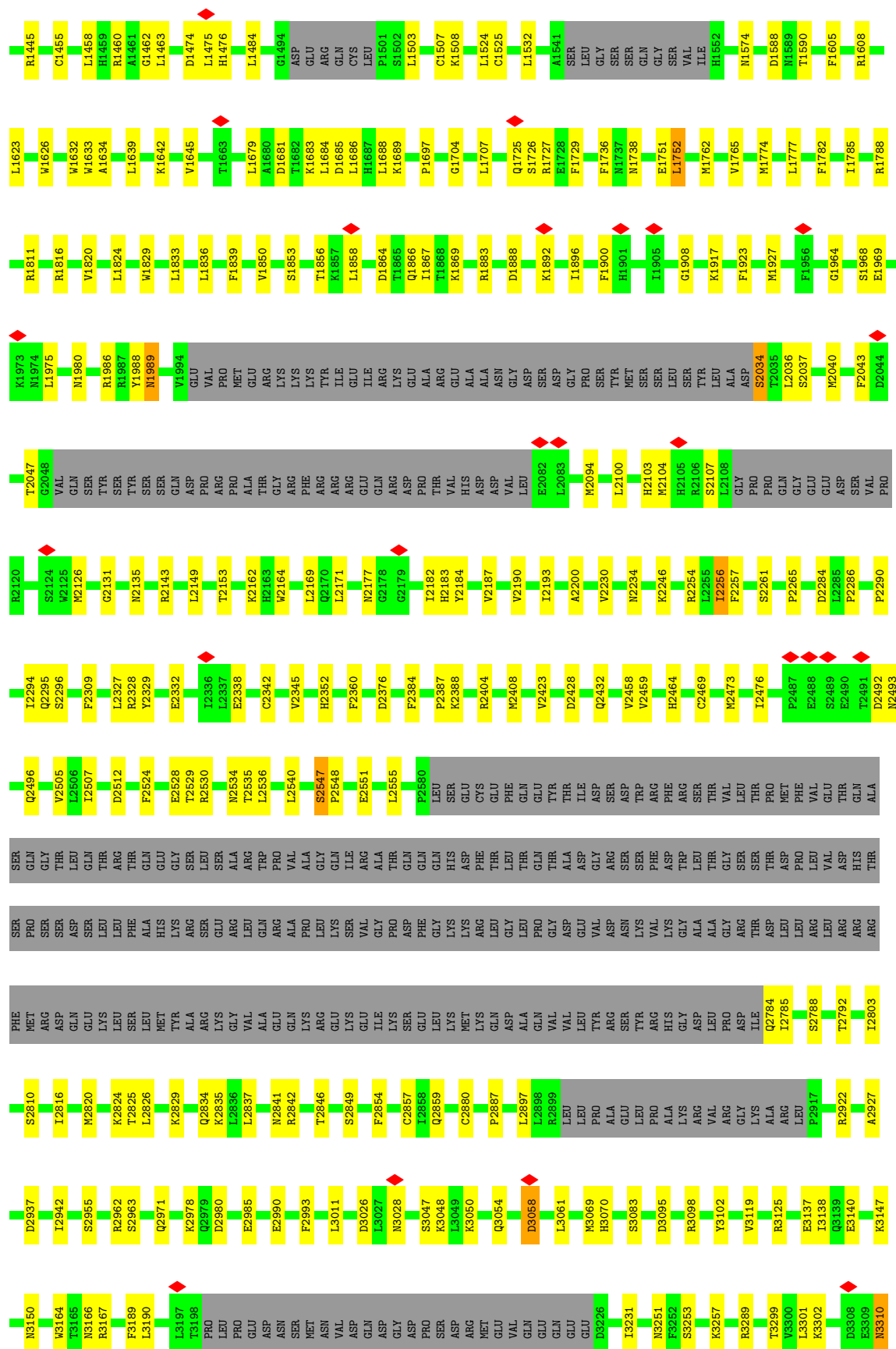
Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	13	Total	C	N	O	P	0	0
			269	128	58	71	12		
5	G	16	Total	C	N	O	P	0	0
			330	157	68	90	15		

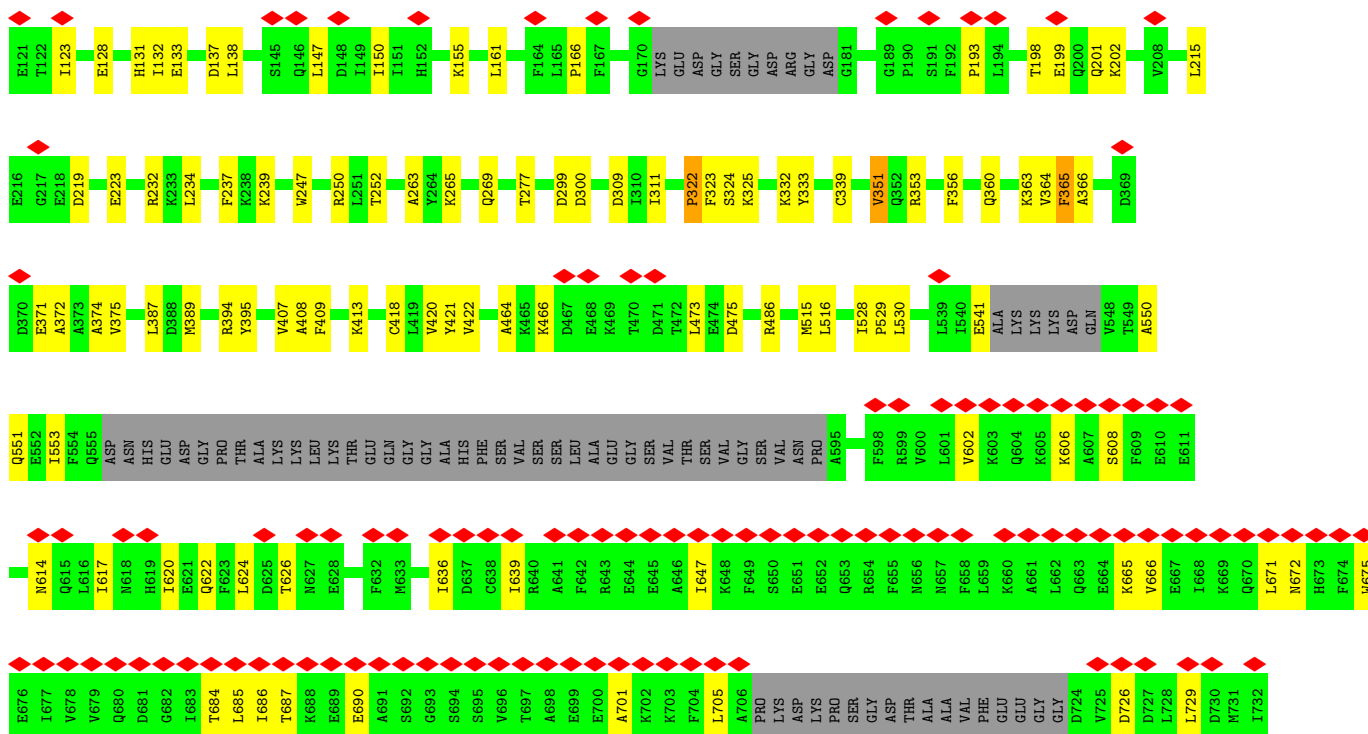
3 Residue-property plots

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.

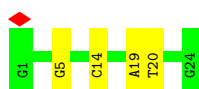
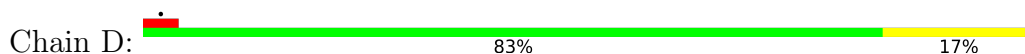
- Molecule 1: DNA-dependent protein kinase catalytic subunit



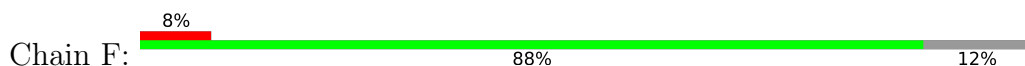




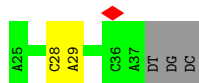
• Molecule 4: DNA (5'-D(P*GP*CP*AP*TP*GP*CP*TP*CP*TP*AP*CP*TP*GP*CP*TP*T
P*CP*GP*AP*TP*AP*TP*CP*G)-3')



• Molecule 4: DNA (5'-D(P*GP*CP*AP*TP*GP*CP*TP*CP*TP*AP*CP*TP*GP*CP*TP*T
P*CP*GP*AP*TP*AP*TP*CP*G)-3')



• Molecule 5: DNA (5'-D(P*AP*AP*GP*CP*AP*GP*TP*AP*GP*AP*GP*CP*A)-3')



• Molecule 5: DNA (5'-D(P*AP*AP*GP*CP*AP*GP*TP*AP*GP*AP*GP*CP*A)-3')



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138985	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	0.104	Depositor
Minimum map value	-0.055	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	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	0.32	0/29394	0.63	29/39755 (0.1%)
2	B	0.29	0/4031	0.63	5/5429 (0.1%)
3	C	0.24	0/5351	0.62	5/7213 (0.1%)
4	D	0.33	0/540	0.50	0/831
4	F	0.32	0/473	0.48	0/727
5	E	0.27	0/304	0.42	0/468
5	G	0.31	0/372	0.45	0/573
All	All	0.30	0/40465	0.62	39/54996 (0.1%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	GLU	CA-C-N	11.64	134.39	119.84
1	A	214	GLU	C-N-CA	11.64	134.39	119.84
1	A	2887	PRO	CB-CA-C	11.39	131.41	112.62
1	A	3311	ASN	N-CA-C	-10.55	88.33	110.80
1	A	739	ASN	N-CA-C	-9.56	101.29	113.72
1	A	1475	LEU	O-C-N	7.41	129.71	122.07
1	A	3641	ASP	N-CA-C	-7.29	106.31	114.62
2	B	498	MET	O-C-N	7.21	129.53	122.03
1	A	738	HIS	O-C-N	6.82	129.03	121.87
2	B	497	LEU	N-CA-C	-6.80	95.20	107.98
1	A	2528	GLU	CA-C-N	6.79	134.50	121.54
1	A	2528	GLU	C-N-CA	6.79	134.50	121.54
1	A	1923	PHE	CA-CB-CG	6.51	120.31	113.80
3	C	364	VAL	CA-C-N	-6.26	109.59	121.54
3	C	364	VAL	C-N-CA	-6.26	109.59	121.54
1	A	3310	ASN	N-CA-C	6.19	118.37	108.41
1	A	190	ILE	N-CA-C	-6.17	106.49	112.29
2	B	244	ARG	CA-C-N	5.98	132.96	121.54
2	B	244	ARG	C-N-CA	5.98	132.96	121.54
1	A	100	ILE	N-CA-C	-5.78	105.75	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	866	ILE	N-CA-C	-5.67	107.29	112.96
1	A	2423	VAL	N-CA-C	-5.62	106.84	113.42
1	A	215	PRO	N-CA-C	5.61	124.03	112.47
1	A	2534	ASN	CA-C-N	5.58	132.20	121.54
1	A	2534	ASN	C-N-CA	5.58	132.20	121.54
1	A	4029	GLN	CA-C-N	5.58	130.33	122.46
1	A	4029	GLN	C-N-CA	5.58	130.33	122.46
1	A	4030	GLU	N-CA-C	5.57	118.87	111.30
1	A	3700	GLU	CA-C-N	5.38	132.09	122.13
1	A	3700	GLU	C-N-CA	5.38	132.09	122.13
1	A	2825	THR	CA-C-N	5.34	131.75	121.54
1	A	2825	THR	C-N-CA	5.34	131.75	121.54
1	A	2034	SER	CA-C-N	5.29	131.65	121.54
1	A	2034	SER	C-N-CA	5.29	131.65	121.54
1	A	3894	PRO	CB-CA-C	5.17	120.28	112.21
3	C	685	LEU	CA-C-N	5.14	128.20	120.69
3	C	685	LEU	C-N-CA	5.14	128.20	120.69
2	B	216	PHE	N-CA-C	5.09	119.14	111.81
3	C	364	VAL	O-C-N	-5.07	116.74	122.72

