



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 05:29 AM UTC

PDB ID : 7TYR / pdb_00007tyr
EMDB ID : EMD-26192
Title : Cryo-EM structure of the basal state of the Artemis:DNA-PKcs complex (see COMPND 13/14)
Authors : Watanabe, G.; Lieber, M.R.; Williams, D.R.
Deposited on : 2022-02-14
Resolution : 3.33 Å(reported)
Based on initial model : 5LUQ

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

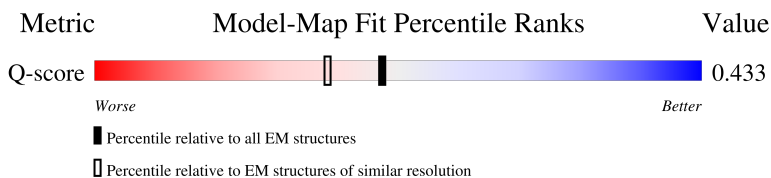
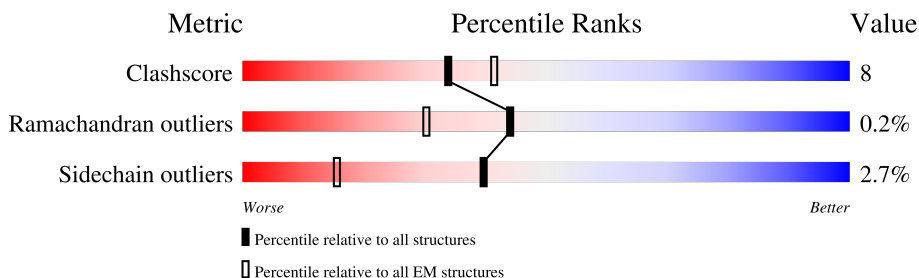
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.33 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	14484 (2.83 - 3.83)

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	C	707	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 31610 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	3905	Total	C	N	O	S	1	0
			31173	19935	5272	5764	202		

- Molecule 2 is a protein called Protein artemis.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	52	Total	C	N	O	0	0
			437	279	76	82		

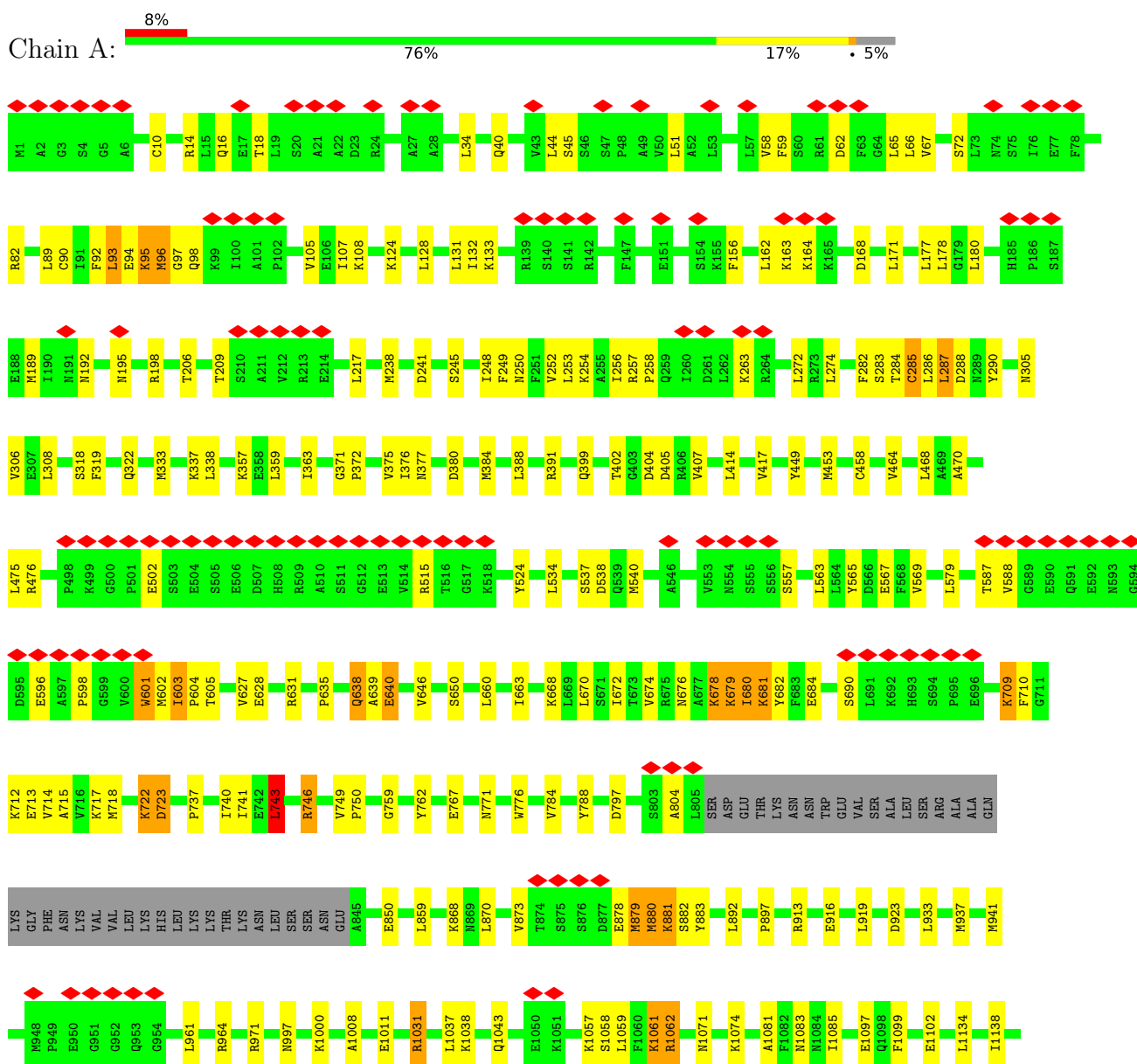
There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	693	GLU	-	expression tag	UNP Q96SD1
C	694	ASN	-	expression tag	UNP Q96SD1
C	695	LEU	-	expression tag	UNP Q96SD1
C	696	TYR	-	expression tag	UNP Q96SD1
C	697	PHE	-	expression tag	UNP Q96SD1
C	698	GLN	-	expression tag	UNP Q96SD1
C	699	GLY	-	expression tag	UNP Q96SD1
C	700	HIS	-	expression tag	UNP Q96SD1
C	701	HIS	-	expression tag	UNP Q96SD1
C	702	HIS	-	expression tag	UNP Q96SD1
C	703	HIS	-	expression tag	UNP Q96SD1
C	704	HIS	-	expression tag	UNP Q96SD1
C	705	HIS	-	expression tag	UNP Q96SD1
C	706	HIS	-	expression tag	UNP Q96SD1
C	707	HIS	-	expression tag	UNP Q96SD1

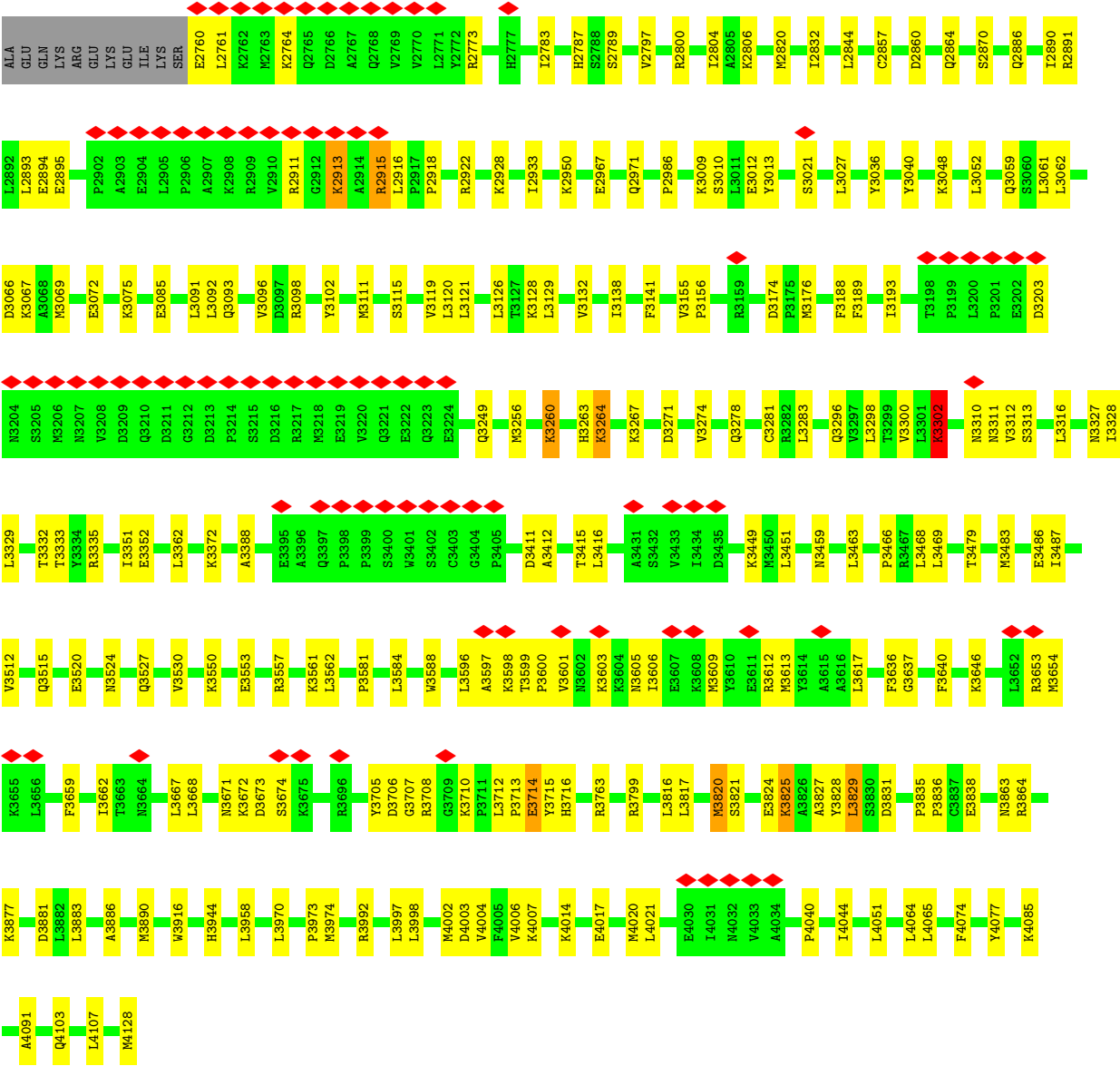
3 Residue-property plots

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.

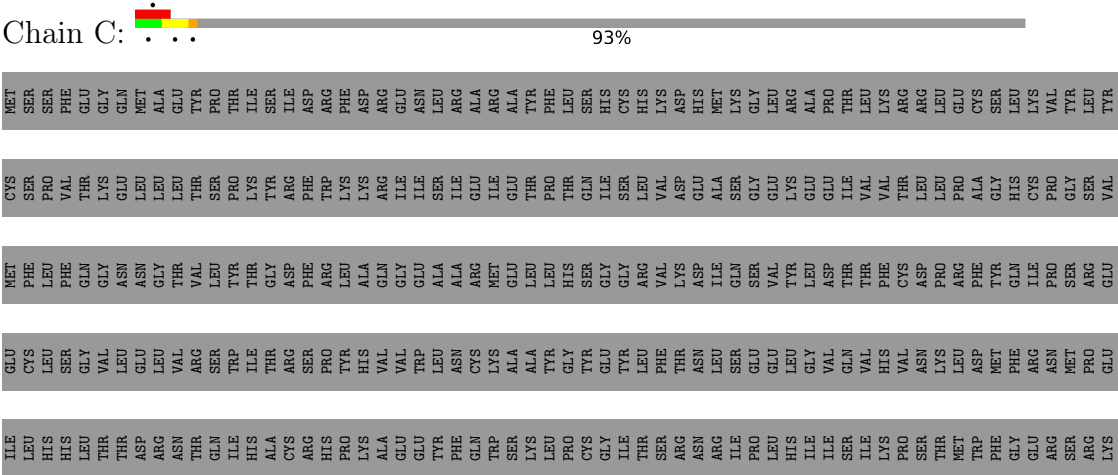
- Molecule 1: DNA-dependent protein kinase catalytic subunit







● Molecule 2: Protein artemis



THR	ASN	VAL	ILE	VAL	ARG	THR	GLY	GLU	SER	TYR	ARG	ALA	CYS	PHE	SER	PHE	HIS	SER	SER	TYR	THR	GLU	ILE	LYS	ASP	PHE	LEU	SER	TYR	PRO	ASN	VAL	ILE	PRO	VAL	GLY	THR	THR	MET	ASP	LYS	VAL	VAL	GLU	ILE	LEU	LYS	PRO	LEU	CYS	ARG																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
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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	103485	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 ($e^-/\text{\AA}^2$)	60.0	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	46296	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.449	Depositor
Minimum map value	-1.114	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	552.96, 552.96, 552.96	wwPDB
Map dimensions	512, 512, 512	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](#)

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	0.26	0/31831	0.48	6/43042 (0.0%)
2	C	0.81	0/452	1.17	0/614
All	All	0.28	0/32283	0.49	6/43656 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3715	TYR	N-CA-C	-6.72	103.96	111.28
1	A	723	ASP	CB-CA-C	-6.18	109.45	116.63
1	A	3714	GLU	CB-CA-C	5.63	118.54	110.04
1	A	3302	LYS	N-CA-C	-5.49	105.38	111.36
1	A	1938	ARG	N-CA-C	-5.08	105.63	111.07
1	A	285	CYS	N-CA-C	-5.01	105.90	111.36

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	31173	0	31434	497	0
2	C	437	0	424	36	0
All	All	31610	0	31858	520	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 8.

