



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:18 PM UTC

PDB ID : 5OJS / pdb_00005ojs
EMDB ID : EMD-3824
Title : Cryo-EM structure of the SAGA and NuA4 coactivator subunit Tra1
Authors : Diaz-Santin, L.M.; Lukyanova, N.; Aciyan, E.; Cheung, A.C.M.
Deposited on : 2017-07-24
Resolution : 3.70 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

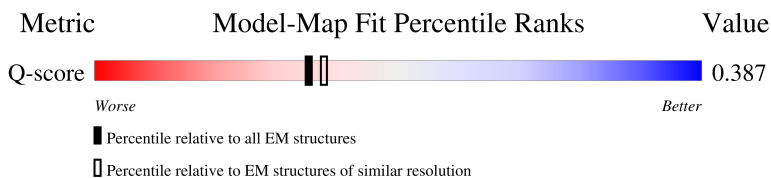
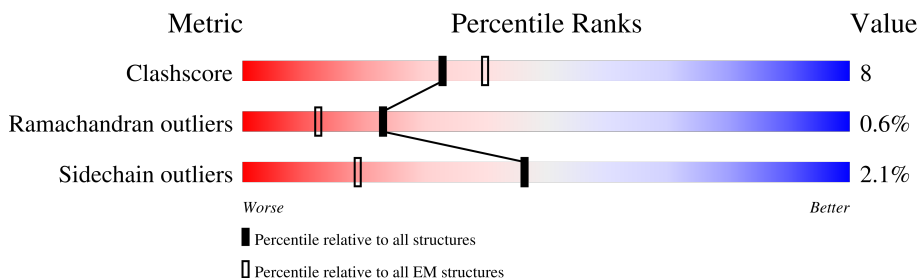
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	T	3767	16% 69% 22% 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 28407 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.

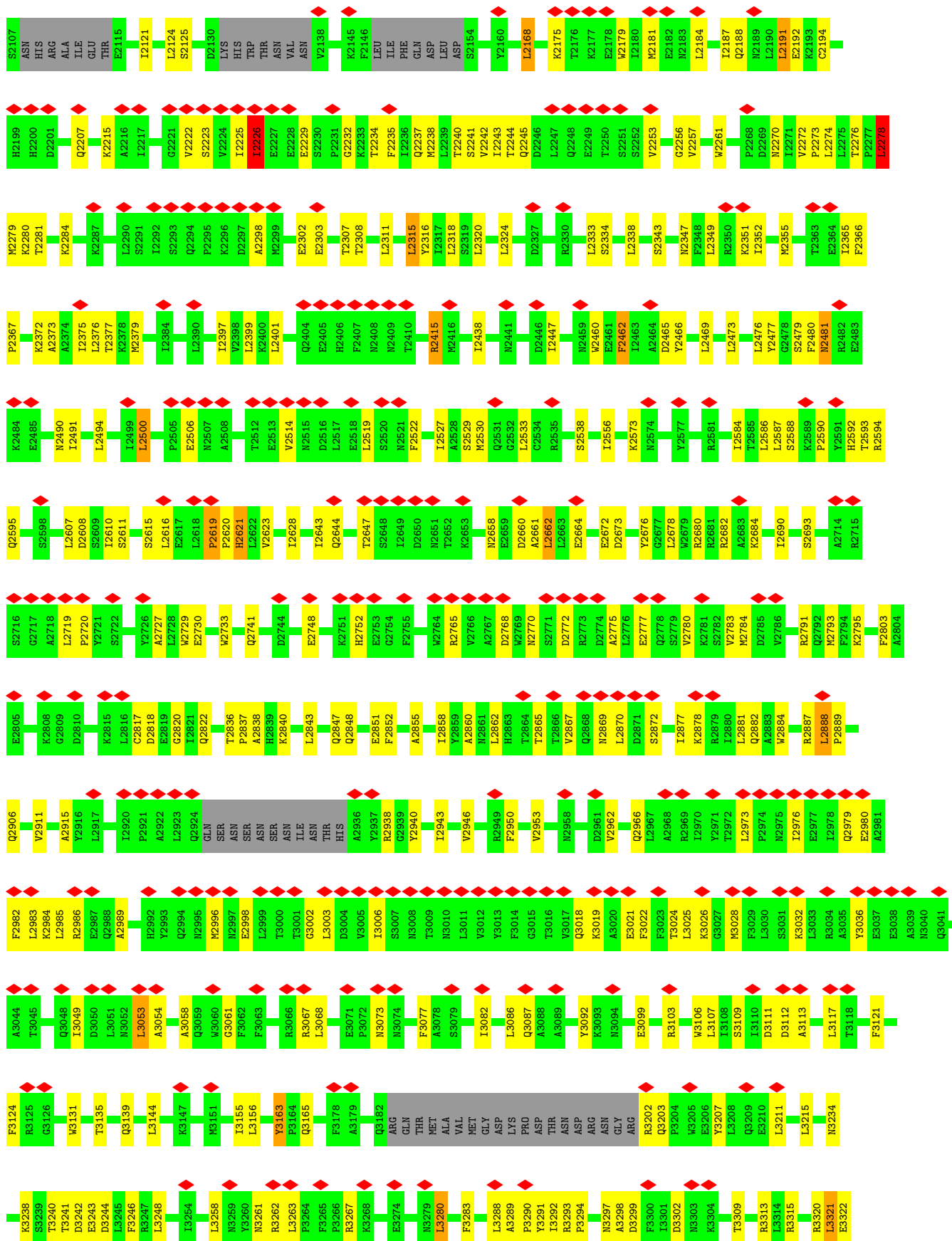
- Molecule 1 is a protein called Transcription-associated protein 1.

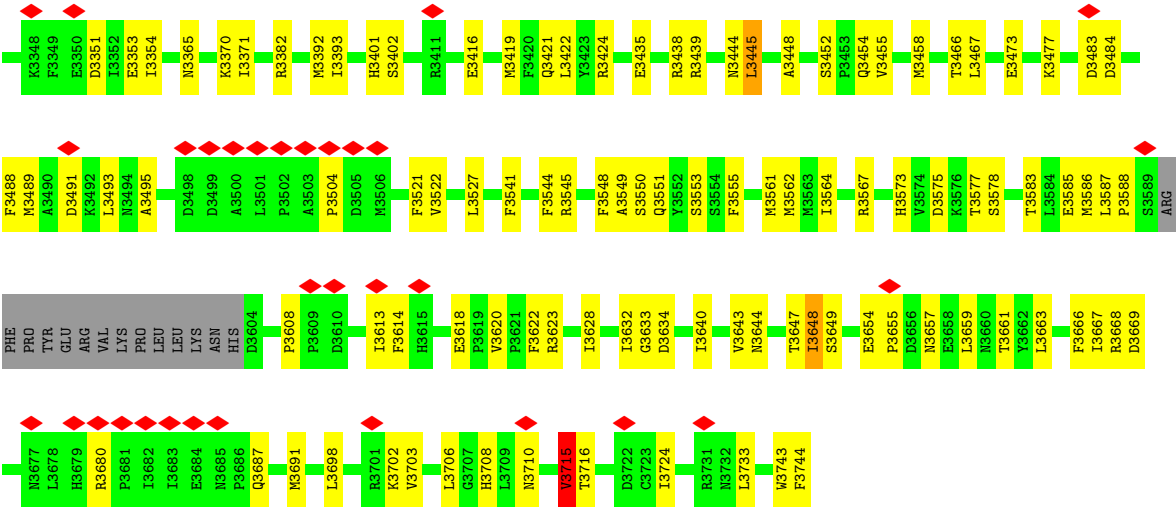
Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	3473	Total	C	N	O	S	0	0
			28407	18391	4718	5178	120		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	-22	MET	-	initiating methionine	UNP P38811
T	-21	ASP	-	expression tag	UNP P38811
T	-20	TYR	-	expression tag	UNP P38811
T	-19	LYS	-	expression tag	UNP P38811
T	-18	ASP	-	expression tag	UNP P38811
T	-17	HIS	-	expression tag	UNP P38811
T	-16	ASP	-	expression tag	UNP P38811
T	-15	GLY	-	expression tag	UNP P38811
T	-14	ASP	-	expression tag	UNP P38811
T	-13	TYR	-	expression tag	UNP P38811
T	-12	LYS	-	expression tag	UNP P38811
T	-11	ASP	-	expression tag	UNP P38811
T	-10	HIS	-	expression tag	UNP P38811
T	-9	ASP	-	expression tag	UNP P38811
T	-8	ILE	-	expression tag	UNP P38811
T	-7	ASP	-	expression tag	UNP P38811
T	-6	TYR	-	expression tag	UNP P38811
T	-5	LYS	-	expression tag	UNP P38811
T	-4	ASP	-	expression tag	UNP P38811
T	-3	ASP	-	expression tag	UNP P38811