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	28808	0	29022	346	0
2	B	3954	0	4042	69	0
3	C	5251	0	5269	79	0
4	D	484	0	274	3	0
4	F	425	0	240	0	0
5	E	269	0	146	1	0
5	G	330	0	180	0	0
All	All	39521	0	39173	480	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 6.

All (480) 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:3352:GLU:HG3	1:A:3355:LYS:HG3	1.38	1.00
1:A:7:GLY:N	1:A:10:CYS:HG	1.69	0.90
1:A:3352:GLU:HG3	1:A:3355:LYS:CG	2.13	0.77
1:A:1416:GLU:O	1:A:1420:ARG:HB2	1.86	0.74
2:B:495:LEU:HB3	2:B:497:LEU:CD2	2.24	0.68
2:B:165:ARG:HA	2:B:199:PHE:O	1.94	0.68
2:B:495:LEU:HB3	2:B:497:LEU:HD23	1.76	0.68
1:A:1151:ARG:HD2	1:A:1163:LEU:H	1.60	0.66
1:A:3586:LYS:HG2	1:A:3667:LEU:HD21	1.78	0.66
3:C:387:LEU:HB3	3:C:389:MET:HG2	1.78	0.66
1:A:3647:GLY:HA2	1:A:3651:LEU:HB2	1.78	0.65
1:A:1206:LEU:O	1:A:1210:ASP:HB2	1.95	0.65
2:B:264:ASN:HD22	3:C:530:LEU:HD13	1.62	0.65
1:A:3630:ARG:HG2	1:A:3632:PHE:H	1.63	0.64
1:A:4028:ILE:HG22	1:A:4029:GLN:HG2	1.81	0.63
1:A:1356:TRP:HE1	1:A:1409:SER:HB2	1.63	0.62
3:C:408:ALA:HA	3:C:420:VAL:O	1.99	0.62
1:A:901:MET:HE1	1:A:2816:ILE:HG23	1.82	0.61
2:B:35:ARG:NH2	2:B:80:ARG:O	2.34	0.61
3:C:409:PHE:HB2	3:C:420:VAL:HG22	1.84	0.60
1:A:1178:ARG:NH1	1:A:1183:CYS:SG	2.75	0.60
1:A:54:GLN:HA	1:A:57:LEU:HB3	1.84	0.60
2:B:36:ASP:OD1	2:B:36:ASP:N	2.35	0.59
2:B:368:VAL:HG13	2:B:434:LEU:HD11	1.84	0.59
1:A:1375:THR:HA	1:A:1379:PRO:HB3	1.84	0.59
1:A:3648:GLY:O	1:A:3653:ARG:NH1	2.36	0.59
1:A:2524:PHE:O	1:A:2530:ARG:NH2	2.36	0.59
1:A:2536:LEU:HD21	1:A:2820:MET:HE3	1.85	0.59
2:B:204:HIS:O	2:B:237:SER:N	2.36	0.59
1:A:215:PRO:HD3	3:C:550:ALA:HB2	1.85	0.59
1:A:1704:GLY:HA2	1:A:1707:LEU:HB3	1.85	0.59
1:A:859:LEU:O	1:A:867:ASN:ND2	2.36	0.59
1:A:791:ASP:OD1	1:A:791:ASP:N	2.36	0.59
3:C:466:LYS:HA	3:C:473:LEU:HA	1.85	0.59
3:C:684:THR:HG21	3:C:705:LEU:HD21	1.84	0.59
1:A:1266:CYS:SG	1:A:1267:TYR:N	2.75	0.58
1:A:3959:MET:SD	1:A:3959:MET:N	2.73	0.58
2:B:413:LEU:HB3	2:B:432:PHE:HD2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3755:GLY:HA2	1:A:3799:ARG:HB2	1.86	0.58
3:C:11:VAL:HB	3:C:132:ILE:HG12	1.85	0.58
2:B:241:ASP:OD1	2:B:241:ASP:N	2.37	0.58
1:A:3831:ASP:HB3	1:A:3834:ALA:HB2	1.86	0.58
1:A:1684:LEU:HB3	1:A:1688:LEU:HB2	1.86	0.58
1:A:1969:GLU:HB2	1:A:1975:LEU:HB3	1.85	0.58
1:A:3050:LYS:O	1:A:3054:GLN:NE2	2.37	0.57
1:A:3327:ASN:HB2	1:A:3388:ALA:HB2	1.86	0.57
1:A:72:SER:O	1:A:82:ARG:NH1	2.37	0.57
3:C:131:HIS:NE2	3:C:133:GLU:OE2	2.38	0.57
1:A:1274:ARG:NH1	1:A:1351:THR:OG1	2.38	0.57
1:A:3515:GLN:NE2	1:A:3551:ASN:OD1	2.38	0.57
3:C:407:VAL:O	3:C:421:TYR:HA	2.05	0.57
1:A:998:ASN:HA	1:A:1001:PHE:HB2	1.87	0.57
1:A:1190:LEU:O	1:A:1194:PHE:HB2	2.05	0.56
1:A:3119:VAL:O	1:A:3125:ARG:NH2	2.38	0.56
1:A:3289:ARG:NH1	1:A:3993:SER:OG	2.38	0.56
1:A:1261:LEU:HD13	1:A:1337:VAL:HG12	1.88	0.56
1:A:3595:GLU:OE2	1:A:3602:ASN:ND2	2.37	0.56
2:B:48:MET:SD	2:B:48:MET:N	2.77	0.56
3:C:76:ASN:ND2	3:C:103:GLN:O	2.38	0.56
1:A:1829:TRP:O	1:A:1883:ARG:NH2	2.38	0.56
1:A:2177:ASN:HB3	1:A:2182:ILE:HG12	1.86	0.56
1:A:3299:THR:HA	1:A:3302:LYS:HE3	1.87	0.56
1:A:2458:VAL:HG11	1:A:2476:ILE:HD11	1.86	0.56
2:B:245:LYS:O	2:B:245:LYS:HG3	2.05	0.56
3:C:265:LYS:NZ	3:C:360:GLN:OE1	2.37	0.56
1:A:1681:ASP:HB3	1:A:1683:LYS:HE3	1.87	0.56
1:A:1751:GLU:O	1:A:1788:ARG:NH2	2.39	0.56
1:A:2143:ARG:HG2	1:A:2171:LEU:HD21	1.88	0.56
1:A:3314:SER:O	1:A:3318:LYS:NZ	2.39	0.56
2:B:144:SER:HB3	2:B:186:ALA:HA	1.88	0.56
2:B:399:ARG:NH2	3:C:516:LEU:O	2.38	0.56
1:A:657:SER:HA	1:A:660:LEU:HB2	1.88	0.56
1:A:901:MET:SD	1:A:2535:THR:OG1	2.63	0.56
1:A:3190:LEU:HD22	1:A:3231:ILE:HG23	1.88	0.56
1:A:3352:GLU:HB3	1:A:3355:LYS:HB2	1.87	0.56
1:A:2963:SER:OG	1:A:3251:ASN:ND2	2.39	0.55
1:A:1104:LEU:HD12	1:A:1134:LEU:HD23	1.88	0.55
1:A:10:CYS:SG	1:A:14:ARG:NH2	2.73	0.55
1:A:4083:GLY:HA3	1:A:4091:ALA:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:SER:HB2	2:B:332:GLU:HG3	1.88	0.55
1:A:723:ASP:OD1	1:A:723:ASP:N	2.37	0.55
1:A:1021:VAL:O	1:A:1021:VAL:HG13	2.06	0.55
1:A:1833:LEU:HB3	1:A:1836:LEU:HB2	1.88	0.55
1:A:2810:SER:HG	1:A:2857:CYS:HG	1.53	0.55
1:A:3360:LEU:HG	1:A:3373:VAL:HG11	1.88	0.55
1:A:1129:ASP:O	1:A:1133:HIS:ND1	2.40	0.55
1:A:3573:ASN:HB3	1:A:3627:ALA:HB2	1.89	0.55
2:B:495:LEU:CB	2:B:497:LEU:HD21	2.37	0.55
3:C:137:ASP:HA	3:C:166:PRO:HD3	1.89	0.55
1:A:442:GLN:NE2	1:A:457:CYS:SG	2.79	0.55
1:A:2230:VAL:O	1:A:2234:ASN:ND2	2.40	0.55
1:A:3484:THR:HG22	1:A:3513:ALA:HA	1.88	0.55
3:C:66:ASN:ND2	3:C:68:LEU:O	2.38	0.55
1:A:1228:GLY:HA3	1:A:1259:LEU:HD13	1.89	0.55
3:C:371:GLU:HB2	3:C:374:ALA:HB3	1.87	0.55
1:A:3253:SER:O	1:A:3257:LYS:NZ	2.39	0.54
3:C:57:VAL:HG22	3:C:79:VAL:HG12	1.89	0.54
1:A:1071:ASN:O	1:A:1075:ARG:NH1	2.41	0.54
1:A:1075:ARG:NH2	1:A:1117:ASP:OD1	2.38	0.54
5:E:28:DC:H2"	5:E:29:DA:C8	2.42	0.54
2:B:74:LYS:HE2	2:B:83:LEU:HD11	1.89	0.54
1:A:2376:ASP:OD1	1:A:2404:ARG:NH2	2.41	0.54
1:A:526:ASP:OD1	1:A:526:ASP:N	2.39	0.54
1:A:3378:TYR:OH	1:A:3426:LYS:NZ	2.40	0.54
1:A:4088:ASN:ND2	1:A:4113:ASP:OD2	2.39	0.54
1:A:414:LEU:HD12	1:A:464:VAL:HG21	1.88	0.54
1:A:621:SER:O	1:A:625:ASN:ND2	2.40	0.54
2:B:219:ASP:OD1	2:B:219:ASP:N	2.40	0.54
1:A:7:GLY:N	1:A:10:CYS:SG	2.76	0.54
1:A:3813:LYS:HB2	1:A:3925:LEU:HB3	1.89	0.54
2:B:95:ASN:HD21	2:B:99:PHE:HB2	1.73	0.54
1:A:1400:VAL:HG11	1:A:1460:ARG:HG2	1.90	0.54
1:A:14:ARG:HA	1:A:17:GLU:HB2	1.90	0.54
1:A:1414:ILE:O	1:A:1418:HIS:ND1	2.36	0.54
3:C:219:ASP:OD1	3:C:219:ASP:N	2.35	0.54
1:A:212:VAL:HG12	1:A:213:ARG:HB2	1.88	0.53
1:A:3714:GLU:O	1:A:3718:ARG:NH1	2.42	0.53