All (520) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:381:VAL:HG13	2:C:382:HIS:ND1	1.35	1.35
2:C:381:VAL:CG1	2:C:382:HIS:ND1	2.17	1.07
2:C:365:THR:HG23	2:C:367:PRO:HD2	1.38	1.03
1:A:2911:ARG:CZ	1:A:2913:LYS:HE3	1.93	0.98
2:C:369:TYR:HB2	2:C:371:PRO:HD3	1.51	0.92
1:A:2161:ALA:C	1:A:2163:HIS:H	1.81	0.87
2:C:381:VAL:HG13	2:C:382:HIS:CE1	2.10	0.85
1:A:2911:ARG:NH2	1:A:2913:LYS:HE3	1.91	0.85
2:C:402:ARG:H	2:C:402:ARG:HD3	1.43	0.84
2:C:366:GLU:HG2	2:C:367:PRO:HD3	1.61	0.83
1:A:90:CYS:HA	1:A:93:LEU:HD23	1.62	0.81
1:A:3827:ALA:O	1:A:3831:ASP:HB3	1.80	0.81
1:A:1212:LEU:HD21	1:A:1220:LEU:HD22	1.61	0.81
1:A:284:THR:HA	1:A:287:LEU:HB2	1.62	0.81
1:A:1529:VAL:HG21	1:A:1581:GLU:HG2	1.67	0.76
1:A:3093:GLN:HA	2:C:377:ARG:HD2	1.68	0.76
1:A:746:ARG:HG2	1:A:788:TYR:HE1	1.52	0.74
1:A:3010:SER:HA	2:C:402:ARG:HD2	1.69	0.74
1:A:2911:ARG:NH1	1:A:2913:LYS:HE3	2.05	0.72
1:A:1057:LYS:HG3	1:A:1061:LYS:HD3	1.72	0.71
1:A:2341:LEU:HD21	1:A:2371:PHE:CE2	2.28	0.69
1:A:881:LYS:C	1:A:883:TYR:H	2.02	0.68
1:A:2097:LEU:HD11	1:A:2149:LEU:HD11	1.75	0.68
1:A:305:ASN:OD1	1:A:306:VAL:N	2.27	0.68
2:C:402:ARG:HD3	2:C:402:ARG:N	2.06	0.68
1:A:1212:LEU:HD11	1:A:1220:LEU:HB2	1.73	0.68
1:A:1206:LEU:HD23	1:A:1209:LYS:HZ3	1.59	0.66
1:A:3098:ARG:HH21	2:C:368:LYS:HG3	1.59	0.66
1:A:596:GLU:HG3	1:A:598:PRO:HD2	1.77	0.66
1:A:1773:VAL:HG13	1:A:1774:MET:HG3	1.76	0.66
1:A:680:ILE:O	1:A:681:LYS:HB2	1.95	0.66
1:A:2161:ALA:O	1:A:2163:HIS:N	2.28	0.66
1:A:89:LEU:HD21	1:A:107:ILE:HD12	1.78	0.66
1:A:1750:LEU:HD12	1:A:1762:MET:HG3	1.77	0.66
1:A:2820:MET:HE2	1:A:2832:ILE:HD13	1.76	0.66
1:A:3520:GLU:O	1:A:3524:ASN:ND2	2.27	0.66
1:A:2911:ARG:CZ	1:A:2913:LYS:CE	2.71	0.65
1:A:2161:ALA:C	1:A:2163:HIS:N	2.49	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3944:HIS:NE2	1:A:4020:MET:SD	2.70	0.64
1:A:879:MET:HE1	1:A:3120:LEU:HG	1.79	0.64
1:A:923:ASP:OD2	1:A:2800:ARG:NH1	2.31	0.63
1:A:3138:ILE:HD13	1:A:3189:PHE:HZ	1.62	0.63
1:A:1749:ALA:O	1:A:1753:SER:HB2	1.99	0.63
1:A:797:ASP:HB2	1:A:870:LEU:HG	1.80	0.63
1:A:1528:LEU:HD21	1:A:1567:ILE:HG23	1.79	0.63
1:A:3599:THR:C	1:A:3601:VAL:N	2.56	0.62
1:A:1169:VAL:HA	1:A:1172:LEU:HD12	1.81	0.62
1:A:1945:TYR:HE1	1:A:1971:PRO:HB3	1.65	0.61
1:A:1134:LEU:O	1:A:1138:ILE:HD12	1.99	0.61
1:A:1977:ILE:HG13	1:A:1979:GLU:H	1.64	0.61
1:A:45:SER:HB2	1:A:51:LEU:HD11	1.82	0.61
1:A:189:MET:SD	1:A:192:ASN:ND2	2.72	0.61
1:A:3085:GLU:OE1	1:A:3085:GLU:N	2.32	0.61
1:A:2911:ARG:NH2	1:A:2913:LYS:CE	2.64	0.60
1:A:2894:GLU:HB3	1:A:3973:PRO:HG3	1.83	0.60
1:A:1211:VAL:O	1:A:1214:GLU:HG3	2.02	0.60
1:A:2915:ARG:NH2	1:A:2918:PRO:HD3	2.17	0.60
1:A:880:MET:O	1:A:883:TYR:HB2	2.02	0.60
1:A:3093:GLN:HA	2:C:377:ARG:CD	2.32	0.60
1:A:3636:PHE:HZ	1:A:3668:LEU:HB3	1.67	0.60
1:A:458:CYS:HB2	1:A:540:MET:HE1	1.84	0.59
2:C:381:VAL:CG1	2:C:382:HIS:CE1	2.79	0.59
1:A:997:ASN:OD1	1:A:1043:GLN:NE2	2.35	0.59
1:A:2165:LEU:HA	1:A:2193:ILE:HD11	1.83	0.59
1:A:2173:ALA:HB2	1:A:2215:LEU:HB2	1.84	0.59
1:A:2160:TYR:O	1:A:2163:HIS:HB2	2.01	0.59
1:A:2393:LEU:HA	1:A:2396:LEU:HD12	1.85	0.59
1:A:414:LEU:HG	1:A:464:VAL:HG21	1.84	0.59
1:A:1532:LEU:HD11	1:A:1567:ILE:HG21	1.84	0.59
1:A:1905:ILE:HG23	1:A:1906:THR:HG23	1.85	0.59
1:A:1097:GLU:O	1:A:1151:ARG:NH1	2.35	0.59
1:A:2322:VAL:HA	1:A:2325:LEU:HD12	1.84	0.59
1:A:1960:LYS:HG3	1:A:2104:MET:HE1	1.84	0.59
1:A:3588:TRP:NE1	1:A:3609:MET:SD	2.74	0.58
2:C:365:THR:CG2	2:C:367:PRO:HD2	2.25	0.58
1:A:1529:VAL:CG2	1:A:1581:GLU:HG2	2.34	0.58
1:A:333:MET:SD	1:A:333:MET:N	2.74	0.58
1:A:1828:LEU:HB3	1:A:1879:VAL:HG11	1.85	0.58
1:A:2123:PRO:HG2	1:A:2126:MET:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2156:VAL:O	1:A:2159:PRO:HD2	2.03	0.58
1:A:3817:LEU:HD22	1:A:3825:LYS:HD2	1.86	0.57
1:A:72:SER:O	1:A:82:ARG:NH1	2.37	0.57
1:A:1153:LEU:HD11	1:A:1159:PRO:HA	1.87	0.57
1:A:2470:ARG:NH1	1:A:2512:ASP:OD1	2.38	0.57
1:A:3828:TYR:HD1	1:A:3829:LEU:HD23	1.69	0.57
1:A:3411:ASP:O	1:A:3415:THR:OG1	2.23	0.57
1:A:3527:GLN:HA	1:A:3530:VAL:HG12	1.85	0.57
1:A:1851:LEU:O	1:A:1870:LYS:NZ	2.35	0.57
1:A:2155:GLU:O	1:A:2159:PRO:HD3	2.04	0.57
1:A:749:VAL:HB	1:A:750:PRO:HD3	1.86	0.57
1:A:1606:ARG:HB2	1:A:2042:GLN:HE22	1.70	0.57
1:A:1945:TYR:CE1	1:A:1971:PRO:HB3	2.39	0.57
1:A:1859:ASN:ND2	1:A:1861:SER:OG	2.38	0.57
1:A:217:LEU:HD22	1:A:263:LYS:HG2	1.87	0.56
1:A:1241:LEU:HG	1:A:1296:PHE:CE1	2.41	0.56
1:A:3021:SER:HB3	2:C:408:PRO:HG3	1.86	0.56
1:A:2890:ILE:O	1:A:2894:GLU:HG3	2.05	0.56
1:A:2313:LYS:HB3	1:A:2314:GLU:OE1	2.05	0.56
1:A:3066:ASP:OD1	1:A:3067:LYS:N	2.39	0.56
1:A:95:LYS:HG3	1:A:96:MET:N	2.20	0.56
1:A:3351:ILE:HD12	1:A:3352:GLU:H	1.70	0.56
1:A:3466:PRO:HA	1:A:3469:LEU:HD12	1.88	0.56
1:A:2326:ILE:O	1:A:2330:VAL:HG13	2.06	0.56
1:A:1442:GLN:OE1	1:A:1445:ARG:NH2	2.38	0.56
1:A:1743:MET:HE1	1:A:1765:VAL:HG11	1.88	0.56
1:A:681:LYS:O	1:A:684:GLU:HG2	2.05	0.56
1:A:2171:LEU:O	1:A:2177:ASN:ND2	2.39	0.56
2:C:365:THR:HG23	2:C:367:PRO:CD	2.23	0.56
1:A:3817:LEU:HD21	1:A:3829:LEU:HD21	1.86	0.56
2:C:378:ALA:O	2:C:379:ARG:HB2	2.06	0.56
1:A:2361:ILE:HD11	1:A:2382:VAL:HG22	1.87	0.55
1:A:1071:ASN:HB3	1:A:1074:LYS:HG3	1.88	0.55
1:A:1081:ALA:O	1:A:1085:ILE:HG13	2.07	0.55
1:A:3048:LYS:HD3	1:A:3061:LEU:HB2	1.88	0.55
1:A:206:THR:O	1:A:209:THR:OG1	2.22	0.55
1:A:2323:LEU:HB3	1:A:2344:LEU:HD11	1.88	0.55
1:A:3013:TYR:CD2	2:C:402:ARG:HG2	2.41	0.55
1:A:3883:LEU:HD13	1:A:3970:LEU:HD22	1.89	0.55
1:A:515:ARG:NH1	1:A:2057:GLN:OE1	2.40	0.55
1:A:2439:ILE:HA	1:A:2442:MET:HE2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:ILE:HD13	1:A:1031:ARG:HG2	1.89	0.55
1:A:2891:ARG:O	1:A:2895:GLU:HG2	2.07	0.55
1:A:2154:GLU:HA	1:A:2157:PHE:HD2	1.72	0.55
1:A:1424:THR:HG22	1:A:1426:GLN:H	1.71	0.54
1:A:1487:VAL:HG11	1:A:1515:LEU:HD13	1.89	0.54
1:A:2482:ASP:O	1:A:2485:ARG:HG2	2.07	0.54
1:A:2143:ARG:HE	1:A:2171:LEU:HD13	1.73	0.54
1:A:3838:GLU:OE1	1:A:3877:LYS:NZ	2.40	0.54
1:A:1208:LEU:O	1:A:1212:LEU:HB2	2.07	0.54
1:A:538:ASP:N	1:A:538:ASP:OD1	2.36	0.54
1:A:670:LEU:O	1:A:674:VAL:HG23	2.06	0.54
1:A:3174:ASP:O	1:A:3249:GLN:NE2	2.38	0.54
1:A:2950:LYS:HE2	1:A:2986:PRO:HG3	1.89	0.54
1:A:4017:GLU:O	1:A:4021:LEU:HB2	2.08	0.54
1:A:2087:GLU:OE2	1:A:2087:GLU:N	2.40	0.54
1:A:565:TYR:O	1:A:569:VAL:HG23	2.08	0.53
1:A:1397:ASP:O	1:A:1401:ASN:ND2	2.34	0.53
1:A:1696:LEU:HD11	1:A:1710:LEU:HD11	1.89	0.53
1:A:1837:ARG:NH1	1:A:1888:ASP:OD2	2.41	0.53
1:A:3835:PRO:N	1:A:3836:PRO:HD2	2.23	0.53
1:A:156:PHE:HB3	1:A:178:LEU:HD11	1.90	0.53
1:A:252:VAL:HG21	1:A:274:LEU:HD22	1.89	0.53
1:A:3763:ARG:HH22	1:A:4004:VAL:HG12	1.72	0.53
1:A:3300:VAL:HB	1:A:3333:THR:HG23	1.91	0.53
1:A:3816:LEU:HD13	1:A:4128:MET:HE2	1.91	0.53
1:A:1493:PRO:HD2	1:A:1538:LEU:HD23	1.91	0.53
1:A:2104:MET:HA	1:A:2108:LEU:HD23	1.89	0.53
1:A:3667:LEU:O	1:A:3671:ASN:ND2	2.42	0.53
1:A:3599:THR:O	1:A:3600:PRO:C	2.50	0.53
1:A:868:LYS:HG2	1:A:3126:LEU:HD11	1.91	0.52
1:A:2159:PRO:O	1:A:2160:TYR:HB2	2.09	0.52
1:A:1234:GLY:HA2	1:A:1259:LEU:HD13	1.91	0.52
1:A:1102:GLU:HA	1:A:1154:PRO:HB3	1.92	0.52
1:A:286:LEU:HD23	1:A:287:LEU:H	1.74	0.52
1:A:476:ARG:HE	1:A:563:LEU:HD11	1.75	0.52
1:A:131:LEU:HD23	1:A:177:LEU:HD21	1.92	0.52
1:A:2123:PRO:HD3	1:A:2160:TYR:CZ	2.45	0.52
1:A:252:VAL:O	1:A:256:ILE:HG12	2.10	0.52
1:A:635:PRO:HA	1:A:676:ASN:HD21	1.75	0.52
1:A:3091:LEU:HD21	1:A:3141:PHE:HE2	1.75	0.51
1:A:1876:ILE:HG22	1:A:1880:MET:HE1	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1212:LEU:O	1:A:1216:GLY:N	2.43	0.51
1:A:1855:PHE:HE1	1:A:1870:LYS:HE3	1.76	0.51
1:A:1057:LYS:HD3	1:A:1099:PHE:HZ	1.74	0.51
1:A:3668:LEU:O	1:A:3672:LYS:HB2	2.11	0.51
1:A:1154:PRO:HD3	1:A:1163:LEU:HD21	1.92	0.51
1:A:3883:LEU:HB3	1:A:3970:LEU:HD13	1.92	0.51
1:A:238:MET:HA	1:A:241:ASP:HB3	1.92	0.51
1:A:2806:LYS:HG3	1:A:2857:CYS:HB2	1.91	0.51
1:A:3581:PRO:HA	1:A:3584:LEU:HD12	1.92	0.51
1:A:14:ARG:HD3	1:A:34:LEU:HD21	1.92	0.51
1:A:162:LEU:HD23	1:A:164:LYS:H	1.76	0.51
1:A:3553:GLU:O	1:A:3557:ARG:HG3	2.11	0.51