T	-2	ASP	-	expression tag	UNP P38811
T	-1	ASP	-	expression tag	UNP P38811
T	0	LYS	-	expression tag	UNP P38811







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	182285	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 ($e^-/\text{\AA}^2$)	1.4	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.208	Depositor
Minimum map value	-0.123	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	307.4, 307.4, 307.4	wwPDB
Map dimensions	290, 290, 290	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	T	0.32	0/29026	0.78	29/39323 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	T	0	50

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	1157	ILE	CA-C-N	15.47	139.17	119.84
1	T	1157	ILE	C-N-CA	15.47	139.17	119.84
1	T	2888	LEU	CA-C-N	9.59	131.82	119.84
1	T	2888	LEU	C-N-CA	9.59	131.82	119.84
1	T	3053	LEU	CA-CB-CG	7.23	141.60	116.30
1	T	3715	VAL	CA-C-N	7.08	135.07	121.54
1	T	3715	VAL	C-N-CA	7.08	135.07	121.54
1	T	1825	LEU	CA-CB-CG	7.03	140.90	116.30
1	T	3163	TYR	CA-C-N	5.77	127.05	119.84
1	T	3163	TYR	C-N-CA	5.77	127.05	119.84
1	T	970	THR	CA-C-N	5.74	132.50	121.54
1	T	970	THR	C-N-CA	5.74	132.50	121.54
1	T	2278	LEU	CA-CB-CG	5.72	136.32	116.30
1	T	3163	TYR	N-CA-C	5.52	122.00	109.81
1	T	38	LEU	CA-CB-CG	5.38	135.14	116.30
1	T	3716	THR	N-CA-C	-5.30	99.51	110.80
1	T	3716	THR	N-CA-CB	5.26	119.37	110.49
1	T	848	THR	CA-C-N	5.22	131.51	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	848	THR	C-N-CA	5.22	131.51	121.54
1	T	3302	ASP	CA-C-N	5.14	131.35	121.54
1	T	3302	ASP	C-N-CA	5.14	131.35	121.54
1	T	1958	ASN	CA-C-N	5.12	131.31	121.54
1	T	1958	ASN	C-N-CA	5.12	131.31	121.54
1	T	776	PHE	N-CA-C	5.11	121.11	109.81
1	T	3444	ASN	CA-C-N	5.08	139.56	121.59
1	T	3444	ASN	C-N-CA	5.08	139.56	121.59