1:A:76:ILE:O	1:A:79:ARG:NH1	2.42	0.53
2:B:262:LYS:HZ1	2:B:346:MET:HE2	1.74	0.53
2:B:249:LYS:NZ	2:B:250:GLU:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1143:VAL:HG23	1:A:1197:LEU:HD21	1.90	0.53
1:A:4006:VAL:HA	1:A:4011:PHE:HZ	1.73	0.53
1:A:1100:VAL:HA	1:A:1103:ALA:HB3	1.90	0.53
1:A:2034:SER:N	1:A:2037:SER:HG	2.05	0.53
1:A:4049:ARG:NH2	1:A:4062:ASP:OD2	2.38	0.53
3:C:111:LEU:HD11	3:C:150:ILE:HD12	1.91	0.53
1:A:2962:ARG:NH1	1:A:4101:GLU:OE2	2.42	0.53
2:B:95:ASN:OD1	2:B:95:ASN:N	2.41	0.53
1:A:1267:TYR:HE2	1:A:1290:LEU:HD13	1.73	0.53
1:A:1820:VAL:HG23	1:A:1824:LEU:HD11	1.90	0.52
2:B:143:LEU:HD23	2:B:182:LYS:HE3	1.90	0.52
3:C:687:THR:HG22	3:C:701:ALA:HB2	1.90	0.52
1:A:2103:HIS:O	1:A:2107:SER:CB	2.58	0.52
1:A:572:VAL:HG23	1:A:626:LEU:HD11	1.92	0.52
1:A:2978:LYS:NZ	1:A:2985:GLU:OE2	2.43	0.52
2:B:59:PRO:HA	2:B:62:MET:HE2	1.92	0.52
2:B:49:PHE:O	2:B:128:GLN:NE2	2.42	0.52
1:A:1169:VAL:HA	1:A:1172:LEU:HD12	1.92	0.52
2:B:453:MET:HE3	2:B:454:ALA:H	1.74	0.52
1:A:60:SER:OG	1:A:63:PHE:O	2.26	0.52
1:A:278:HIS:HB3	1:A:281:GLN:HG3	1.92	0.52
1:A:3654:MET:HE3	1:A:3656:LEU:HB2	1.92	0.52
1:A:3652:LEU:HD22	1:A:3653:ARG:HH21	1.75	0.51
1:A:2384:PHE:O	1:A:2388:LYS:NZ	2.43	0.51
1:A:4010:SER:O	1:A:4015:ASN:ND2	2.43	0.51
3:C:250:ARG:HH21	3:C:252:THR:HG21	1.75	0.51
1:A:9:ARG:HA	1:A:12:LEU:HD13	1.92	0.51
1:A:603:ILE:HG13	1:A:1083:ASN:HB3	1.91	0.51
1:A:2254:ARG:HA	1:A:2257:PHE:HB3	1.92	0.51
1:A:2493:ASN:HA	1:A:2496:GLN:HE21	1.74	0.51
1:A:3602:ASN:N	1:A:3602:ASN:OD1	2.42	0.51
2:B:55:ASP:OD1	2:B:55:ASP:N	2.43	0.51
1:A:142:ARG:HE	1:A:143:LEU:H	1.58	0.51
1:A:1634:ALA:O	1:A:1642:LYS:NZ	2.43	0.51
1:A:1440:ASP:OD1	1:A:1440:ASP:N	2.35	0.51
1:A:3048:LYS:HB3	1:A:3061:LEU:HD22	1.92	0.51
1:A:3147:LYS:HB3	1:A:3150:ASN:HB2	1.93	0.51
2:B:505:ASP:OD2	3:C:333:TYR:OH	2.28	0.51
1:A:739:ASN:OD1	1:A:739:ASN:N	2.44	0.51
1:A:3137:GLU:OE2	1:A:3167:ARG:NH2	2.42	0.51
2:B:52:GLN:HE22	2:B:207:LYS:HA	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:624:LEU:HD12	3:C:665:LYS:HE2	1.92	0.51
1:A:3026:ASP:N	1:A:3026:ASP:OD1	2.44	0.51
1:A:1206:LEU:O	1:A:1210:ASP:CB	2.58	0.51
1:A:1685:ASP:H	1:A:1688:LEU:HD12	1.75	0.51
1:A:1726:SER:OG	1:A:1727:ARG:N	2.44	0.51
1:A:1986:ARG:NH2	1:A:1988:TYR:OH	2.43	0.51
1:A:3508:LYS:NZ	1:A:3509:ASP:O	2.44	0.51
2:B:480:ASN:O	2:B:484:GLN:HB2	2.11	0.51
3:C:223:GLU:OE2	3:C:239:LYS:NZ	2.43	0.50
1:A:1407:LYS:NZ	1:A:1462:GLY:O	2.44	0.50
1:A:2131:GLY:O	1:A:2135:ASN:ND2	2.44	0.50
3:C:6:ASN:ND2	3:C:128:GLU:OE1	2.43	0.50
1:A:1019:ASP:OD1	1:A:1019:ASP:N	2.43	0.50
1:A:2824:LYS:O	1:A:2829:LYS:NZ	2.38	0.50
1:A:3354:ASP:OD1	1:A:3354:ASP:N	2.44	0.50
1:A:1836:LEU:HD21	1:A:1839:PHE:HB3	1.93	0.50
3:C:17:GLY:O	3:C:20:MET:HB3	2.11	0.50
1:A:189:MET:HG2	1:A:192:ASN:HD21	1.77	0.50
1:A:738:HIS:ND1	1:A:741:ILE:O	2.44	0.50
1:A:2507:ILE:HG21	1:A:2547:SER:HB3	1.93	0.50
2:B:266:ASP:OD1	2:B:266:ASP:N	2.43	0.50
1:A:1418:HIS:O	1:A:1422:LYS:NZ	2.36	0.50
1:A:1888:ASP:OD1	1:A:1888:ASP:N	2.42	0.50
2:B:245:LYS:O	2:B:246:VAL:HG22	2.11	0.50
2:B:288:LEU:HB3	3:C:311:ILE:HG13	1.93	0.50
1:A:16:GLN:NE2	1:A:62:ASP:O	2.45	0.49
1:A:889:GLU:O	1:A:891:ARG:NH1	2.45	0.49
1:A:2149:LEU:O	1:A:2153:THR:OG1	2.29	0.49
1:A:2897:LEU:HD11	1:A:2922:ARG:HB3	1.94	0.49
1:A:3588:TRP:NE1	1:A:3609:MET:SD	2.80	0.49
2:B:35:ARG:HH22	2:B:80:ARG:HB2	1.77	0.49
2:B:86:VAL:HG13	2:B:104:VAL:HG12	1.93	0.49
3:C:63:GLY:O	3:C:78:THR:OG1	2.30	0.49
1:A:66:LEU:HD11	1:A:110:THR:HG21	1.94	0.49
1:A:399:GLN:HG3	1:A:400:THR:HG23	1.94	0.49
1:A:2428:ASP:O	1:A:2432:GLN:NE2	2.44	0.49
1:A:3140:GLU:OE2	1:A:3164:TRP:NE1	2.45	0.49
2:B:194:ARG:NH1	2:B:219:ASP:O	2.46	0.49
2:B:202:LEU:HG	2:B:221:ILE:HD12	1.94	0.49
1:A:2100:LEU:HG	1:A:2104:MET:HE3	1.93	0.49
1:A:1068:LEU:HD21	1:A:1106:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1178:ARG:HG2	1:A:1180:GLN:H	1.77	0.49
1:A:1588:ASP:N	1:A:1588:ASP:OD1	2.46	0.49
1:A:2290:PRO:HB3	1:A:2295:GLN:HA	1.94	0.49
1:A:1503:LEU:HD13	1:A:1508:LYS:HE2	1.94	0.48
2:B:507:THR:OG1	3:C:394:ARG:NH1	2.45	0.48
1:A:2551:GLU:OE2	1:A:2849:SER:OG	2.30	0.48
1:A:2990:GLU:HA	1:A:2993:PHE:HB3	1.95	0.48
1:A:3468:LEU:HA	1:A:3471:ILE:HG22	1.95	0.48
1:A:3700:GLU:OE2	1:A:3716:HIS:ND1	2.36	0.48
2:B:107:GLU:O	2:B:115:ARG:NH1	2.37	0.48
3:C:199:GLU:HA	3:C:202:LYS:HD2	1.95	0.48
1:A:1455:CYS:HA	1:A:1458:LEU:HD12	1.95	0.48
1:A:535:LEU:O	1:A:561:ASN:ND2	2.46	0.48
1:A:1440:ASP:O	1:A:1445:ARG:NH1	2.46	0.48
2:B:326:GLN:HE21	2:B:328:ILE:HD11	1.77	0.48
1:A:100:ILE:HG22	1:A:103:TYR:HB2	1.96	0.48
1:A:737:PRO:O	1:A:739:ASN:OD1	2.32	0.48
1:A:1853:SER:OG	1:A:1866:GLN:NE2	2.46	0.48
1:A:2859:GLN:NE2	1:A:2880:CYS:SG	2.77	0.48
1:A:333:MET:SD	1:A:333:MET:N	2.76	0.48
1:A:1045:THR:OG1	1:A:1048:GLN:NE2	2.46	0.48
1:A:1265:GLU:OE2	1:A:1340:ARG:NE	2.42	0.48
1:A:268:PRO:HB2	1:A:308:LEU:HD11	1.96	0.48
1:A:4011:PHE:HA	1:A:4015:ASN:HD22	1.78	0.48
1:A:169:THR:OG1	4:D:14:DC:OP1	2.30	0.48
1:A:1359:LEU:HB3	1:A:1363:LEU:HD21	1.95	0.48
1:A:2103:HIS:O	1:A:2107:SER:HB3	2.13	0.48
1:A:2265:PRO:HB3	1:A:2309:PHE:CG	2.49	0.48
1:A:3590:ASN:HA	1:A:3593:ARG:HG2	1.94	0.48
1:A:2162:LYS:HA	1:A:2200:ALA:HB2	1.96	0.48
1:A:1167:ASP:OD1	1:A:1167:ASP:N	2.44	0.48
2:B:416:GLN:NE2	2:B:433:GLN:OE1	2.40	0.48
1:A:191:ASN:OD1	1:A:191:ASN:N	2.47	0.47
3:C:636:ILE:HA	3:C:639:ILE:HG12	1.95	0.47
1:A:1250:LEU:O	1:A:1253:THR:OG1	2.28	0.47
1:A:2290:PRO:HD3	1:A:2296:SER:HB3	1.95	0.47
1:A:2540:LEU:HD11	1:A:2835:LYS:HD2	1.95	0.47
1:A:2555:LEU:HD21	1:A:2854:PHE:HD1	1.79	0.47