1:A:859:LEU:HD21	1:A:870:LEU:HD13	1.93	0.51
1:A:2517:LEU:HA	1:A:2520:ILE:HG13	1.92	0.51
2:C:376:LYS:H	2:C:377:ARG:HH21	1.58	0.50
1:A:746:ARG:HG2	1:A:788:TYR:CE1	2.39	0.50
1:A:3069:MET:HA	1:A:3075:LYS:HB2	1.91	0.50
1:A:3296:GLN:O	1:A:3300:VAL:HG22	2.11	0.50
2:C:364:SER:O	2:C:365:THR:HG22	2.11	0.50
1:A:1059:LEU:HA	1:A:1062:ARG:HD2	1.93	0.50
1:A:1407:LYS:HD3	1:A:1463:LEU:HD21	1.94	0.50
1:A:2341:LEU:HD21	1:A:2371:PHE:HE2	1.74	0.50
1:A:1448:LEU:HD21	1:A:1514:LEU:HD11	1.93	0.50
1:A:2057:GLN:HG3	1:A:2059:PRO:HD2	1.93	0.50
1:A:2459:VAL:HG21	1:A:2501:LEU:HD21	1.94	0.50
1:A:3256:MET:HE2	1:A:3283:LEU:HD23	1.92	0.50
1:A:3705:TYR:HD1	1:A:3712:LEU:HD13	1.75	0.50
1:A:16:GLN:NE2	1:A:62:ASP:O	2.42	0.50
1:A:249:PHE:CZ	1:A:253:LEU:HD13	2.46	0.50
1:A:879:MET:HE3	1:A:3119:VAL:HG23	1.92	0.50
1:A:3817:LEU:HD23	1:A:3820:MET:HE1	1.94	0.50
1:A:3992:ARG:NH1	1:A:4103:GLN:OE1	2.45	0.50
1:A:470:ALA:HB1	1:A:1546:SER:HB2	1.93	0.50
1:A:2158:ARG:O	1:A:2161:ALA:HB2	2.10	0.50
1:A:93:LEU:HD21	1:A:133:LYS:CB	2.42	0.50
1:A:3637:GLY:HA2	1:A:3640:PHE:CZ	2.47	0.50
2:C:376:LYS:H	2:C:377:ARG:NH2	2.09	0.50
1:A:1675:TYR:OH	1:A:1692:ALA:O	2.24	0.50
1:A:1972:GLU:HB3	1:A:2142:ILE:HD12	1.94	0.50
1:A:2105:HIS:CE1	1:A:2156:VAL:HA	2.46	0.50
1:A:2327:LEU:O	1:A:2330:VAL:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2797:VAL:HG13	1:A:2804:ILE:HG21	1.93	0.50
1:A:4085:LYS:NZ	1:A:4091:ALA:O	2.45	0.50
1:A:668:LYS:O	1:A:672:ILE:HG13	2.12	0.49
1:A:1508:LYS:HE2	1:A:1562:LEU:HD22	1.94	0.49
1:A:2348:GLN:HG3	1:A:2360:PHE:CE1	2.47	0.49
1:A:3012:GLU:OE2	1:A:3048:LYS:NZ	2.44	0.49
1:A:3313:SER:HA	1:A:3316:LEU:HD12	1.93	0.49
1:A:168:ASP:OD1	1:A:168:ASP:N	2.45	0.49
1:A:363:ILE:HG12	1:A:388:LEU:HD11	1.94	0.49
1:A:1164:CYS:SG	1:A:1165:LEU:N	2.86	0.49
1:A:4065:LEU:HA	1:A:4074:PHE:HE2	1.77	0.49
1:A:380:ASP:O	1:A:384:MET:HG3	2.12	0.49
1:A:2150:VAL:HG11	1:A:2168:LEU:HD11	1.94	0.49
1:A:3062:LEU:HD22	1:A:3093:GLN:HE21	1.77	0.49
1:A:3886:ALA:O	1:A:3890:MET:HG3	2.13	0.49
2:C:377:ARG:H	2:C:377:ARG:NE	2.11	0.49
1:A:557:SER:HB3	1:A:1545:SER:H	1.78	0.49
1:A:1696:LEU:HD21	1:A:1714:LEU:HD21	1.94	0.49
1:A:1938:ARG:CZ	1:A:1938:ARG:HB3	2.41	0.49
1:A:3612:ARG:HH11	1:A:3799:ARG:HH12	1.61	0.49
2:C:374:LYS:HD2	2:C:376:LYS:HZ1	1.77	0.49
1:A:881:LYS:C	1:A:883:TYR:N	2.66	0.49
1:A:933:LEU:HG	1:A:937:MET:HE2	1.94	0.49
1:A:2350:LYS:HG3	1:A:2351:GLN:N	2.27	0.49
1:A:2567:SER:HA	1:A:2572:TYR:CG	2.48	0.49
1:A:3998:LEU:O	1:A:4002:MET:HG3	2.13	0.49
1:A:58:VAL:HG13	1:A:65:LEU:HD23	1.95	0.48
1:A:1213:LYS:HD2	1:A:1213:LYS:HA	1.46	0.48
1:A:1528:LEU:HD12	1:A:1531:LEU:HD11	1.94	0.48
1:A:2886:GLN:HB2	1:A:2933:ILE:HD13	1.95	0.48
1:A:3328:ILE:HD11	1:A:3412:ALA:HB2	1.94	0.48
1:A:3713:PRO:O	1:A:3714:GLU:HB3	2.12	0.48
1:A:892:LEU:HD11	1:A:941:MET:HG3	1.94	0.48
1:A:1376:LEU:HD21	1:A:1403:MET:HE1	1.95	0.48
1:A:2402:LEU:HD13	1:A:2438:ILE:HG13	1.94	0.48
1:A:746:ARG:HH21	1:A:749:VAL:HG11	1.78	0.48
1:A:1849:ASP:HA	1:A:1852:LYS:HG2	1.95	0.48
1:A:2481:HIS:CE1	1:A:2485:ARG:HH21	2.31	0.48
1:A:3613:MET:O	1:A:3617:LEU:N	2.35	0.48
1:A:1984:LEU:HD22	1:A:2185:MET:HB2	1.95	0.48
1:A:2893:LEU:HD22	1:A:2922:ARG:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:377:ARG:CD	2:C:377:ARG:H	2.26	0.48
1:A:601:TRP:HE3	1:A:602:MET:H	1.61	0.48
1:A:4006:VAL:HG11	1:A:4044:ILE:HB	1.96	0.48
1:A:1794:GLN:OE1	1:A:1832:SER:OG	2.27	0.48
1:A:2474:TYR:HD1	1:A:2477:LEU:HD12	1.79	0.48
1:A:767:GLU:HG3	1:A:771:ASN:HD21	1.78	0.48
1:A:3468:LEU:HB3	1:A:3483:MET:HE1	1.95	0.48
1:A:3916:TRP:CE2	1:A:4107:LEU:HD21	2.48	0.48
1:A:1711:ARG:NH1	1:A:1715:GLU:OE2	2.47	0.48
1:A:2933:ILE:HD11	1:A:3121:LEU:HD13	1.95	0.48
1:A:881:LYS:O	1:A:883:TYR:N	2.47	0.47
1:A:2158:ARG:HG2	1:A:2196:TRP:NE1	2.29	0.47
1:A:2318:ALA:O	1:A:2322:VAL:HG23	2.14	0.47
1:A:1356:TRP:HB2	1:A:1411:TYR:HE1	1.78	0.47
1:A:1498:GLN:OE1	1:A:1541:ALA:N	2.48	0.47
1:A:3155:VAL:HG23	1:A:3156:PRO:HD3	1.95	0.47
1:A:3302:LYS:HE3	2:C:393:PHE:O	2.14	0.47
1:A:62:ASP:HA	1:A:67:VAL:HG21	1.96	0.47
1:A:2044:ASP:OD1	1:A:2051:SER:OG	2.25	0.47
1:A:93:LEU:HD21	1:A:133:LYS:HB2	1.97	0.47
1:A:257:ARG:HE	1:A:258:PRO:HD2	1.80	0.47
1:A:3332:THR:HG23	1:A:3335:ARG:HH21	1.80	0.47
1:A:10:CYS:SG	1:A:2390:HIS:ND1	2.87	0.47
1:A:92:PHE:O	1:A:96:MET:HG3	2.14	0.47
1:A:1472:SER:OG	1:A:1474:ASP:OD2	2.27	0.47
1:A:1058:SER:O	1:A:1062:ARG:HG3	2.14	0.47
1:A:767:GLU:O	1:A:771:ASN:ND2	2.48	0.47
1:A:2412:TYR:CE2	1:A:2450:GLU:HG2	2.50	0.47
1:A:3557:ARG:O	1:A:3561:LYS:HG3	2.15	0.47
1:A:2860:ASP:O	1:A:2864:GLN:HG2	2.14	0.47
1:A:3606:ILE:HD12	1:A:3606:ILE:H	1.80	0.47
1:A:97:GLY:O	1:A:98:GLN:C	2.58	0.47
1:A:2304:VAL:HG13	1:A:2347:LYS:HD3	1.97	0.47
1:A:1239:PRO:HD2	1:A:1243:TYR:CE1	2.49	0.46
1:A:2474:TYR:O	1:A:2478:MET:HG3	2.15	0.46
1:A:66:LEU:H	1:A:66:LEU:HD12	1.81	0.46
1:A:710:PHE:O	1:A:714:VAL:HG23	2.15	0.46
1:A:3302:LYS:HB3	1:A:3302:LYS:HE2	1.54	0.46
1:A:3072:GLU:OE1	1:A:3072:GLU:N	2.46	0.46
1:A:3603:LYS:HD3	1:A:3605:ASN:HB2	1.97	0.46
1:A:646:VAL:O	1:A:650:SER:OG	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1241:LEU:HG	1:A:1241:LEU:H	1.60	0.46
1:A:1723:PRO:O	1:A:1768:ARG:NH2	2.48	0.46
2:C:401:LEU:HB2	2:C:402:ARG:NH1	2.30	0.46
1:A:372:PRO:O	1:A:376:ILE:HG12	2.16	0.46
1:A:359:LEU:HD11	1:A:391:ARG:HH21	1.80	0.46
1:A:3260:LYS:HG3	2:C:395:ASP:CG	2.40	0.46
1:A:3013:TYR:CB	2:C:402:ARG:HE	2.27	0.46
1:A:105:VAL:HG12	1:A:108:LYS:HE3	1.98	0.46
1:A:602:MET:SD	1:A:603:ILE:HG23	2.56	0.46
1:A:1188:ILE:HG21	1:A:1269:THR:HG21	1.98	0.46
1:A:1936:ARG:HA	1:A:1939:LEU:HD12	1.98	0.46
1:A:2269:ASP:OD1	1:A:2269:ASP:N	2.48	0.46
1:A:1920:TYR:OH	1:A:1962:TYR:O	2.27	0.46
1:A:3706:ASP:OD1	1:A:3707:GLY:N	2.49	0.46
1:A:449:TYR:HB3	1:A:453:MET:HB3	1.98	0.45
1:A:1332:TYR:O	1:A:1336:THR:OG1	2.34	0.45
1:A:250:ASN:O	1:A:254:LYS:HG2	2.16	0.45
1:A:1840:PHE:O	1:A:1844:VAL:HG23	2.17	0.45
1:A:2773:ARG:NE	1:A:2789:SER:OG	2.43	0.45
2:C:366:GLU:CD	2:C:366:GLU:H	2.24	0.45
1:A:1186:LYS:O	1:A:1190:LEU:HD23	2.16	0.45
1:A:1459:HIS:CE1	1:A:1520:ALA:HB1	2.51	0.45
1:A:3821:SER:OG	1:A:3824:GLU:HG3	2.17	0.45
1:A:913:ARG:NH1	1:A:916:GLU:OE1	2.49	0.45
1:A:1765:VAL:HA	1:A:1768:ARG:HD3	1.96	0.45
1:A:2338:GLU:HG3	1:A:2341:LEU:HB2	1.98	0.45
1:A:249:PHE:HB2	1:A:282:PHE:CD1	2.51	0.45
1:A:604:PRO:HG2	1:A:1083:ASN:HB3	1.98	0.45
1:A:878:GLU:OE2	1:A:881:LYS:HB3	2.17	0.45
1:A:1791:CYS:O	1:A:1795:VAL:HG12	2.16	0.45
1:A:1972:GLU:HG3	1:A:2132:LYS:HD3	1.98	0.45
1:A:59:PHE:HD1	1:A:66:LEU:HD11	1.82	0.45
1:A:1976:LEU:HD22	1:A:2142:ILE:HD13	1.99	0.45
1:A:3092:LEU:O	2:C:377:ARG:HG3	2.16	0.45
1:A:3479:THR:O	1:A:3479:THR:OG1	2.35	0.45
1:A:4003:ASP:O	1:A:4007:LYS:HG2	2.17	0.45
1:A:217:LEU:HD13	1:A:263:LYS:HE3	1.98	0.45
1:A:3091:LEU:HD23	1:A:3188:PHE:HE2	1.81	0.45
1:A:3451:LEU:HD12	1:A:3486:GLU:HB3	1.99	0.45
1:A:286:LEU:HD12	1:A:319:PHE:CD1	2.52	0.45
1:A:601:TRP:HE3	1:A:602:MET:N	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1452:VAL:HG23	1:A:1517:LEU:HD22	1.99	0.45
1:A:2027:SER:OG	1:A:2028:LEU:N	2.49	0.45
1:A:391:ARG:HD2	1:A:391:ARG:HA	1.82	0.45
1:A:603:ILE:HG21	1:A:1031:ARG:HD2	1.99	0.45
1:A:2100:LEU:O	1:A:2104:MET:HG2	2.17	0.45
1:A:3596:LEU:O	1:A:3597:ALA:HB3	2.17	0.45
1:A:1686:LEU:HD23	1:A:1738:ASN:HB3	1.99	0.44
1:A:3091:LEU:HD21	1:A:3141:PHE:CE2	2.52	0.44
1:A:709:LYS:HG3	1:A:710:PHE:N	2.30	0.44
1:A:2761:LEU:HD23	1:A:2764:LYS:HB2	1.99	0.44
1:A:3052:LEU:HD12	1:A:3061:LEU:HD23	1.99	0.44
1:A:132:ILE:HG12	1:A:180:LEU:HD22	1.99	0.44
1:A:660:LEU:HB3	1:A:663:ILE:HD12	1.98	0.44
1:A:2022:PRO:HB2	1:A:2052:TYR:HB3	1.98	0.44
1:A:124:LYS:O	1:A:128:LEU:HD13	2.17	0.44
1:A:1264:LEU:HD22	1:A:1344:PHE:HD2	1.81	0.44
1:A:1724:MET:HA	1:A:1768:ARG:HH21	1.83	0.44
1:A:2596:ARG:HD2	1:A:2761:LEU:HD22	1.99	0.44
1:A:3459:ASN:O	1:A:3463:LEU:HG	2.18	0.44
1:A:404:ASP:N	1:A:404:ASP:OD1	2.51	0.44
1:A:3027:LEU:HD21	1:A:3048:LYS:HE3	1.99	0.44
1:A:93:LEU:HG	1:A:94:GLU:N	2.33	0.44
1:A:95:LYS:HE2	1:A:95:LYS:HB2	1.62	0.44
1:A:2870:SER:O	1:A:2870:SER:OG	2.25	0.44