1	T	2573	LYS	CA-C-N	5.07	131.22	121.54
1	T	2573	LYS	C-N-CA	5.07	131.22	121.54
1	T	2415	ARG	CA-CB-CG	-5.01	104.08	114.10

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	T	1070	ARG	Peptide
1	T	1136	PRO	Peptide
1	T	1157	ILE	Peptide
1	T	1227	SER	Peptide
1	T	1297	SER	Peptide
1	T	1346	PRO	Peptide
1	T	1357	ILE	Peptide
1	T	1473	LEU	Peptide
1	T	1543	LEU	Peptide
1	T	1635	GLU	Peptide
1	T	1660	VAL	Peptide
1	T	1710	SER	Peptide
1	T	1770	ILE	Peptide
1	T	1773	SER	Peptide
1	T	1795	CYS	Peptide
1	T	1850	ALA	Peptide
1	T	1900	LEU	Peptide
1	T	2225	ILE	Peptide
1	T	2226	ILE	Peptide
1	T	227	CYS	Peptide
1	T	2315	LEU	Peptide
1	T	2343	SER	Peptide
1	T	2366	PHE	Peptide
1	T	246	LEU	Peptide
1	T	2462	PHE	Peptide
1	T	2615	SER	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	T	2619	PRO	Peptide
1	T	2888	LEU	Peptide
1	T	2973	LEU	Peptide
1	T	2976	ILE	Peptide
1	T	3163	TYR	Peptide
1	T	3238	LYS	Peptide
1	T	3290	PRO	Peptide
1	T	346	GLU	Peptide
1	T	3504	PRO	Peptide
1	T	3608	PRO	Peptide
1	T	3618	GLU	Peptide
1	T	3633	GLY	Peptide
1	T	3654	GLU	Peptide
1	T	3680	ARG	Peptide
1	T	3715	VAL	Peptide
1	T	380	GLY	Peptide
1	T	693	MET	Peptide
1	T	694	ASP	Peptide
1	T	72	GLU	Peptide
1	T	750	ASP	Peptide
1	T	776	PHE	Peptide
1	T	847	LEU	Peptide
1	T	851	LEU	Peptide
1	T	935	GLN	Peptide

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	T	28407	0	28803	482	0
All	All	28407	0	28803	482	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 (482) 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:T:118:CYS:O	1:T:122:LEU:HB2	1.70	0.91
1:T:2188:GLN:O	1:T:2192:GLU:HB3	1.71	0.89
1:T:3293:ARG:O	1:T:3297:ASN:HB2	1.73	0.89
1:T:3258:LEU:O	1:T:3262:ARG:HB2	1.72	0.89
1:T:1902:LYS:O	1:T:1906:TYR:HB2	1.74	0.87