1:A:3069:MET:O	1:A:3070:HIS:ND1	2.48	0.47
2:B:495:LEU:HD22	2:B:497:LEU:HD21	1.97	0.47
1:A:3448:GLU:HG2	1:A:3482:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3471:ILE:O	1:A:3475:TYR:HB2	2.13	0.47
1:A:3751:LEU:HB3	1:A:3803:ILE:HG23	1.95	0.47
1:A:671:SER:HA	1:A:674:VAL:HG12	1.97	0.47
1:A:3457:ASN:OD1	1:A:3494:GLN:NE2	2.47	0.47
1:A:2246:LYS:NZ	1:A:2284:ASP:OD2	2.47	0.47
1:A:2937:ASP:OD1	1:A:3784:ARG:NH2	2.46	0.47
1:A:3786:LEU:HD22	1:A:3910:LEU:HD22	1.97	0.47
3:C:351:VAL:HG21	3:C:407:VAL:HG21	1.97	0.47
1:A:2103:HIS:O	1:A:2107:SER:OG	2.32	0.47
1:A:2459:VAL:HB	1:A:2505:VAL:HG21	1.96	0.47
2:B:375:VAL:HG12	3:C:541:GLU:HB2	1.96	0.47
1:A:1407:LYS:HD3	1:A:1463:LEU:HD12	1.96	0.47
3:C:309:ASP:OD1	3:C:309:ASP:N	2.39	0.47
3:C:365:PHE:CD2	3:C:366:ALA:N	2.83	0.47
3:C:672:ASN:HA	3:C:675:TRP:HB2	1.96	0.47
1:A:583:LEU:HA	1:A:614:PRO:HA	1.97	0.46
1:A:1071:ASN:HD22	1:A:1074:LYS:HG3	1.80	0.46
1:A:1762:MET:HA	1:A:1765:VAL:HG12	1.97	0.46
1:A:2327:LEU:HD11	1:A:2345:VAL:HG11	1.96	0.46
1:A:3620:PRO:HG2	1:A:3621:LYS:HE2	1.96	0.46
1:A:3761:ASP:HA	1:A:3764:VAL:HG22	1.97	0.46
1:A:1782:PHE:HA	1:A:1785:ILE:HD12	1.96	0.46
1:A:3658:ASP:OD1	1:A:3658:ASP:N	2.47	0.46
1:A:4044:ILE:O	1:A:4048:LYS:HB2	2.15	0.46
3:C:11:VAL:O	3:C:132:ILE:HA	2.15	0.46
3:C:666:VAL:O	3:C:675:TRP:NE1	2.40	0.46
1:A:2184:TYR:HA	1:A:2187:VAL:HG22	1.97	0.46
1:A:4099:SER:O	1:A:4103:GLN:HB2	2.15	0.46
1:A:962:TYR:HA	1:A:965:THR:HG22	1.97	0.46
1:A:1686:LEU:HB3	1:A:1738:ASN:HD21	1.80	0.46
1:A:2837:LEU:O	1:A:2841:ASN:ND2	2.35	0.46
1:A:211:ALA:HB2	3:C:551:GLN:HE21	1.81	0.46
3:C:39:THR:O	3:C:43:GLN:HB2	2.15	0.46
1:A:96:MET:SD	1:A:96:MET:N	2.89	0.46
1:A:3492:CYS:SG	1:A:3524:ASN:ND2	2.88	0.46
1:A:3796:MET:HE3	1:A:3796:MET:HB2	1.65	0.46
1:A:704:PHE:HD1	1:A:704:PHE:O	1.99	0.46
1:A:873:VAL:HG13	1:A:874:THR:H	1.80	0.46
1:A:1896:ILE:HD12	1:A:1908:GLY:HA2	1.97	0.46
1:A:3289:ARG:NH1	1:A:3993:SER:O	2.49	0.46
3:C:6:ASN:HB3	3:C:7:LYS:H	1.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LYS:HA	1:A:263:LYS:HD2	1.76	0.46
1:A:2169:LEU:HD21	1:A:2193:ILE:HG21	1.98	0.46
2:B:140:ASP:OD1	2:B:140:ASP:N	2.42	0.46
2:B:263:LEU:HB2	2:B:267:ILE:HG13	1.97	0.46
2:B:407:PRO:HG2	3:C:486:ARG:HD2	1.97	0.46
1:A:3530:VAL:HG11	1:A:3568:ILE:HG21	1.99	0.45
1:A:3885:ARG:HA	1:A:3888:VAL:HG12	1.98	0.45
2:B:160:LYS:HB2	2:B:160:LYS:HE3	1.78	0.45
1:A:2927:ALA:HB2	1:A:2942:ILE:HD11	1.98	0.45
1:A:3883:LEU:HB3	1:A:3970:LEU:HD13	1.98	0.45
2:B:83:LEU:HD12	2:B:111:PRO:HD3	1.99	0.45
3:C:686:ILE:HD12	3:C:690:GLU:HB2	1.99	0.45
1:A:1917:LYS:O	1:A:1917:LYS:NZ	2.46	0.45
1:A:2126:MET:HG3	1:A:2164:TRP:HE1	1.80	0.45
1:A:976:VAL:O	1:A:981:ARG:NH1	2.49	0.45
1:A:300:TRP:HD1	1:A:303:HIS:HD2	1.64	0.45
3:C:528:ILE:HG23	3:C:529:PRO:HD3	1.98	0.45
3:C:666:VAL:HA	3:C:671:LEU:HD21	1.99	0.45
1:A:317:GLU:OE2	1:A:364:ARG:NE	2.42	0.45
1:A:1856:THR:HG22	1:A:1858:LEU:HD22	1.97	0.45
2:B:93:ASP:HB3	2:B:101:ASN:H	1.82	0.45
3:C:69:SER:HA	3:C:74:TYR:HB2	1.99	0.45
1:A:1507:CYS:SG	1:A:1508:LYS:N	2.90	0.45
1:A:2338:GLU:O	1:A:2342:CYS:CB	2.65	0.45
1:A:4115:ASN:OD1	1:A:4119:ARG:NH2	2.49	0.45
1:A:238:MET:HE2	1:A:238:MET:HB3	1.88	0.45
1:A:858:MET:HE3	1:A:858:MET:HB3	1.76	0.45
1:A:1623:LEU:HA	1:A:1626:TRP:HD1	1.82	0.45
3:C:464:ALA:HA	3:C:475:ASP:HA	1.99	0.45
2:B:495:LEU:CB	2:B:497:LEU:CD2	2.90	0.45
3:C:198:THR:OG1	3:C:201:GLN:OE1	2.26	0.45
1:A:532:ARG:O	1:A:536:SER:OG	2.32	0.44
1:A:704:PHE:O	1:A:704:PHE:CD1	2.70	0.44
1:A:1212:LEU:HD13	1:A:1220:LEU:HB2	1.99	0.44
1:A:1590:THR:OG1	1:A:1632:TRP:NE1	2.46	0.44
1:A:1633:TRP:HA	1:A:1642:LYS:HZ2	1.81	0.44
1:A:3680:LEU:HD22	1:A:3724:GLU:HG2	1.99	0.44
1:A:3772:ASN:HA	1:A:3775:LEU:HB2	1.98	0.44
3:C:356:PHE:HD2	3:C:422:VAL:HG11	1.81	0.44
1:A:65:LEU:HD11	1:A:89:LEU:HD21	1.98	0.44
1:A:1816:ARG:HA	1:A:1816:ARG:HD2	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1892:LYS:HD2	1:A:1896:ILE:HD11	1.99	0.44
1:A:3095:ASP:N	1:A:3095:ASP:OD1	2.50	0.44
1:A:3447:VAL:HG22	1:A:3468:LEU:HD22	1.99	0.44
1:A:3958:LEU:O	1:A:4110:GLN:NE2	2.50	0.44
1:A:4029:GLN:HB3	1:A:4030:GLU:H	1.47	0.44
2:B:363:ARG:HH11	3:C:269:GLN:HE22	1.65	0.44
1:A:1392:MET:HE3	1:A:1392:MET:HB3	1.92	0.44
1:A:1697:PRO:HG3	1:A:1752:LEU:HD21	2.00	0.44
2:B:342:ASP:OD1	2:B:342:ASP:N	2.50	0.44
1:A:2043:PHE:O	1:A:2047:THR:OG1	2.31	0.44
1:A:238:MET:SD	1:A:283:SER:N	2.91	0.44
1:A:1386:ILE:HG23	1:A:1392:MET:HG3	2.00	0.44
1:A:2842:ARG:O	1:A:2846:THR:OG1	2.31	0.44
1:A:215:PRO:HG2	3:C:553:ILE:HG21	2.00	0.44
1:A:678:LYS:HD2	1:A:737:PRO:HA	1.99	0.44
1:A:1850:VAL:HA	1:A:1853:SER:HB3	1.98	0.44
1:A:9:ARG:HB3	1:A:63:PHE:HE2	1.83	0.44
1:A:68:PHE:HA	1:A:71:LYS:HG2	2.00	0.44
1:A:1869:LYS:HE3	1:A:1869:LYS:HB2	1.87	0.44
1:A:1964:GLY:O	1:A:1968:SER:OG	2.36	0.44
3:C:365:PHE:HB3	3:C:418:CYS:SG	2.57	0.44
1:A:2492:ASP:O	1:A:2496:GLN:NE2	2.51	0.43
1:A:2788:SER:O	1:A:2792:THR:OG1	2.34	0.43
1:A:3531:TYR:HB3	1:A:3796:MET:HA	2.00	0.43
2:B:207:LYS:HB2	2:B:213:ILE:HD11	2.00	0.43
1:A:436:GLU:HA	1:A:439:VAL:HG12	2.00	0.43
1:A:2512:ASP:OD1	1:A:2512:ASP:N	2.48	0.43
1:A:3629:ARG:HH12	1:A:3634:GLN:HG3	1.84	0.43
1:A:3767:LEU:HD13	1:A:3918:LEU:HD22	2.00	0.43
3:C:363:LYS:HG2	3:C:420:VAL:HG12	1.99	0.43
2:B:485:GLN:NE2	3:C:332:LYS:O	2.39	0.43
3:C:16:VAL:HG13	3:C:58:LEU:HD11	2.01	0.43
3:C:602:VAL:HA	3:C:606:LYS:HD2	2.00	0.43
1:A:93:LEU:HD12	1:A:100:ILE:HD13	2.00	0.43
1:A:208:MET:HE3	1:A:208:MET:HB2	1.91	0.43
1:A:335:LYS:HE2	1:A:376:ILE:HD11	1.99	0.43
1:A:913:ARG:HH22	1:A:2803:ILE:HG13	1.83	0.43
1:A:1525:CYS:SG	1:A:1574:ASN:ND2	2.91	0.43