1:A:3372:LYS:HA	1:A:3372:LYS:HD2	1.82	0.44
1:A:3646:LYS:HA	1:A:3646:LYS:HD3	1.86	0.44
1:A:638:GLN:O	1:A:639:ALA:HB3	2.18	0.44
1:A:1239:PRO:HD2	1:A:1243:TYR:CZ	2.53	0.44
1:A:3974:MET:HE2	1:A:3974:MET:HB2	1.91	0.44
1:A:377:ASN:ND2	1:A:380:ASP:OD1	2.44	0.43
1:A:502:GLU:HG3	1:A:2760:GLU:HA	2.00	0.43
1:A:1689:LYS:HE2	1:A:1717:LEU:HD13	1.99	0.43
1:A:1973:LYS:H	1:A:1973:LYS:HG3	1.63	0.43
1:A:2095:ALA:HB3	1:A:2096:PRO:HD3	2.00	0.43
1:A:2967:GLU:OE2	1:A:2971:GLN:NE2	2.42	0.43
1:A:3362:LEU:HD23	1:A:3362:LEU:HA	1.85	0.43
1:A:3863:ASN:OD1	1:A:3864:ARG:N	2.51	0.43
2:C:368:LYS:O	2:C:369:TYR:C	2.61	0.43
1:A:305:ASN:HB3	1:A:308:LEU:HB3	2.00	0.43
1:A:414:LEU:HA	1:A:417:VAL:HG22	2.00	0.43
1:A:1212:LEU:HD12	1:A:1212:LEU:HA	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3036:TYR:HA	1:A:3040:TYR:HD2	1.83	0.43
1:A:1240:THR:HG23	1:A:1243:TYR:HE1	1.82	0.43
1:A:3659:PHE:O	1:A:3662:ILE:HG12	2.19	0.43
1:A:3820:MET:HE2	1:A:3820:MET:HB2	1.77	0.43
1:A:287:LEU:HG	1:A:337:LYS:NZ	2.32	0.43
1:A:468:LEU:HD22	1:A:475:LEU:HB3	1.99	0.43
1:A:850:GLU:H	1:A:850:GLU:CD	2.26	0.43
1:A:2304:VAL:HG22	1:A:2347:LYS:HG3	1.99	0.43
1:A:2482:ASP:CG	1:A:2530:ARG:HH21	2.26	0.43
1:A:3298:LEU:HD21	1:A:3351:ILE:HG12	1.99	0.43
1:A:741:ILE:HG21	1:A:776:TRP:CE2	2.53	0.43
1:A:759:GLY:HA2	1:A:762:TYR:O	2.17	0.43
1:A:1367:HIS:O	1:A:1371:VAL:HG22	2.19	0.43
1:A:1038:LYS:HB3	1:A:1038:LYS:HE2	1.77	0.43
1:A:2913:LYS:HB3	1:A:2913:LYS:HE2	1.68	0.43
1:A:1820:VAL:HA	1:A:1824:LEU:HB3	2.00	0.43
1:A:1500:LEU:HD12	1:A:1501:PRO:HD2	2.00	0.43
1:A:1627:LYS:HE3	1:A:1627:LYS:HB3	1.77	0.43
1:A:1857:LYS:HE2	1:A:1857:LYS:HB3	1.85	0.43
1:A:3487:ILE:HD12	1:A:3487:ILE:HA	1.86	0.43
1:A:3530:VAL:HA	1:A:3562:LEU:HD13	2.00	0.43
1:A:3562:LEU:HD23	1:A:3562:LEU:HA	1.87	0.43
1:A:245:SER:O	1:A:248:ILE:HG22	2.19	0.43
1:A:631:ARG:HH12	1:A:668:LYS:HB3	1.82	0.43
1:A:2361:ILE:HG12	1:A:2397:CYS:SG	2.58	0.43
1:A:2474:TYR:HE2	1:A:2517:LEU:HD13	1.84	0.43
1:A:4014:LYS:O	1:A:4017:GLU:HG3	2.18	0.43
1:A:96:MET:HE2	1:A:96:MET:HB2	1.73	0.42
1:A:722:LYS:HE3	1:A:722:LYS:HB3	1.48	0.42
1:A:1202:ARG:HH21	1:A:1207:TRP:HA	1.84	0.42
1:A:1515:LEU:HG	1:A:1519:PHE:CE2	2.54	0.42
1:A:3010:SER:CA	2:C:402:ARG:HD2	2.44	0.42
1:A:3193:ILE:HD12	1:A:3193:ILE:HA	1.89	0.42
1:A:1942:CYS:SG	1:A:1975:LEU:HG	2.59	0.42
1:A:2249:LEU:HD23	1:A:2249:LEU:HA	1.85	0.42
1:A:2500:LYS:HB3	1:A:2500:LYS:HE3	1.60	0.42
1:A:256:ILE:HG23	1:A:272:LEU:HD11	2.01	0.42
1:A:1301:ILE:O	1:A:1334:LYS:NZ	2.52	0.42
1:A:1633:TRP:HB3	1:A:1645:VAL:HG11	2.01	0.42
1:A:2347:LYS:HB3	1:A:2347:LYS:HE3	1.48	0.42
1:A:2513:GLU:H	1:A:2513:GLU:HG2	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3310:ASN:HA	1:A:3313:SER:HB2	2.02	0.42
1:A:59:PHE:HA	1:A:66:LEU:HD11	2.02	0.42
1:A:405:ASP:OD1	1:A:405:ASP:N	2.50	0.42
1:A:676:ASN:HA	1:A:679:LYS:HE3	2.01	0.42
1:A:1639:LEU:O	1:A:1643:MET:HG3	2.20	0.42
1:A:1762:MET:HB3	1:A:1778:PHE:HE2	1.83	0.42
1:A:678:LYS:HE2	1:A:737:PRO:HA	2.02	0.42
1:A:1202:ARG:NH2	1:A:1210:ASP:OD1	2.52	0.42
1:A:2101:VAL:HG21	1:A:2149:LEU:HD21	2.02	0.42
1:A:2302:ALA:HA	1:A:2305:ASN:ND2	2.35	0.42
1:A:2374:LEU:O	1:A:2377:ARG:HD2	2.19	0.42
1:A:2394:LYS:HD3	1:A:2423:VAL:HG13	2.02	0.42
1:A:3203:ASP:OD1	1:A:3203:ASP:N	2.43	0.42
1:A:638:GLN:HB3	1:A:640:GLU:CD	2.44	0.42
1:A:897:PRO:HG3	1:A:2787:HIS:HD2	1.85	0.42
1:A:919:LEU:HD21	1:A:971:ARG:HB3	2.02	0.42
1:A:2247:ASP:N	1:A:2247:ASP:OD1	2.53	0.42
1:A:338:LEU:HD13	1:A:372:PRO:HB2	2.01	0.42
1:A:1565:GLU:CD	1:A:1565:GLU:H	2.28	0.42
1:A:1724:MET:HB3	1:A:1725:GLN:OE1	2.20	0.42
1:A:2327:LEU:HD13	1:A:2341:LEU:HG	2.02	0.42
1:A:2341:LEU:HD23	1:A:2374:LEU:HD12	2.01	0.42
1:A:3111:MET:O	1:A:3115:SER:OG	2.31	0.42
1:A:3263:HIS:O	1:A:3264:LYS:C	2.63	0.42
1:A:3817:LEU:HA	1:A:3820:MET:HE2	2.02	0.42
1:A:14:ARG:O	1:A:18:THR:OG1	2.33	0.42
1:A:680:ILE:HD12	1:A:680:ILE:HA	1.88	0.42
1:A:1519:PHE:HB3	1:A:1570:GLU:OE1	2.19	0.42
1:A:3327:ASN:HB3	1:A:3388:ALA:HB2	2.01	0.42
1:A:3550:LYS:HD2	1:A:3550:LYS:HA	1.84	0.42
1:A:1407:LYS:HE2	1:A:1407:LYS:HB3	1.82	0.41
1:A:2373:PRO:O	1:A:2376:ASP:HB2	2.20	0.41
1:A:2928:LYS:HB2	1:A:2928:LYS:HE3	1.82	0.41
1:A:4006:VAL:HG22	1:A:4040:PRO:HB3	2.02	0.41
1:A:1000:LYS:HD3	1:A:1000:LYS:HA	1.80	0.41
1:A:1797:LEU:O	1:A:1801:VAL:HG23	2.20	0.41
1:A:2126:MET:HG2	1:A:2164:TRP:HZ2	1.85	0.41
1:A:371:GLY:O	1:A:375:VAL:HG13	2.20	0.41
1:A:713:GLU:O	1:A:717:LYS:HG3	2.20	0.41
1:A:1981:LEU:HD23	1:A:1981:LEU:H	1.86	0.41
1:A:2428:ASP:OD2	1:A:2431:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3098:ARG:HH22	2:C:369:TYR:HA	1.85	0.41
1:A:3281:CYS:HB2	1:A:3329:LEU:HD13	2.02	0.41
1:A:163:LYS:HZ3	1:A:171:LEU:HD21	1.85	0.41
1:A:563:LEU:O	1:A:567:GLU:HG2	2.20	0.41
1:A:3013:TYR:HB3	2:C:402:ARG:HE	1.86	0.41
1:A:690:SER:O	1:A:690:SER:OG	2.36	0.41
1:A:740:ILE:HA	1:A:743:LEU:HD22	2.01	0.41
1:A:1008:ALA:HA	1:A:1011:GLU:HG2	2.01	0.41
1:A:1037:LEU:HD22	1:A:1085:ILE:HG23	2.02	0.41
1:A:2394:LYS:HE3	1:A:2394:LYS:HB2	1.87	0.41
1:A:3463:LEU:HB2	1:A:3997:LEU:HD11	2.03	0.41
1:A:40:GLN:O	1:A:44:LEU:HB2	2.20	0.41
1:A:287:LEU:HD12	1:A:287:LEU:HA	1.87	0.41
1:A:804:ALA:HB2	1:A:3115:SER:HB2	2.02	0.41
1:A:1444:ASP:OD1	1:A:1444:ASP:N	2.52	0.41
1:A:3098:ARG:HD2	1:A:3102:TYR:CE2	2.56	0.41
2:C:383:ARG:HD2	2:C:383:ARG:HA	1.81	0.41
1:A:579:LEU:HD23	1:A:579:LEU:HA	1.87	0.41
1:A:679:LYS:H	1:A:679:LYS:HG3	1.60	0.41
1:A:1851:LEU:HA	1:A:1870:LYS:HD3	2.02	0.41
1:A:3128:LYS:O	1:A:3132:VAL:HG12	2.21	0.41
1:A:3958:LEU:HD22	1:A:4064:LEU:HD11	2.03	0.41
1:A:4128:MET:HE2	1:A:4128:MET:HB3	1.86	0.41
1:A:2055:SER:HB2	1:A:2060:ARG:HH21	1.85	0.41
1:A:357:LYS:H	1:A:357:LYS:HG2	1.65	0.41
1:A:399:GLN:HB2	1:A:2052:TYR:CE2	2.56	0.41
1:A:402:THR:HA	1:A:2018:ASP:HA	2.03	0.41
1:A:603:ILE:O	1:A:603:ILE:HG13	2.15	0.41
1:A:897:PRO:HG3	1:A:2787:HIS:CD2	2.54	0.41
1:A:1966:LEU:HD12	1:A:1966:LEU:HA	1.87	0.41
1:A:2844:LEU:HD23	1:A:2844:LEU:HA	1.90	0.41
1:A:3274:VAL:O	1:A:3278:GLN:HG3	2.20	0.41
1:A:3416:LEU:HD23	1:A:3449:LYS:HZ3	1.86	0.41
1:A:3653:ARG:HH21	1:A:3654:MET:HB2	1.83	0.41
1:A:3992:ARG:HG2	1:A:4051:LEU:O	2.21	0.41
1:A:163:LYS:HD3	1:A:163:LYS:HA	1.81	0.41
1:A:405:ASP:C	1:A:407:VAL:H	2.29	0.41
1:A:534:LEU:O	1:A:537:SER:OG	2.39	0.41
1:A:627:VAL:O	1:A:631:ARG:HG3	2.20	0.41
1:A:743:LEU:HA	1:A:743:LEU:HD12	1.82	0.41
1:A:1545:SER:O	1:A:1545:SER:OG	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2534:ASN:O	1:A:2535:THR:HG22	2.21	0.41
1:A:3311:ASN:OD1	1:A:3312:VAL:N	2.54	0.41
1:A:4064:LEU:HD13	1:A:4077:TYR:HB3	2.03	0.41
1:A:195:ASN:OD1	1:A:198:ARG:NH2	2.45	0.40
1:A:715:ALA:O	1:A:718:MET:HG2	2.21	0.40
1:A:257:ARG:NE	1:A:258:PRO:HD2	2.36	0.40
1:A:290:TYR:CZ	1:A:337:LYS:HG3	2.57	0.40
1:A:468:LEU:HD23	1:A:468:LEU:HA	1.88	0.40
1:A:1923:PHE:CZ	1:A:1945:TYR:HA	2.56	0.40
1:A:2207:LYS:HD2	1:A:2207:LYS:HA	1.81	0.40
1:A:2473:MET:O	1:A:2477:LEU:HG	2.21	0.40
1:A:3881:ASP:OD1	1:A:3881:ASP:N	2.55	0.40
1:A:90:CYS:O	1:A:94:GLU:HG2	2.21	0.40
1:A:1254:LEU:HD12	1:A:1329:ARG:HH21	1.86	0.40
1:A:2294:ILE:HG12	1:A:2295:GLN:HE21	1.86	0.40
1:A:2346:ALA:HA	1:A:2349:LEU:HD23	2.03	0.40
1:A:3512:VAL:HA	1:A:3515:GLN:HG3	2.03	0.40
1:A:3673:ASP:OD1	1:A:3674:SER:N	2.53	0.40
1:A:870:LEU:HD22	1:A:3129:LEU:HD21	2.03	0.40
1:A:1217:VAL:O	1:A:1221:ILE:HG13	2.20	0.40
1:A:2408:MET:HE2	1:A:2408:MET:HB3	2.00	0.40
1:A:2581:LEU:HD11	1:A:2783:ILE:HG23	2.02	0.40
2:C:376:LYS:HD3	2:C:376:LYS:HA	1.79	0.40
1:A:318:SER:O	1:A:322:GLN:HG2	2.22	0.40
1:A:524:TYR:CE1	1:A:628:GLU:HB3	2.57	0.40
1:A:587:THR:HG23	1:A:588:VAL:HG13	2.04	0.40
1:A:2485:ARG:O	1:A:2486:ASP:C	2.64	0.40
1:A:2562:LEU:HD23	1:A:2562:LEU:HA	1.88	0.40
1:A:3176:MET:HA	1:A:3176:MET:HE3	2.02	0.40
1:A:3271:ASP:HA	1:A:3274:VAL:HG12	2.04	0.40
1:A:3708:ARG:O	1:A:3710:LYS:NZ	2.52	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	3896/4128 (94%)	3699 (95%)	191 (5%)	6 (0%)	43	71
2	C	50/707 (7%)	38 (76%)	11 (22%)	1 (2%)	6	28
All	All	3946/4835 (82%)	3737 (95%)	202 (5%)	7 (0%)	44	71