1:T:1404:THR:O	1:T:1408:LEU:HB2	1.73	0.87
1:T:3541:PHE:O	1:T:3544:PHE:HB3	1.80	0.82
1:T:1173:GLU:O	1:T:1177:LEU:HB2	1.82	0.80
1:T:702:ILE:O	1:T:706:LEU:HB2	1.81	0.80
1:T:2473:LEU:O	1:T:2477:TYR:HB2	1.82	0.78
1:T:3473:GLU:O	1:T:3477:LYS:HB2	1.84	0.78
1:T:2372:LYS:O	1:T:2376:LEU:HB2	1.84	0.77
1:T:1838:HIS:O	1:T:1842:TRP:HB2	1.85	0.77
1:T:2590:PRO:HG2	1:T:2592:HIS:HB3	1.70	0.73
1:T:1335:SER:O	1:T:1339:ALA:HB2	1.89	0.73
1:T:2238:MET:O	1:T:2241:SER:HB2	1.90	0.72
1:T:1114:GLN:HG3	1:T:1189:PHE:HD1	1.56	0.71
1:T:397:ASP:O	1:T:401:ASN:HB2	1.92	0.70
1:T:246:LEU:HD12	1:T:247:PRO:HD2	1.75	0.69
1:T:685:TYR:O	1:T:689:MET:HB2	1.93	0.68
1:T:1099:ALA:O	1:T:1103:LEU:HB2	1.94	0.68
1:T:1726:GLN:HE21	1:T:1762:LEU:HB2	1.59	0.68
1:T:1988:PHE:HA	1:T:1991:SER:HB3	1.75	0.68
1:T:695:ASN:HD21	1:T:1540:GLY:HA2	1.59	0.67
1:T:10:PHE:HB2	1:T:13:ARG:HE	1.60	0.67
1:T:2168:LEU:O	1:T:2215:LYS:NZ	2.27	0.67
1:T:3211:LEU:O	1:T:3215:LEU:HB2	1.94	0.67
1:T:447:LEU:O	1:T:451:LYS:HB2	1.95	0.67
1:T:2397:ILE:O	1:T:2401:LEU:HB2	1.94	0.66
1:T:3024:THR:O	1:T:3028:MET:N	2.29	0.66
1:T:476:LYS:HG3	1:T:640:GLU:HG2	1.78	0.65
1:T:1939:ARG:HE	1:T:1985:LEU:HD13	1.59	0.65
1:T:1750:PHE:O	1:T:1799:ARG:NH2	2.30	0.65
1:T:1730:LEU:HD11	1:T:1765:PHE:HB2	1.78	0.64
1:T:3491:ASP:O	1:T:3495:ALA:HB2	1.98	0.64
1:T:2094:GLU:O	1:T:2098:ALA:HB3	1.97	0.64
1:T:3687:GLN:O	1:T:3691:MET:HB2	1.98	0.64
1:T:1293:VAL:HG21	1:T:1326:MET:HG2	1.79	0.64
1:T:730:GLU:HB3	1:T:732:THR:H	1.63	0.64
1:T:1805:ASN:O	1:T:1809:SER:HB2	1.98	0.63
1:T:2980:GLU:O	1:T:2984:LYS:HB2	1.97	0.63
1:T:3315:ARG:NH1	1:T:3483:ASP:OD1	2.32	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:76:ARG:HD3	1:T:117:LEU:HD21	1.80	0.62
1:T:3309:THR:O	1:T:3313:ARG:HB2	1.99	0.62