1:A:1989:ASN:OD1	1:A:1989:ASN:N	2.45	0.43
1:A:67:VAL:HA	1:A:70:ARG:HB2	2.00	0.43
1:A:485:GLN:HE22	1:A:2040:MET:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1082:PHE:HA	1:A:1085:ILE:HG12	2.01	0.43
1:A:1632:TRP:HB3	1:A:1645:VAL:HG21	2.00	0.43
1:A:1927:MET:HE2	1:A:1980:ASN:HD21	1.83	0.43
1:A:3876:SER:O	1:A:3876:SER:OG	2.35	0.43
1:A:1729:PHE:HB2	1:A:1736:PHE:HB2	1.99	0.43
1:A:2784:GLN:HB3	1:A:2785:ILE:H	1.61	0.43
2:B:410:PHE:HB2	2:B:439:PHE:HE1	1.84	0.43
2:B:497:LEU:H	2:B:497:LEU:HG	1.59	0.43
3:C:61:THR:OG1	3:C:62:ASP:N	2.50	0.43
1:A:851:ILE:HD13	1:A:851:ILE:HA	1.89	0.42
1:A:1190:LEU:HA	1:A:1193:LYS:HG2	2.00	0.42
1:A:2387:PRO:O	2:B:158:GLN:NE2	2.46	0.42
1:A:3098:ARG:HE	1:A:3102:TYR:HE2	1.65	0.42
1:A:3138:ILE:HG12	1:A:3189:PHE:HZ	1.84	0.42
1:A:3686:TRP:HH2	1:A:3699:LEU:HD11	1.84	0.42
2:B:143:LEU:O	2:B:145:GLU:N	2.52	0.42
1:A:95:LYS:HA	1:A:834:LEU:HD11	2.00	0.42
1:A:782:ARG:NH1	1:A:3166:ASN:OD1	2.52	0.42
1:A:3011:LEU:HD23	1:A:3047:SER:HB2	2.01	0.42
1:A:3554:PHE:HD1	1:A:3557:ARG:HH21	1.66	0.42
1:A:3829:LEU:HD23	1:A:3829:LEU:HA	1.87	0.42
1:A:346:TYR:HA	1:A:349:ILE:HG22	2.01	0.42
1:A:3623:PRO:HG3	1:A:3633:ILE:HG12	2.02	0.42
2:B:240:GLU:HA	2:B:243:LEU:HD12	2.01	0.42
2:B:245:LYS:O	2:B:246:VAL:CG2	2.67	0.42
1:A:1679:LEU:O	1:A:1689:LYS:NZ	2.46	0.42
1:A:2980:ASP:OD1	1:A:2980:ASP:N	2.46	0.42
2:B:262:LYS:HA	2:B:268:VAL:HG12	2.01	0.42
3:C:116:ASP:O	3:C:120:HIS:ND1	2.49	0.42
1:A:2036:LEU:O	1:A:2040:MET:HB2	2.19	0.42
2:B:51:SER:O	2:B:51:SER:OG	2.38	0.42
3:C:12:LEU:HD13	3:C:38:ILE:HD11	2.02	0.42
1:A:441:MET:HE2	1:A:441:MET:HB2	1.92	0.42
1:A:485:GLN:HE21	1:A:2040:MET:HG3	1.85	0.42
1:A:1900:PHE:HD1	1:A:1900:PHE:HA	1.76	0.42
1:A:1864:ASP:HA	1:A:1867:ILE:HD12	2.01	0.42
1:A:2190:VAL:HA	1:A:2193:ILE:HG22	2.02	0.42
1:A:3883:LEU:HD13	1:A:3970:LEU:HD22	2.01	0.42
3:C:413:LYS:HD3	3:C:413:LYS:HA	1.87	0.42
3:C:606:LYS:NZ	3:C:608:SER:O	2.53	0.42
1:A:2955:SER:O	1:A:2971:GLN:NE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3733:ARG:HH22	1:A:4022:LYS:HD2	1.85	0.41
1:A:3998:LEU:HG	1:A:4002:MET:HE2	2.02	0.41
3:C:232:ARG:HA	3:C:515:MET:HE2	2.01	0.41
1:A:836:LYS:NZ	4:D:5:DG:OP1	2.37	0.41
1:A:3351:ILE:O	1:A:3352:GLU:HB2	2.19	0.41
3:C:353:ARG:HA	3:C:356:PHE:HE1	1.85	0.41
3:C:726:ASP:HA	3:C:729:LEU:HG	2.01	0.41
1:A:205:LYS:O	1:A:209:THR:OG1	2.34	0.41
1:A:410:MET:HE3	1:A:410:MET:HB2	1.88	0.41
1:A:680:ILE:HD12	1:A:680:ILE:HA	1.95	0.41
1:A:2286:PRO:HB3	1:A:2329:TYR:CE2	2.56	0.41
1:A:2464:HIS:ND1	1:A:2469:CYS:SG	2.93	0.41
3:C:45:GLN:HE21	3:C:237:PHE:HE1	1.68	0.41
3:C:132:ILE:O	3:C:161:LEU:HA	2.21	0.41
1:A:848:LEU:HD12	1:A:848:LEU:HA	1.91	0.41
1:A:863:GLY:HA2	1:A:3167:ARG:HG3	2.01	0.41
1:A:1137:ILE:HD12	1:A:1137:ILE:HA	1.94	0.41
1:A:1811:ARG:HE	3:C:626:THR:HG23	1.86	0.41
3:C:108:LEU:HD13	3:C:147:LEU:HD21	2.03	0.41
3:C:372:ALA:HA	3:C:375:VAL:HG12	2.02	0.41
1:A:12:LEU:HD23	1:A:64:GLY:HA2	2.01	0.41
1:A:473:PRO:HA	1:A:476:ARG:HG2	2.01	0.41
1:A:1532:LEU:HD23	1:A:1532:LEU:HA	1.86	0.41
1:A:2473:MET:HE3	1:A:2473:MET:HB3	1.89	0.41
2:B:422:ASP:N	2:B:422:ASP:OD2	2.53	0.41
3:C:155:LYS:NZ	3:C:215:LEU:O	2.49	0.41
3:C:614:ASN:OD1	3:C:614:ASN:N	2.53	0.41
1:A:214:GLU:HA	1:A:215:PRO:HD2	1.73	0.41
1:A:1141:LYS:HD3	1:A:1141:LYS:HA	1.93	0.41
2:B:245:LYS:C	2:B:246:VAL:CG2	2.93	0.41
3:C:339:CYS:O	3:C:395:TYR:HA	2.21	0.41
1:A:117:LYS:HE2	1:A:117:LYS:HB2	1.80	0.41
1:A:862:LEU:HD12	1:A:862:LEU:HA	1.94	0.41
1:A:1605:PHE:O	1:A:1608:ARG:NH2	2.45	0.41
1:A:3489:SER:O	1:A:3489:SER:OG	2.34	0.41
3:C:617:ILE:HA	3:C:620:ILE:HG12	2.01	0.41
1:A:790:LYS:HE2	1:A:790:LYS:HB3	1.88	0.41
1:A:879:MET:H	1:A:879:MET:HG2	1.66	0.41
1:A:1774:MET:HB3	1:A:1777:LEU:HD21	2.02	0.41
1:A:2257:PHE:O	1:A:2261:SER:OG	2.35	0.41
1:A:3620:PRO:HG3	1:A:3638:LYS:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3753:LYS:HE2	1:A:3803:ILE:HG21	2.01	0.41
3:C:247:TRP:HB3	3:C:263:ALA:HB3	2.03	0.41
1:A:1246:GLY:HA2	1:A:1247:PRO:HD3	1.95	0.41
1:A:1474:ASP:OD1	1:A:1474:ASP:N	2.52	0.41
1:A:2256:ILE:H	1:A:2256:ILE:HG12	1.64	0.41
1:A:2352:HIS:HB3	1:A:2360:PHE:HB2	2.03	0.41
2:B:237:SER:OG	2:B:238:LYS:N	2.51	0.41
3:C:324:SER:OG	3:C:325:LYS:N	2.53	0.41
1:A:2328:ARG:NH1	1:A:2332:GLU:OE2	2.55	0.40
1:A:2408:MET:HB3	1:A:2408:MET:HE2	1.87	0.40
3:C:138:LEU:HD23	3:C:138:LEU:HA	1.95	0.40
1:A:96:MET:HB2	1:A:100:ILE:HD11	2.04	0.40
1:A:2094:MET:HE2	1:A:2094:MET:HB2	1.97	0.40
1:A:3582:GLU:OE2	1:A:3671:ASN:ND2	2.55	0.40
1:A:3975:LYS:HA	1:A:3975:LYS:HD3	1.89	0.40
2:B:238:LYS:HZ3	2:B:238:LYS:HG2	1.74	0.40
4:D:19:DA:H2'	4:D:20:DT:H71	2.04	0.40
1:A:76:ILE:HD13	1:A:76:ILE:HA	1.96	0.40
1:A:2834:GLN:HE21	1:A:2834:GLN:HB2	1.59	0.40
1:A:3714:GLU:H	1:A:3714:GLU:HG2	1.79	0.40
1:A:3772:ASN:HD22	1:A:3788:LEU:HB2	1.86	0.40
1:A:3972:LEU:HD23	1:A:3972:LEU:HA	1.91	0.40
2:B:94:LYS:HB3	2:B:103:TYR:CD1	2.57	0.40
3:C:322:PRO:HB2	3:C:323:PHE:H	1.65	0.40
1:A:919:LEU:HD11	1:A:968:VAL:HG23	2.03	0.40
1:A:1484:LEU:HD22	1:A:1524:LEU:HD21	2.03	0.40
1:A:1725:GLN:HG2	3:C:622:GLN:HG3	2.04	0.40
1:A:3962:ARG:NH1	1:A:4128:MET:O	2.55	0.40
1:A:663:ILE:HD13	1:A:663:ILE:HA	1.93	0.40
2:B:358:LYS:HD2	2:B:358:LYS:HA	1.84	0.40
2:B:510:LYS:HE2	2:B:510:LYS:HB2	1.97	0.40
3:C:666:VAL:HB	3:C:675:TRP:CD1	2.56	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	3594/4128 (87%)	3123 (87%)	459 (13%)	12 (0%)	36	69
2	B	486/609 (80%)	409 (84%)	74 (15%)	3 (1%)	21	55
3	C	645/732 (88%)	549 (85%)	92 (14%)	4 (1%)	21	55
All	All	4725/5469 (86%)	4081 (86%)	625 (13%)	19 (0%)	31	64