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	882	SER
1	A	2161	ALA
1	A	2162	LYS
1	A	3716	HIS
1	A	682	TYR
1	A	743	LEU
2	C	365	THR

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	3474/3671 (95%)	3399 (98%)	75 (2%)	45	65
2	C	50/647 (8%)	30 (60%)	20 (40%)	0	0
All	All	3524/4318 (82%)	3429 (97%)	95 (3%)	40	63

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	LEU
1	A	95	LYS
1	A	96	MET
1	A	283	SER
1	A	285	CYS
1	A	287	LEU

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Mol	Chain	Res	Type
1	A	288	ASP
1	A	601	TRP
1	A	603	ILE
1	A	605	THR
1	A	638	GLN
1	A	640	GLU
1	A	678	LYS
1	A	679	LYS
1	A	680	ILE
1	A	681	LYS
1	A	709	LYS
1	A	712	LYS
1	A	722	LYS
1	A	723	ASP
1	A	743	LEU
1	A	746	ARG
1	A	784	VAL
1	A	873	VAL
1	A	879	MET
1	A	880	MET
1	A	881	LYS
1	A	961	LEU
1	A	964	ARG
1	A	1031	ARG
1	A	1061	LYS
1	A	1062	ARG
1	A	1212	LEU
1	A	1213	LYS
1	A	1236	LEU
1	A	1241	LEU
1	A	1466	ASN
1	A	1481	THR
1	A	1524	LEU
1	A	1525	CYS
1	A	1529	VAL
1	A	1751	GLU
1	A	1938	ARG
1	A	2093	CYS
1	A	2094	MET
1	A	2097	LEU
1	A	2126	MET
1	A	2155	GLU

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Mol	Chain	Res	Type
1	A	2156	VAL
1	A	2328	ARG
1	A	2339	GLU
1	A	2341	LEU
1	A	2342	CYS
1	A	2344	LEU
1	A	2347	LYS
1	A	2349	LEU
1	A	2350	LYS
1	A	2374	LEU
1	A	2377	ARG
1	A	2497	GLU
1	A	2500	LYS
1	A	2913	LYS
1	A	2915	ARG
1	A	2916	LEU
1	A	3009	LYS
1	A	3059	GLN
1	A	3096	VAL
1	A	3260	LYS
1	A	3264	LYS
1	A	3267	LYS
1	A	3302	LYS
1	A	3598	LYS
1	A	3820	MET
1	A	3825	LYS
1	A	3829	LEU
2	C	363	GLN
2	C	365	THR
2	C	366	GLU
2	C	368	LYS
2	C	369	TYR
2	C	370	LYS
2	C	372	LEU
2	C	374	LYS
2	C	375	LEU
2	C	376	LYS
2	C	377	ARG
2	C	381	VAL
2	C	384	ASP
2	C	386	GLU
2	C	389	ASP

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Mol	Chain	Res	Type
2	C	392	LEU
2	C	395	ASP
2	C	397	LEU
2	C	399	ILE
2	C	402	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	ASN
1	A	390	GLN
1	A	508	HIS
1	A	638	GLN
1	A	676	ASN
1	A	771	ASN
1	A	857	GLN
1	A	925	GLN
1	A	978	GLN
1	A	1043	GLN
1	A	1205	ASN
1	A	1238	GLN
1	A	1534	ASN
1	A	1611	GLN
1	A	1859	ASN
1	A	1866	GLN
1	A	1946	ASN
1	A	1974	ASN
1	A	2050	GLN
1	A	2183	HIS
1	A	2305	ASN
1	A	2348	GLN
1	A	2426	HIS
1	A	2481	HIS
1	A	2496	GLN
1	A	2523	ASN
1	A	2553	HIS
1	A	2560	ASN
1	A	2579	HIS
1	A	2784	GLN
1	A	2831	ASN
1	A	3004	HIS
1	A	3108	GLN

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Mol	Chain	Res	Type
1	A	3154	GLN
1	A	3494	GLN
1	A	3602	ASN
1	A	4015	ASN
1	A	4018	GLN
1	A	4087	HIS
1	A	4088	ASN
2	C	363	GLN

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 [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

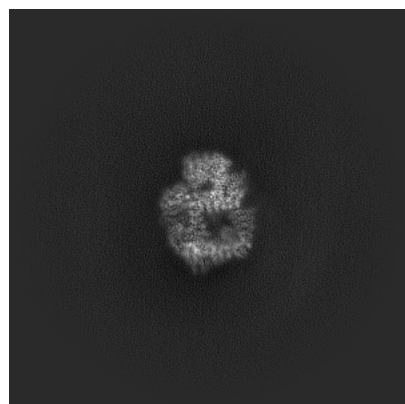
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26192. These allow visual inspection of the internal detail of the map and identification of artifacts.