1:T:2316:TYR:O	1:T:2320:LEU:HB2	2.00	0.62
1:T:3036:TYR:O	1:T:3067:ARG:NH2	2.34	0.61
1:T:1805:ASN:O	1:T:1809:SER:CB	2.48	0.61
1:T:2469:LEU:HB2	1:T:2556:ILE:HD11	1.82	0.61
1:T:790:ASP:O	1:T:794:ASN:HB2	2.01	0.61
1:T:2257:VAL:O	1:T:2261:TRP:HB2	2.00	0.60
1:T:719:LEU:O	1:T:722:VAL:HB	2.00	0.60
1:T:3550:SER:O	1:T:3553:SER:HB2	2.01	0.60
1:T:3698:LEU:O	1:T:3702:LYS:HB2	2.01	0.60
1:T:2690:ILE:HG13	1:T:3715:VAL:HA	1.82	0.60
1:T:1841:ILE:HG21	1:T:1885:ASP:HB3	1.83	0.60
1:T:2660:ASP:HB3	1:T:2682:ARG:HH22	1.66	0.60
1:T:3109:SER:OG	1:T:3668:ARG:NH1	2.35	0.60
1:T:1913:ILE:O	1:T:1956:ARG:NH1	2.35	0.59
1:T:3068:LEU:O	1:T:3073:ASN:ND2	2.35	0.59
1:T:2983:LEU:HA	1:T:2986:ARG:HB3	1.85	0.59
1:T:1217:LYS:HB3	1:T:1263:LEU:HD11	1.84	0.59
1:T:1006:SER:O	1:T:1014:ARG:NH2	2.36	0.59
1:T:1033:ALA:HB1	1:T:2530:MET:HB3	1.84	0.59
1:T:1740:GLN:HE22	1:T:1781:ASN:HB2	1.68	0.59
1:T:1936:VAL:HG22	1:T:1939:ARG:HD2	1.85	0.59
1:T:1945:SER:O	1:T:1949:LEU:HB2	2.03	0.59
1:T:1750:PHE:HZ	1:T:1802:VAL:HG21	1.68	0.58
1:T:2270:ASN:HB3	1:T:2272:VAL:HG23	1.84	0.58
1:T:1801:PHE:HA	1:T:1804:LYS:HG3	1.85	0.58
1:T:3452:SER:HB2	1:T:3455:VAL:H	1.69	0.58
1:T:2729:TRP:O	1:T:2733:TRP:HB2	2.02	0.58
1:T:953:GLY:O	1:T:957:ARG:NH1	2.37	0.58
1:T:2836:THR:HG22	1:T:2838:ALA:H	1.68	0.58
1:T:117:LEU:O	1:T:121:VAL:HB	2.04	0.58
1:T:3622:PHE:HZ	1:T:3724:ILE:HG22	1.68	0.58
1:T:1648:TYR:O	1:T:1652:ILE:HB	2.03	0.57
1:T:2768:ASP:OD1	1:T:2770:ASN:ND2	2.37	0.57
1:T:1966:TRP:HA	1:T:1969:TRP:HD1	1.70	0.57
1:T:2852:PHE:O	1:T:2855:ALA:HB3	2.05	0.57
1:T:2817:CYS:SG	1:T:2818:ASP:N	2.78	0.56
1:T:153:ASN:OD1	1:T:157:GLN:NE2	2.37	0.56
1:T:3424:ARG:NH1	1:T:3445:LEU:O	2.37	0.56
1:T:2465:ASP:N	1:T:2465:ASP:OD1	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:1952:VAL:HA	1:T:1955:GLU:HG2	1.87	0.56