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1476	HIS
1	A	2826	LEU
1	A	3352	GLU
2	B	144	SER
1	A	215	PRO
1	A	3058	ASP
1	A	3311	ASN
2	B	245	LYS
3	C	299	ASP
3	C	322	PRO
1	A	1021	VAL
1	A	3028	ASN
1	A	3083	SER
3	C	300	ASP
1	A	661	PRO
1	A	2548	PRO
1	A	2547	SER
3	C	193	PRO
2	B	499	GLU

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	3174/3671 (86%)	3155 (99%)	19 (1%)	78	80
2	B	444/548 (81%)	437 (98%)	7 (2%)	55	69
3	C	587/649 (90%)	580 (99%)	7 (1%)	63	72
All	All	4205/4868 (86%)	4172 (99%)	33 (1%)	70	77

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
1	A	57	LEU
1	A	100	ILE
1	A	215	PRO
1	A	284	THR
1	A	739	ASN
1	A	1639	LEU
1	A	1752	LEU
1	A	1989	ASN
1	A	2183	HIS
1	A	2256	ILE
1	A	2294	ILE
1	A	2529	THR
1	A	3058	ASP
1	A	3301	LEU
1	A	3310	ASN
1	A	3352	GLU
1	A	3955	VAL
1	A	4031	ILE
2	B	95	ASN
2	B	217	TYR
2	B	269	ILE
2	B	292	THR
2	B	368	VAL
2	B	493	LEU
2	B	497	LEU
3	C	27	ILE
3	C	123	ILE
3	C	234	LEU
3	C	277	THR
3	C	351	VAL
3	C	365	PHE
3	C	647	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	109	ASN
1	A	192	ASN
1	A	207	GLN
1	A	303	HIS
1	A	442	GLN
1	A	485	GLN
1	A	720	GLN
1	A	867	ASN
1	A	1004	GLN
1	A	1048	GLN
1	A	1115	HIS
1	A	1126	GLN
1	A	1509	GLN
1	A	1598	ASN
1	A	1610	ASN
1	A	1624	GLN
1	A	1721	HIS
1	A	1772	HIS
1	A	1866	GLN
1	A	1980	ASN
1	A	2103	HIS
1	A	2135	ASN
1	A	2222	HIS
1	A	2283	ASN
1	A	2348	GLN
1	A	2365	ASN
1	A	2422	GLN
1	A	2432	GLN
1	A	2496	GLN
1	A	2560	ASN
1	A	2834	GLN
1	A	2885	GLN
1	A	3003	ASN
1	A	3059	GLN
1	A	3112	GLN
1	A	3139	GLN
1	A	3251	ASN
1	A	3327	ASN
1	A	3379	GLN
1	A	3383	GLN

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Mol	Chain	Res	Type
1	A	3423	GLN
1	A	3524	ASN
1	A	3527	GLN
1	A	3573	ASN
1	A	3643	HIS
1	A	3671	ASN
1	A	3772	ASN
1	A	3822	GLN
1	A	3966	GLN
1	A	4015	ASN
1	A	4110	GLN
2	B	52	GLN
2	B	152	ASN
2	B	174	ASN
2	B	264	ASN
2	B	326	GLN
2	B	360	HIS
2	B	405	ASN
2	B	489	ASN
3	C	82	HIS
3	C	290	GLN
3	C	330	GLN
3	C	488	GLN
3	C	551	GLN
3	C	627	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.

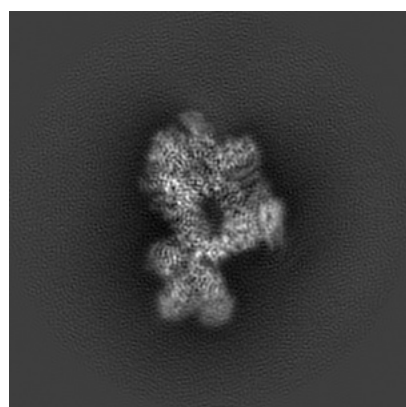
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22626. These allow visual inspection of the internal detail of the map and identification of artifacts.

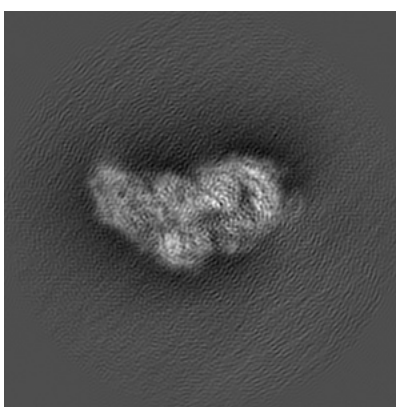
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

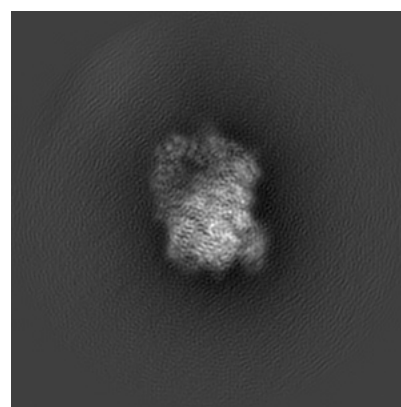
6.1.1 Primary map



X



Y

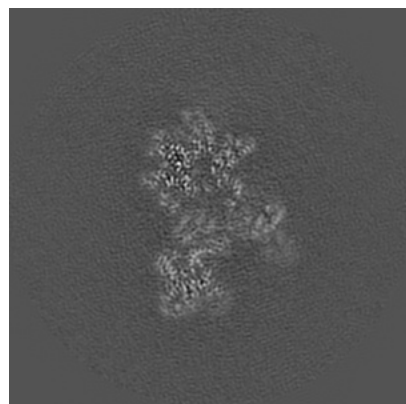


Z

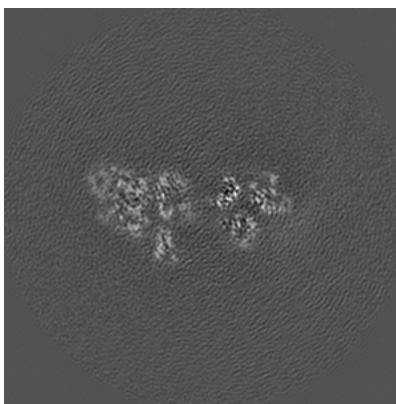
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

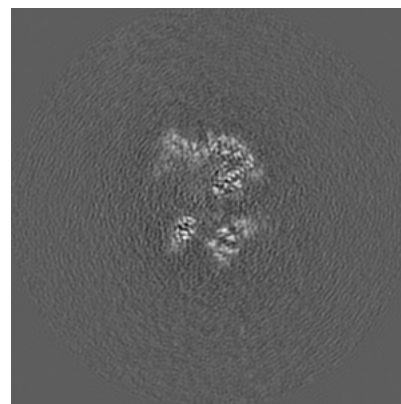
6.2.1 Primary map



X Index: 176



Y Index: 176

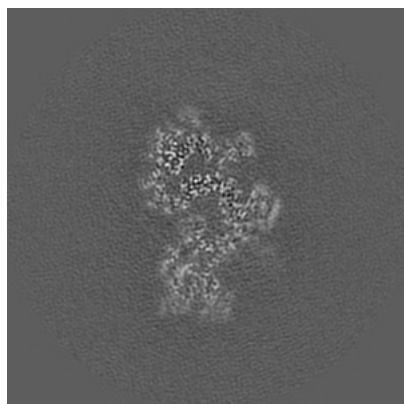


Z Index: 176

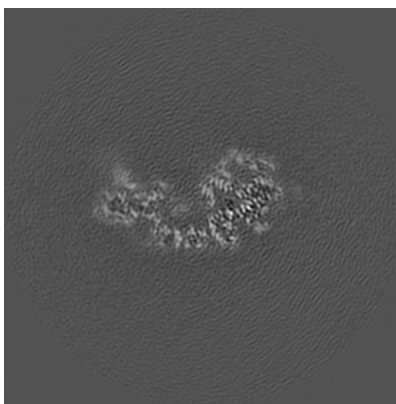
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

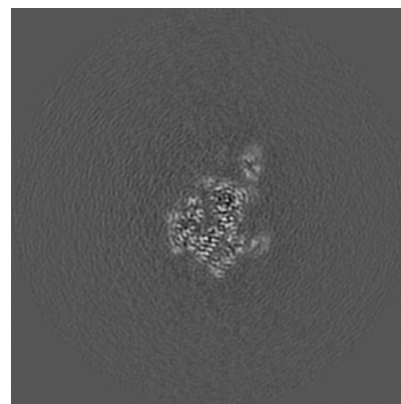
6.3.1 Primary map



X Index: 187



Y Index: 149

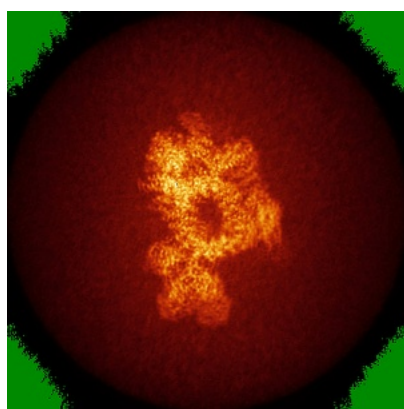


Z Index: 199

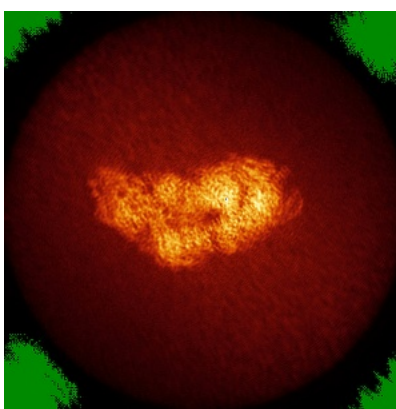
The images above show the largest variance slices of the map in three orthogonal directions.