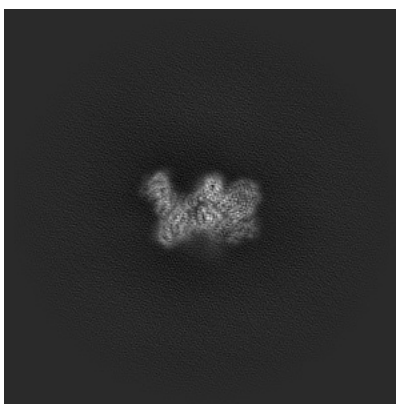
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

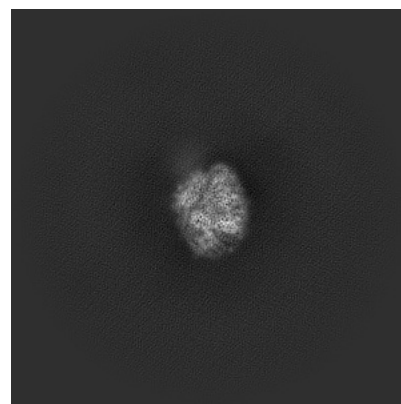
6.1.1 Primary map



X

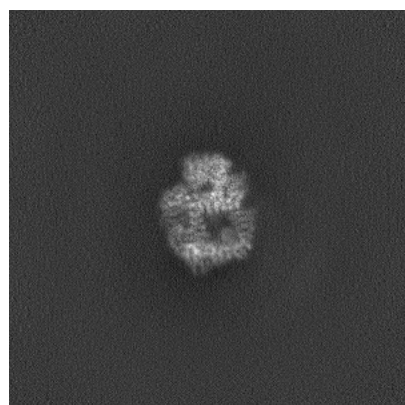


Y

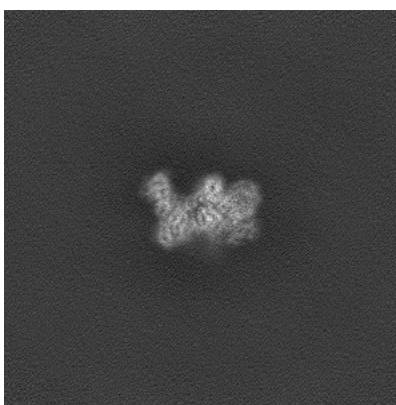


Z

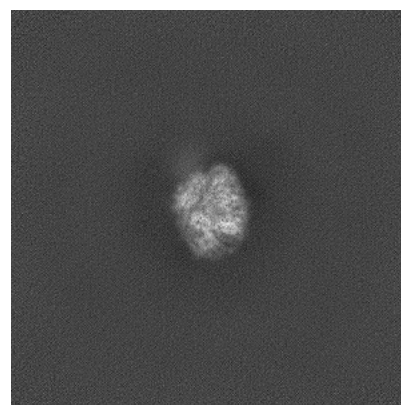
6.1.2 Raw map



X



Y

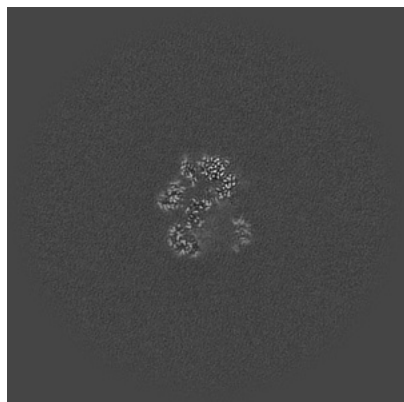


Z

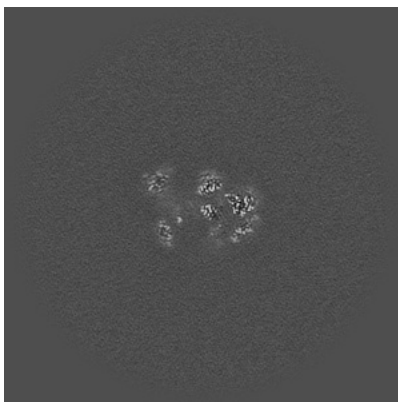
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 256

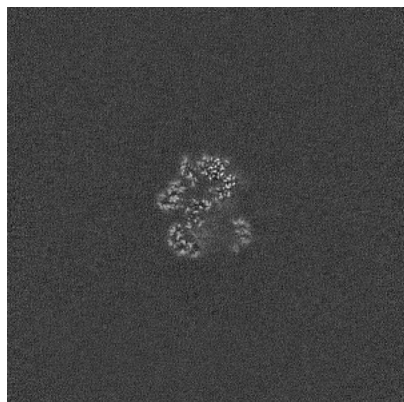


Y Index: 256

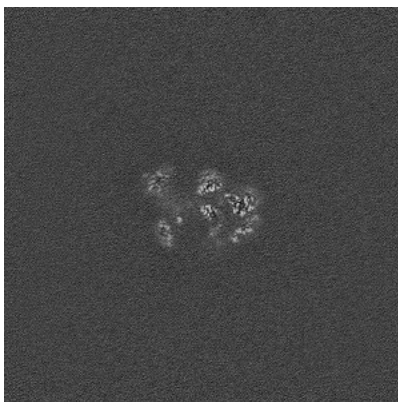


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

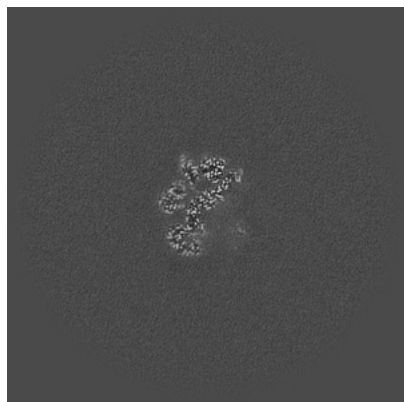


Z Index: 256

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

6.3 Largest variance slices [i](#)

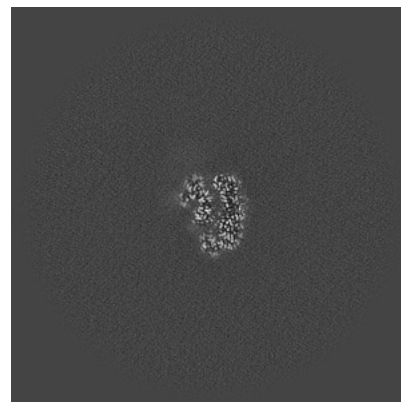
6.3.1 Primary map



X Index: 252

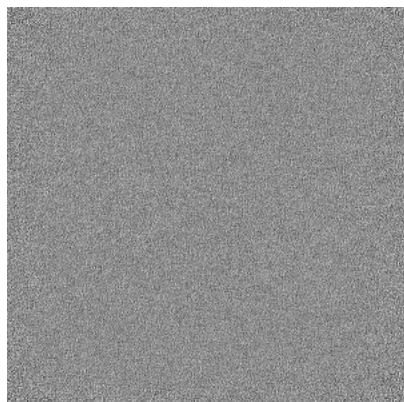


Y Index: 238

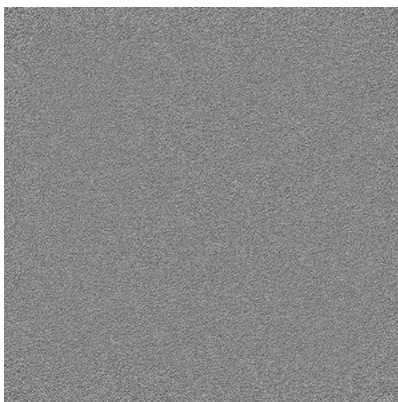


Z Index: 265

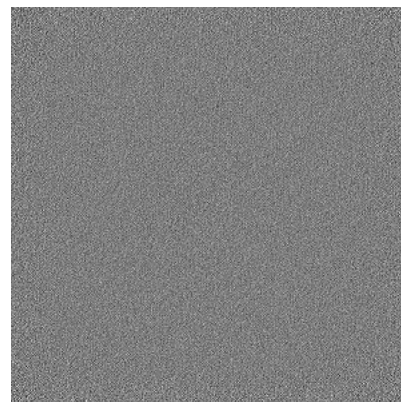
6.3.2 Raw map



X Index: 0



Y Index: 0

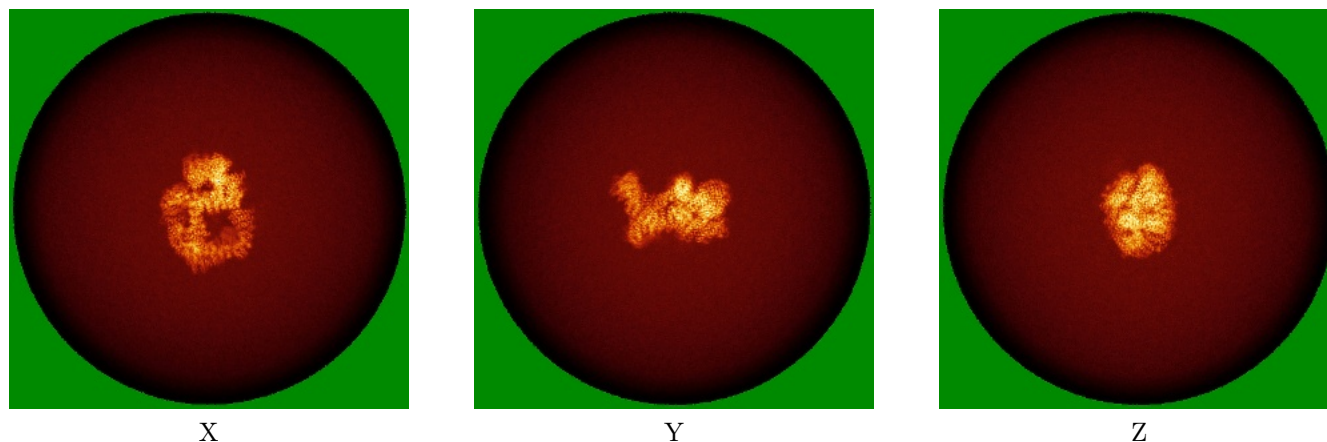


Z Index: 0

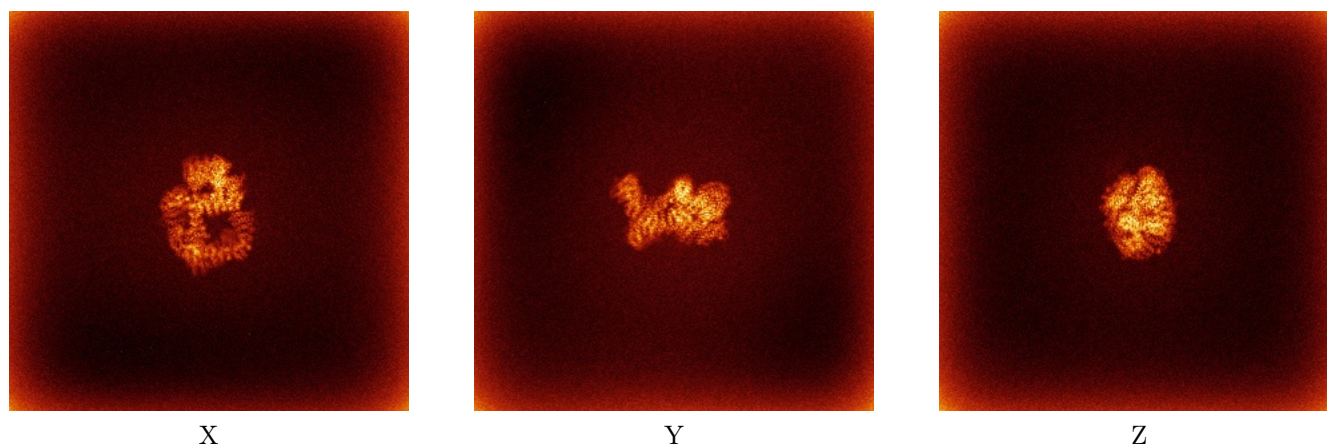
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

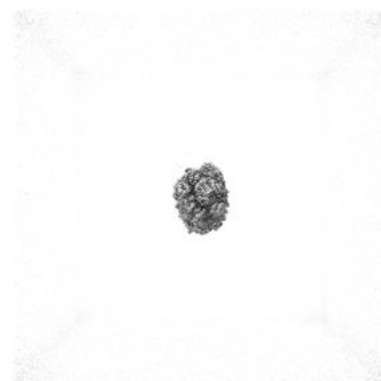
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

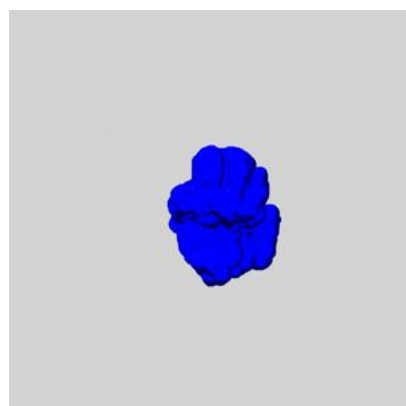
6.6 Mask visualisation [i](#)