1:T:3567:ARG:NH1	1:T:3585:GLU:OE1	2.38	0.56
1:T:3561:MET:HG2	1:T:3562:MET:HG3	1.87	0.56
1:T:956:ASN:HD21	1:T:2843:LEU:HD12	1.70	0.56
1:T:3628:ILE:O	1:T:3632:ILE:HB	2.06	0.56
1:T:2783:VAL:O	1:T:2791:ARG:NH2	2.36	0.56
1:T:1971:LYS:HD3	1:T:2002:LEU:HD23	1.88	0.56
1:T:49:GLN:NE2	1:T:91:THR:OG1	2.39	0.56
1:T:3299:ASP:HB3	1:T:3313:ARG:HD2	1.87	0.56
1:T:1380:GLU:HA	1:T:1383:VAL:HG12	1.88	0.55
1:T:1054:ARG:NH1	1:T:2506:GLU:OE2	2.39	0.55
1:T:1790:VAL:HG23	1:T:1800:ILE:HG23	1.88	0.55
1:T:3435:GLU:O	1:T:3439:ARG:NH1	2.39	0.55
1:T:2741:GLN:OE1	1:T:2765:ARG:NH2	2.39	0.55
1:T:3156:LEU:HD13	1:T:3211:LEU:HD11	1.89	0.55
1:T:355:LEU:HD21	1:T:364:LEU:HD13	1.89	0.55
1:T:445:ARG:O	1:T:449:LEU:HB2	2.06	0.55
1:T:1203:ASP:OD2	1:T:1208:ASN:ND2	2.40	0.55
1:T:1655:ILE:HD11	1:T:1698:MET:HE1	1.89	0.55
1:T:910:ALA:O	1:T:955:ARG:NH2	2.40	0.55
1:T:1337:ILE:HG21	1:T:1357:ILE:HD11	1.87	0.55
1:T:1477:LEU:O	1:T:1481:GLY:N	2.38	0.55
1:T:1015:LYS:NZ	1:T:1094:GLU:O	2.39	0.55
1:T:1416:ILE:HG23	1:T:1444:PHE:HE1	1.71	0.55
1:T:3351:ASP:HB3	1:T:3370:LYS:HG2	1.89	0.55
1:T:222:LYS:NZ	1:T:237:SER:OG	2.40	0.54
1:T:122:LEU:O	1:T:126:PHE:HB2	2.07	0.54
1:T:3058:ALA:O	1:T:3061:GLY:N	2.41	0.54
1:T:3640:ILE:O	1:T:3644:ASN:ND2	2.40	0.54
1:T:1664:SER:O	1:T:1668:ASN:ND2	2.41	0.54
1:T:1391:SER:OG	1:T:1397:GLN:NE2	2.41	0.54
1:T:2593:THR:OG1	1:T:2595:GLN:NE2	2.40	0.54
1:T:1517:GLU:HA	1:T:1520:ARG:HD3	1.89	0.54
1:T:1991:SER:HB2	1:T:2034:LEU:HD11	1.90	0.54
1:T:3521:PHE:HB3	1:T:3522:VAL:HG23	1.89	0.54
1:T:2587:LEU:O	1:T:2594:ARG:NH2	2.41	0.54
1:T:3454:GLN:HG3	1:T:3455:VAL:HG23	1.90	0.54
1:T:1625:CYS:SG	1:T:1675:THR:OG1	2.60	0.54
1:T:2473:LEU:HD23	1:T:2476:LEU:HD11	1.90	0.54
1:T:3135:THR:O	1:T:3421:GLN:NE2	2.40	0.54