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

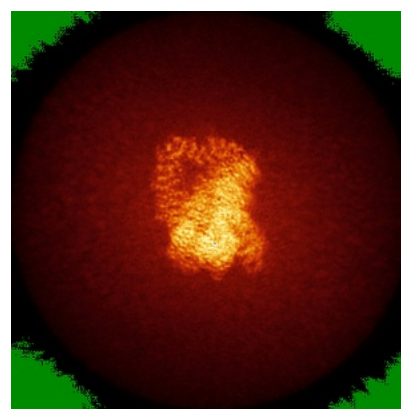
6.4.1 Primary map



X



Y

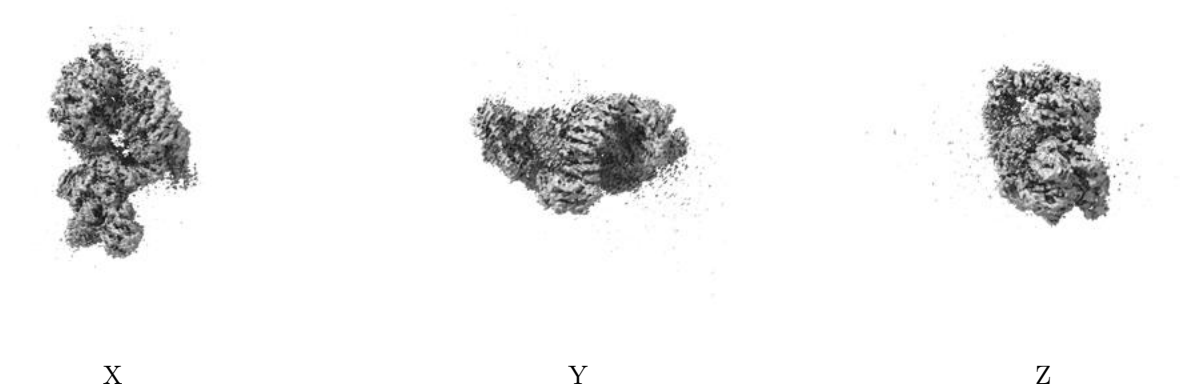


Z

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

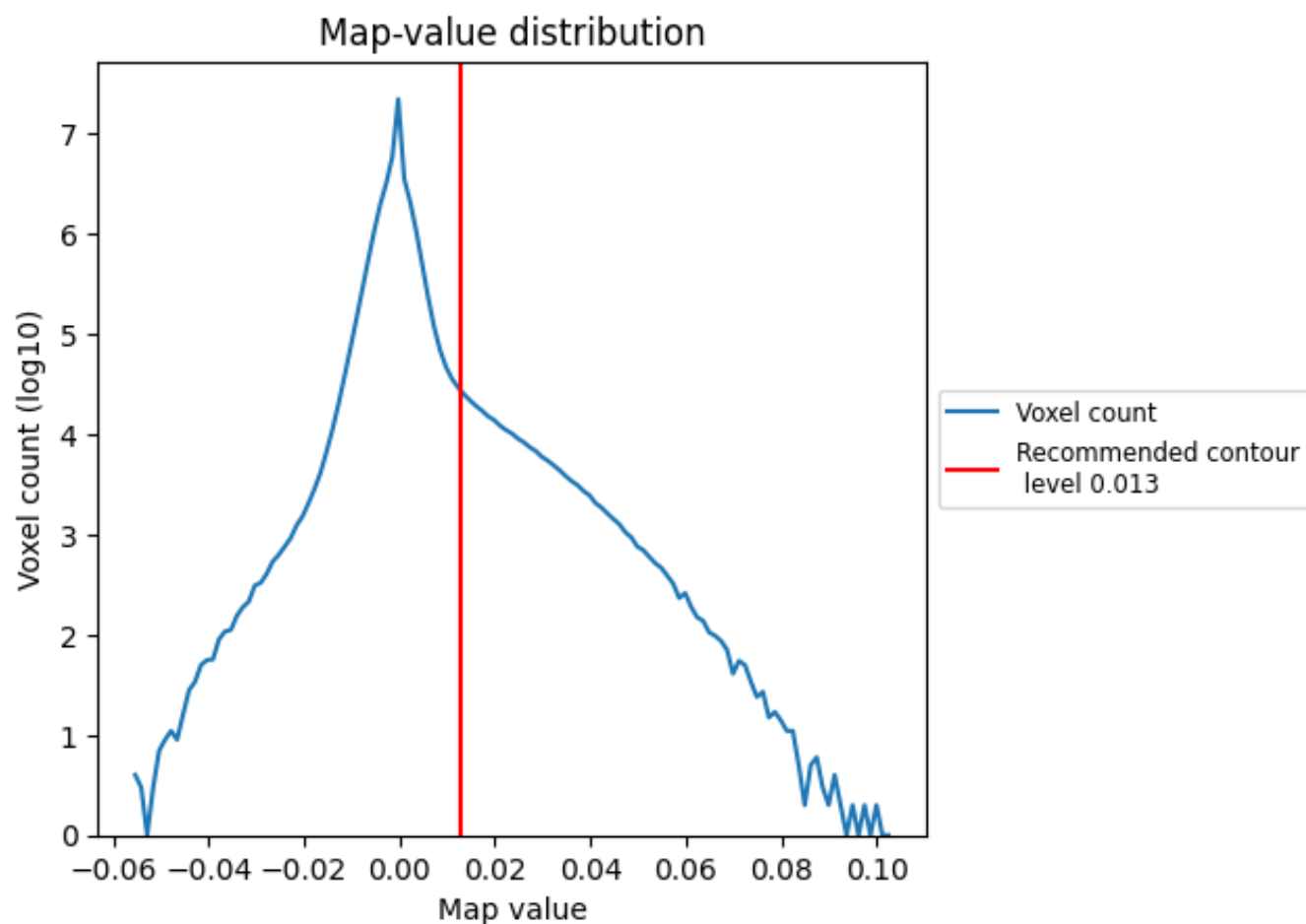
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

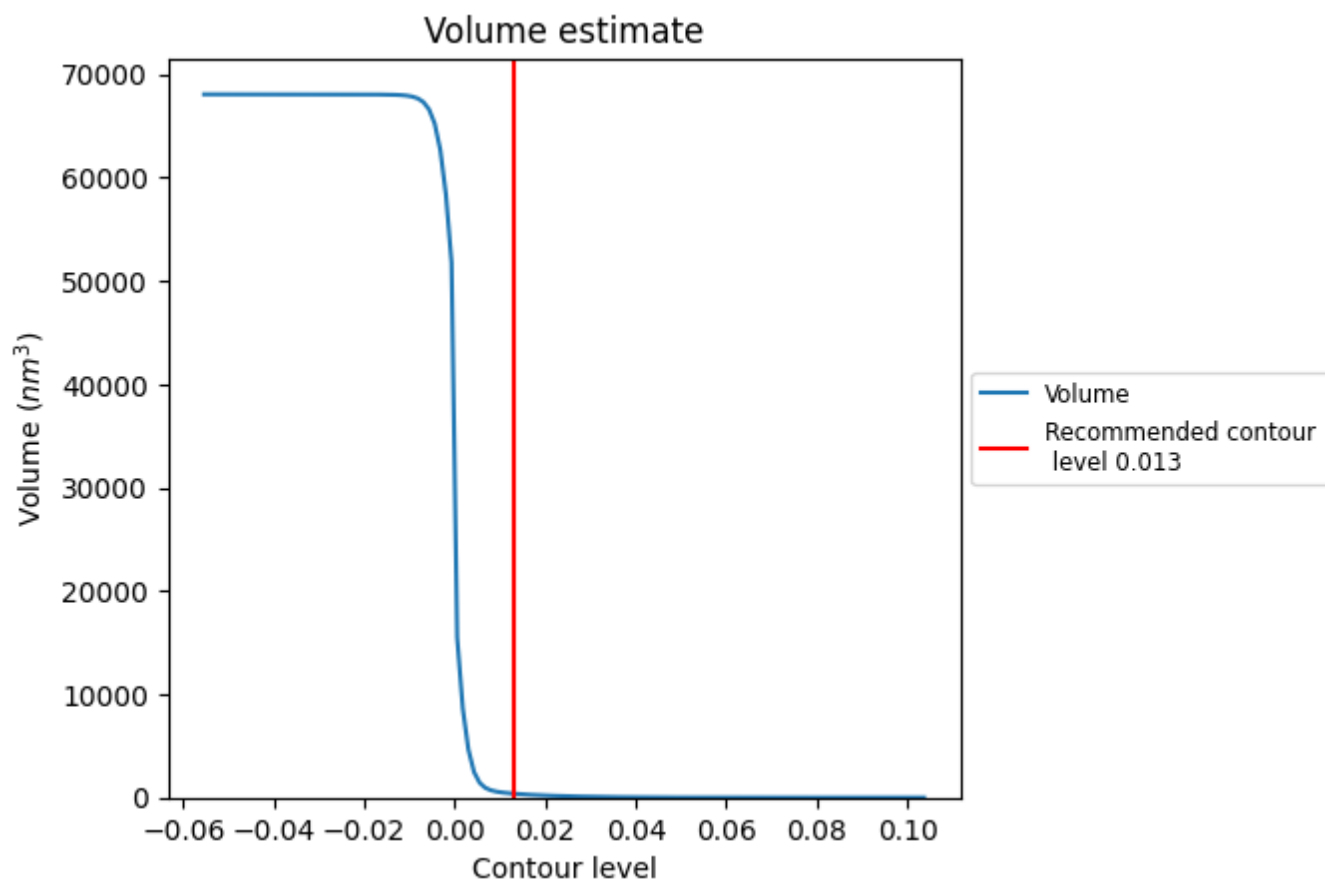
This section contains the results of statistical analysis of the map.