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

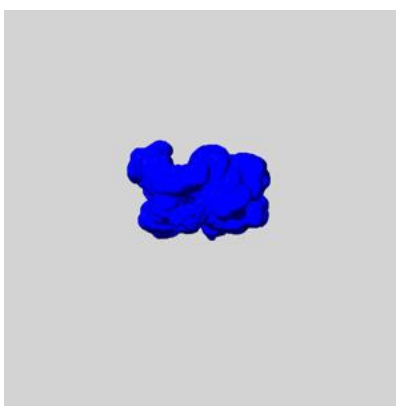
A mask typically either:

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

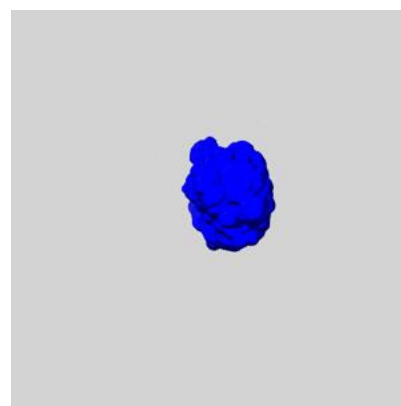
6.6.1 emd_26192_msk_1.map [i](#)



X



Y

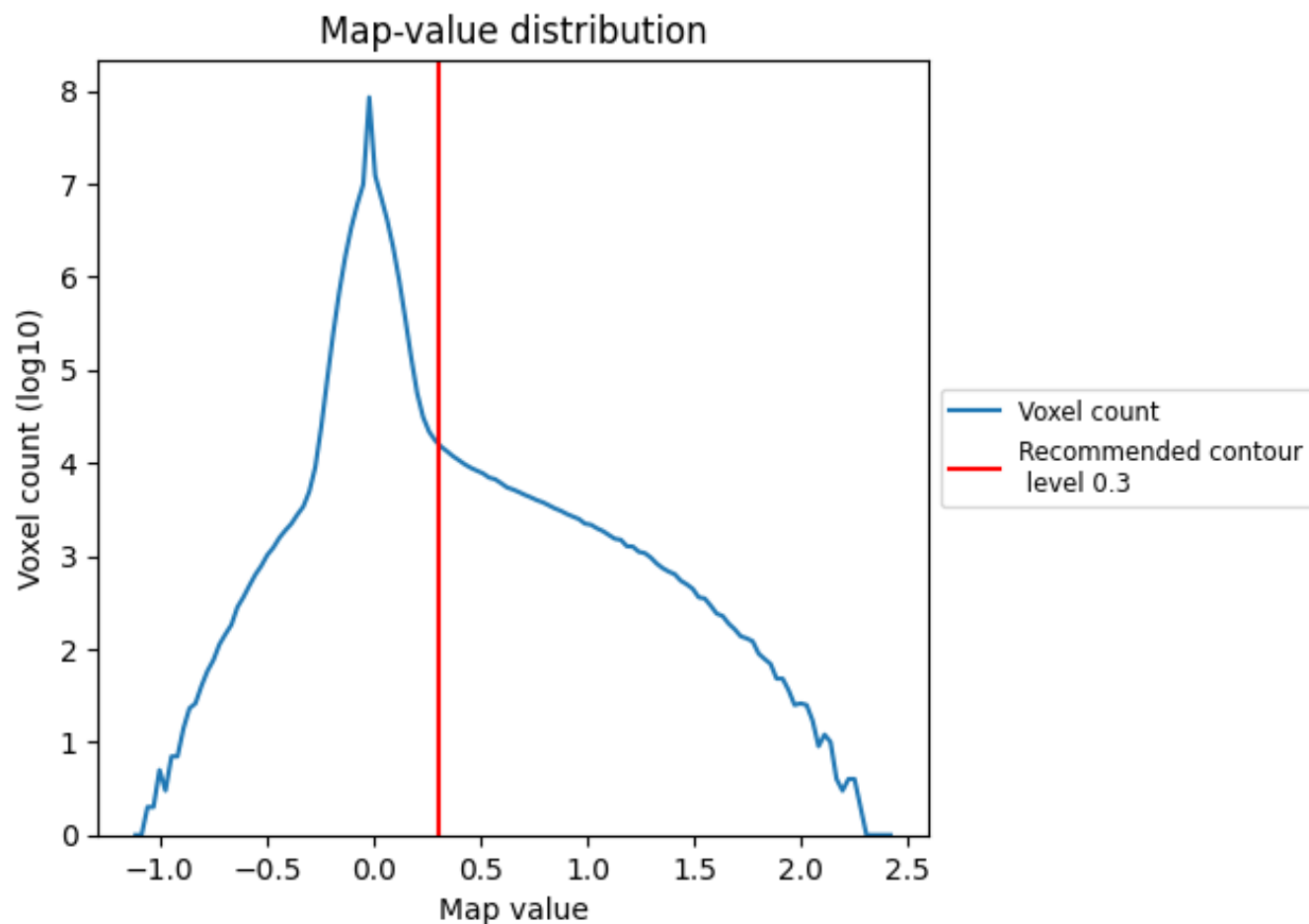


Z

7 Map analysis [i](#)

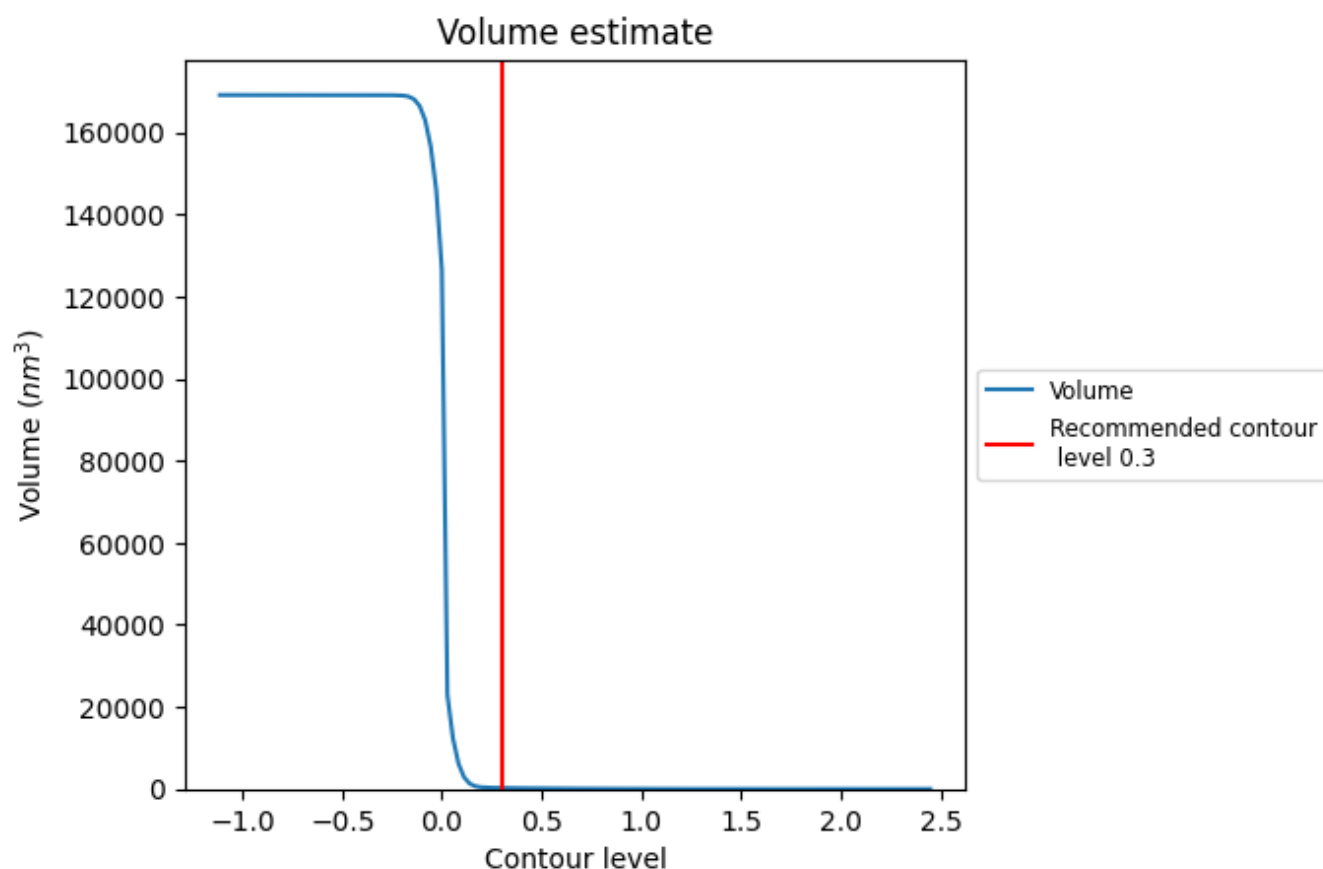
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

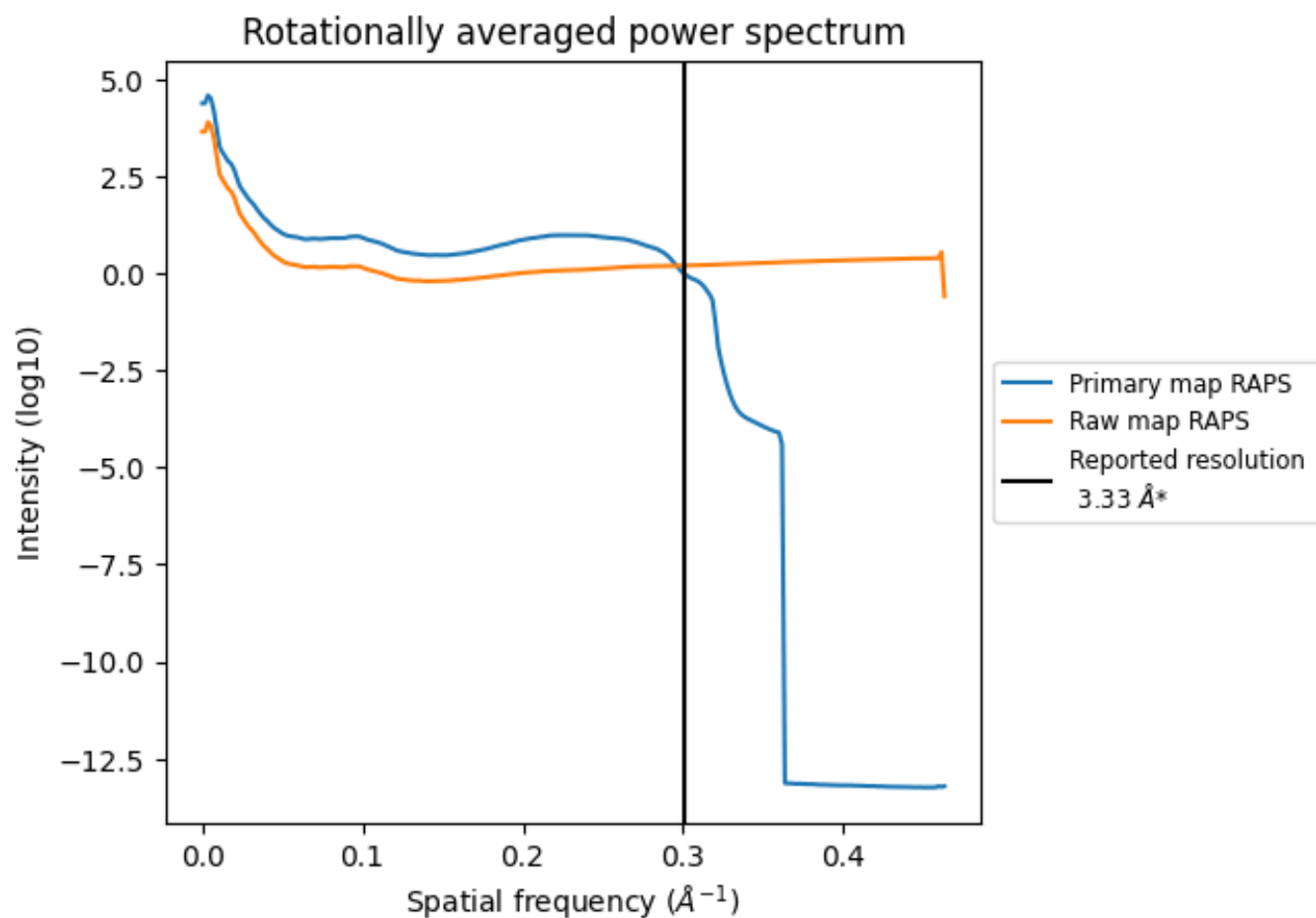
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 240 nm^3 ; this corresponds to an approximate mass of 217 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 ⓘ