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.

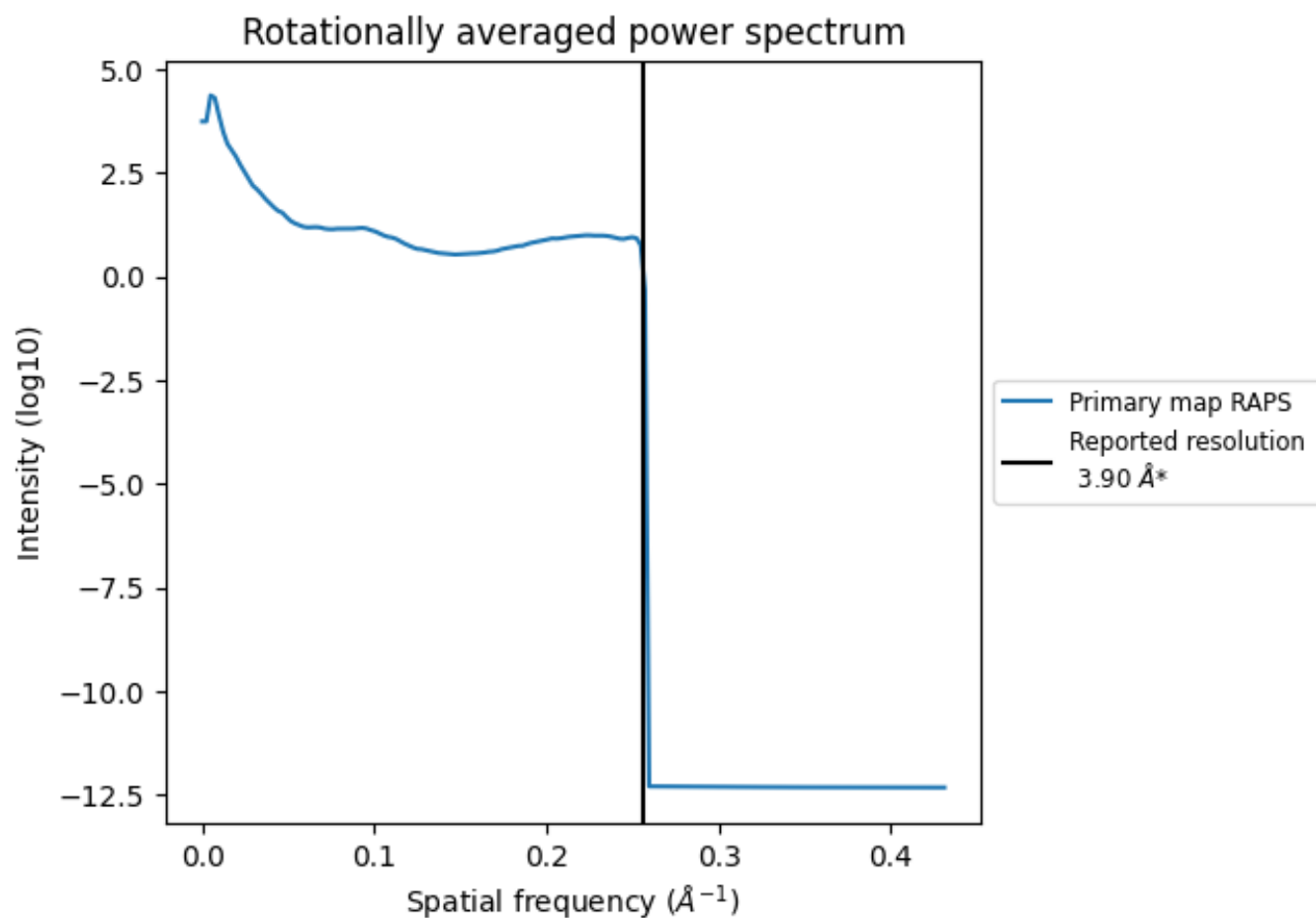
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 378 nm³; this corresponds to an approximate mass of 341 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 0.256 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

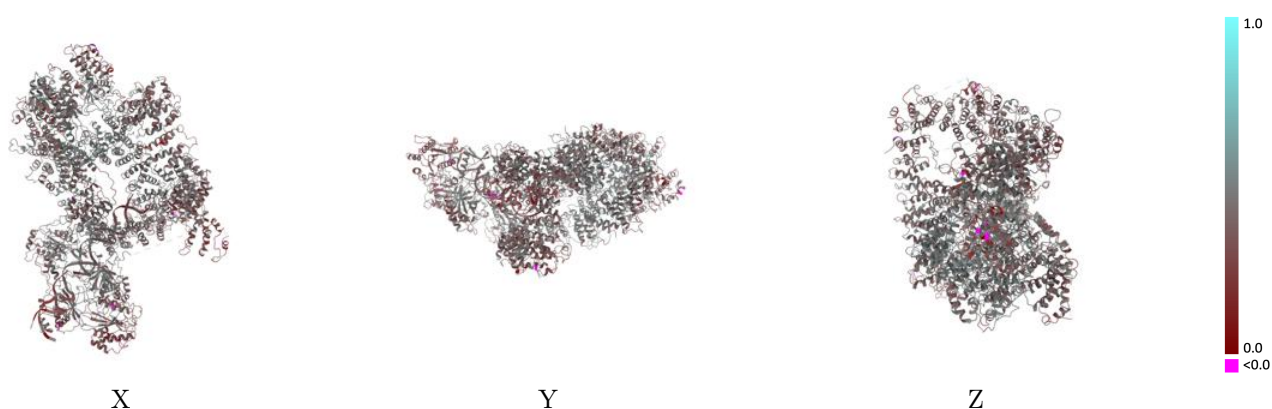
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22626 and PDB model 7K1N. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

This section was not generated.

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

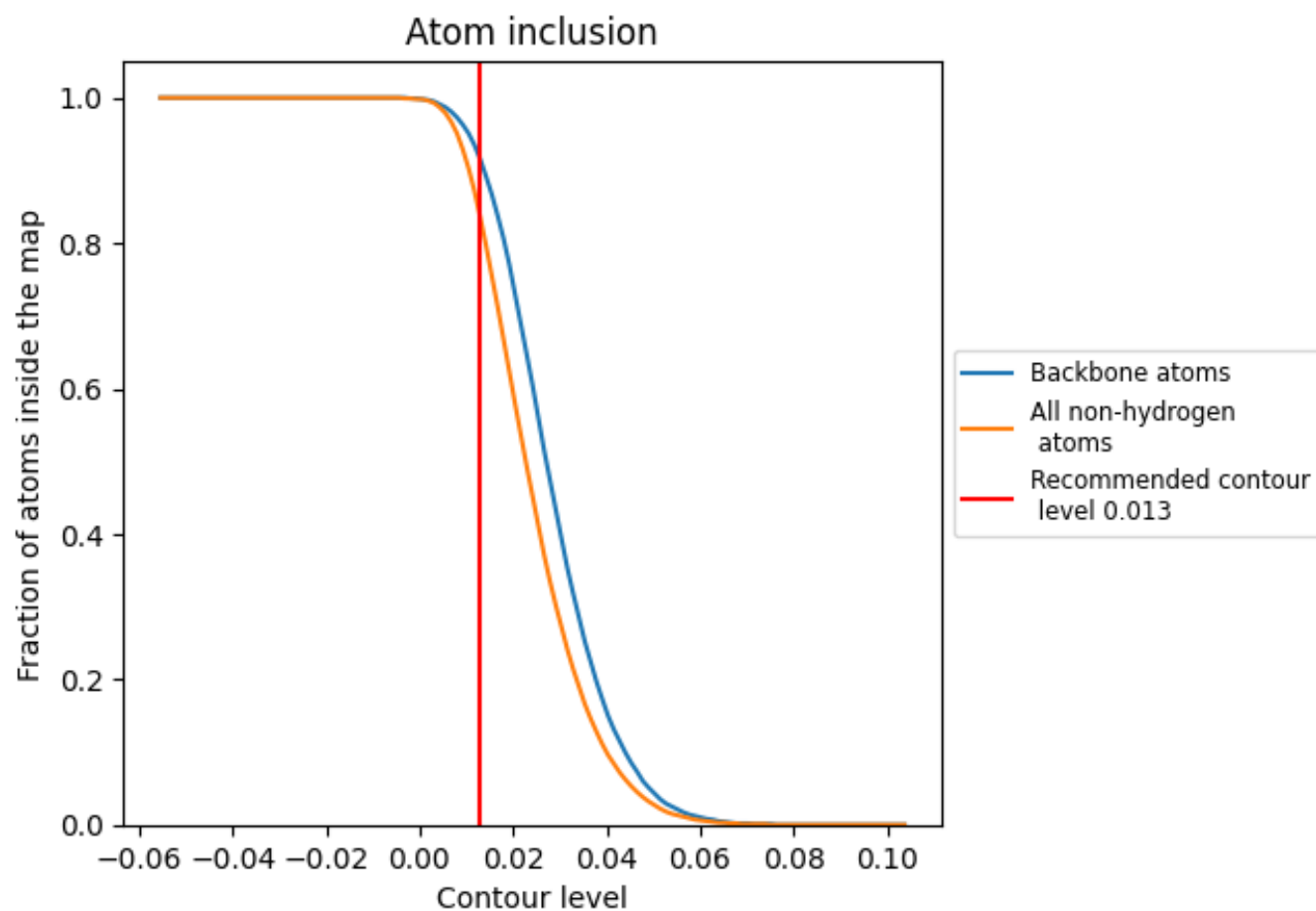


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 84% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8350	0.4170
A	0.8590	0.4300
B	0.8490	0.4160
C	0.6850	0.3710
D	0.8930	0.3510
E	0.7580	0.2840
F	0.8590	0.3510
G	0.9000	0.3430

1.0

0.0

<0.0