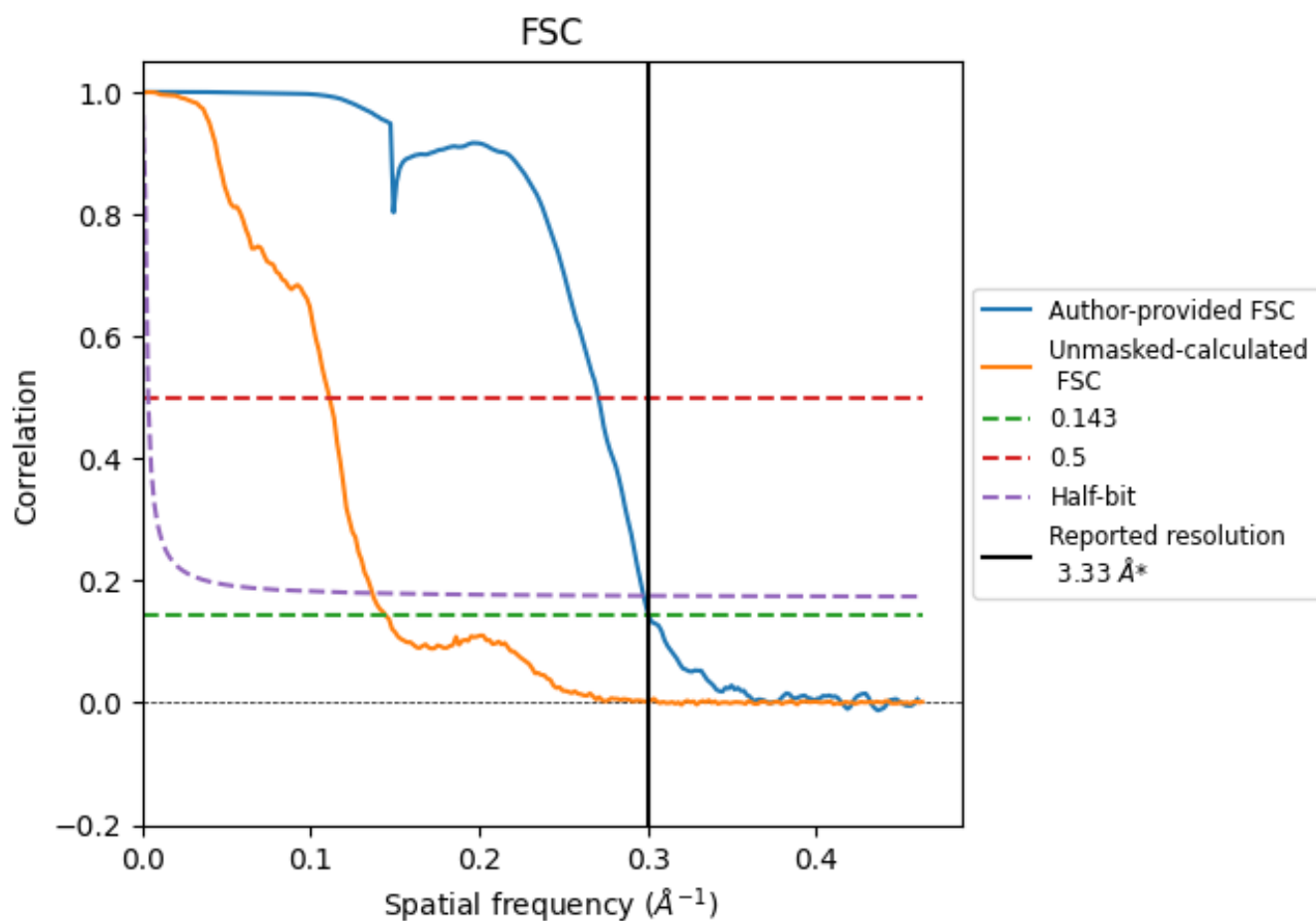


*Reported resolution corresponds to spatial frequency of 0.300 Å⁻¹

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 0.300 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

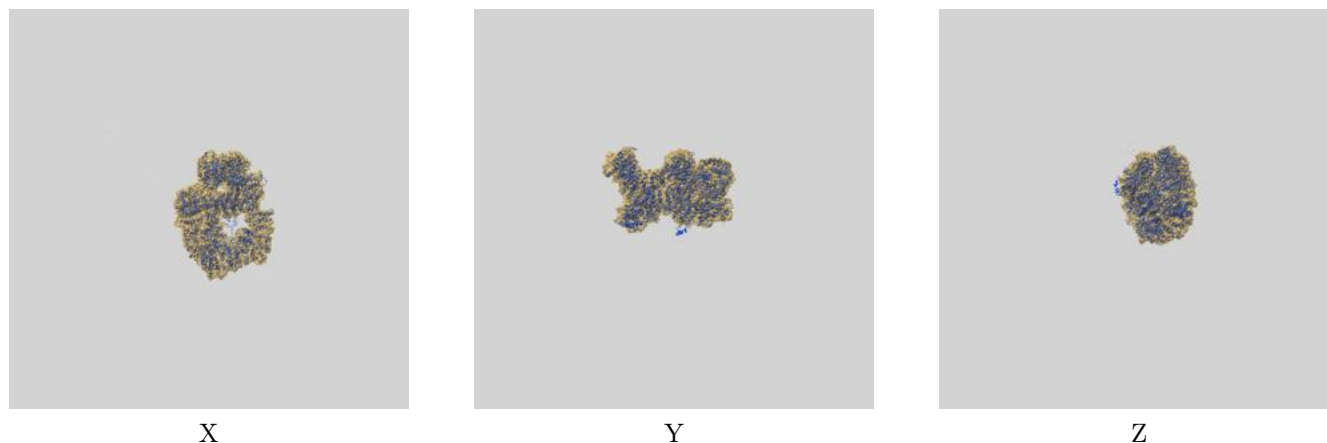
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.33	-	-
Author-provided FSC curve	3.33	3.69	3.36
Unmasked-calculated*	6.93	9.00	7.32

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.93 differs from the reported value 3.33 by more than 10 %

9 Map-model fit [i](#)

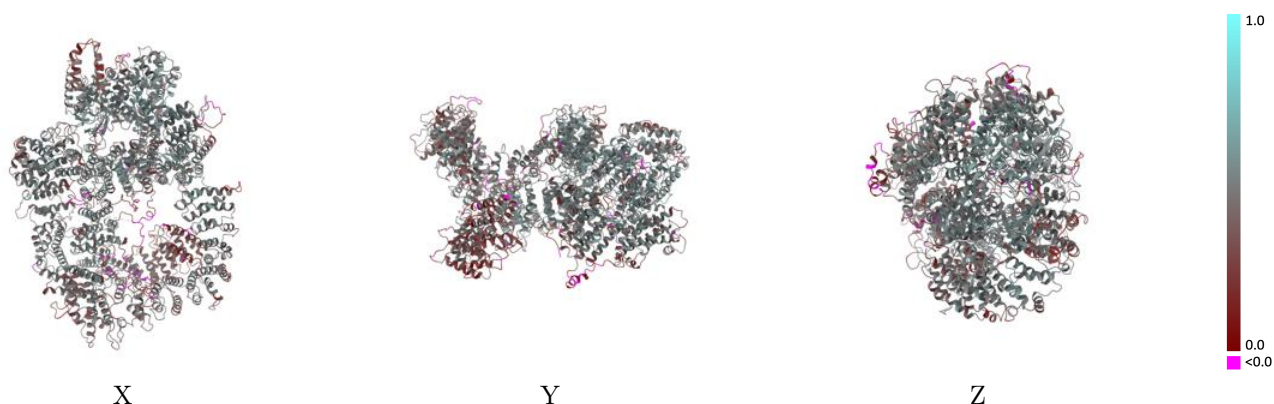
This section contains information regarding the fit between EMDB map EMD-26192 and PDB model 7TYR. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



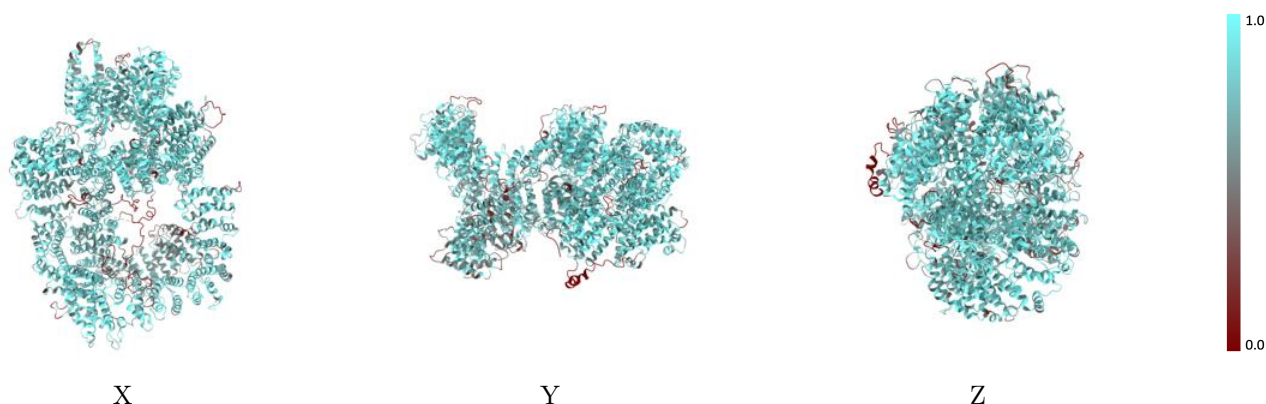
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



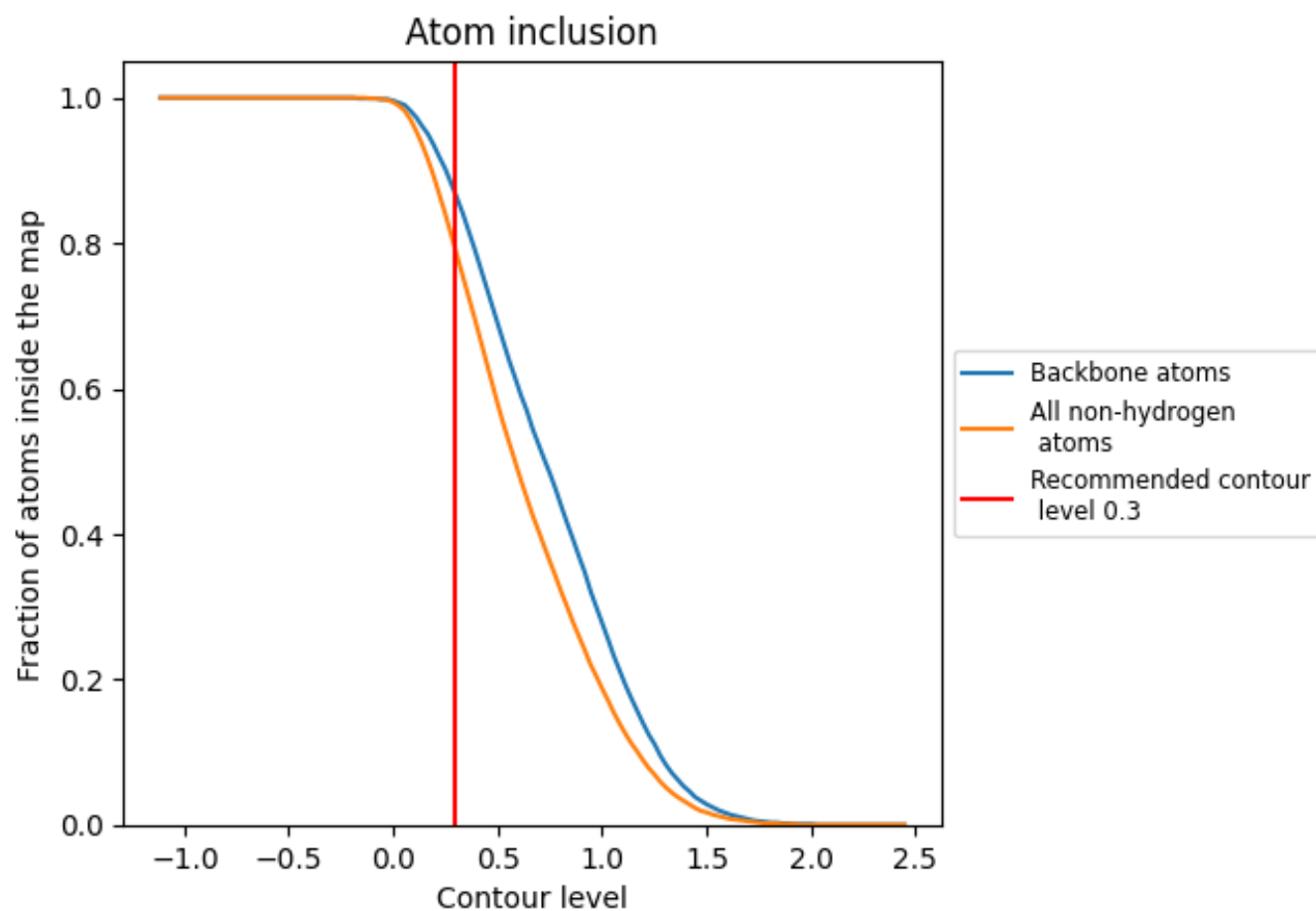
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 79% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7890	0.4330
A	0.7960	0.4360
C	0.3220	0.2170