1:T:2102:ARG:O	1:T:2106:ALA:HB2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:3139:GLN:NE2	1:T:3669:ASP:OD2	2.40	0.54
1:T:934:PRO:HB3	1:T:2822:GLN:HE21	1.74	0.53
1:T:1099:ALA:O	1:T:1103:LEU:CB	2.55	0.53
1:T:3422:LEU:HD11	1:T:3666:PHE:HB3	1.90	0.53
1:T:106:VAL:HG21	1:T:117:LEU:HB2	1.89	0.53
1:T:3545:ARG:HA	1:T:3548:PHE:HB3	1.90	0.53
1:T:1519:GLY:O	1:T:1523:LEU:CB	2.55	0.53
1:T:1580:LEU:HD22	1:T:1592:PHE:HZ	1.73	0.53
1:T:1757:LYS:HE3	1:T:1802:VAL:HG13	1.90	0.53
1:T:1925:GLN:HA	1:T:1928:VAL:HB	1.88	0.53
1:T:474:ARG:O	1:T:474:ARG:NH2	2.40	0.53
1:T:1122:LYS:HE3	1:T:1123:ARG:HH12	1.74	0.53
1:T:1683:GLU:HG3	1:T:1685:LEU:H	1.74	0.53
1:T:1734:GLU:HB3	1:T:1765:PHE:HE1	1.73	0.53
1:T:510:ASN:ND2	1:T:2207:GLN:OE1	2.42	0.53
1:T:1957:MET:HG3	1:T:1961:GLY:HA3	1.90	0.53
1:T:2784:MET:HG3	1:T:2795:LYS:HD3	1.91	0.53
1:T:2529:SER:O	1:T:2533:LEU:N	2.41	0.53
1:T:1593:ARG:O	1:T:1597:ALA:N	2.40	0.53
1:T:3564:ILE:HA	1:T:3588:PRO:HA	1.90	0.53
1:T:468:ILE:HA	1:T:471:TYR:HD2	1.74	0.52
1:T:1216:ILE:HD11	1:T:1241:LEU:HD21	1.91	0.52
1:T:608:PRO:O	1:T:612:THR:N	2.41	0.52
1:T:2349:LEU:HA	1:T:2352:ILE:HG12	1.91	0.52
1:T:3392:MET:HA	1:T:3402:SER:HA	1.90	0.52
1:T:2584:ILE:HG23	1:T:2623:VAL:HG21	1.90	0.52
1:T:1837:LEU:HG	1:T:1840:LYS:HE3	1.92	0.52
1:T:2865:THR:HA	1:T:2867:VAL:HG23	1.91	0.52
1:T:2878:LYS:O	1:T:2882:GLN:HB2	2.10	0.52
1:T:3019:LYS:O	1:T:3022:PHE:HB2	2.09	0.52
1:T:3246:PHE:HB2	1:T:3321:LEU:HD12	1.91	0.52
1:T:619:TRP:CD1	1:T:623:SER:HG	2.28	0.52
1:T:2817:CYS:O	1:T:2820:GLY:N	2.42	0.52
1:T:1:MET:O	1:T:6:GLN:NE2	2.39	0.52
1:T:118:CYS:O	1:T:122:LEU:CB	2.51	0.52
1:T:1520:ARG:HD2	1:T:1569:PHE:HZ	1.75	0.52
1:T:1635:GLU:HA	1:T:1638:GLU:HG2	1.92	0.52
1:T:1726:GLN:HE22	1:T:1758:ALA:HB3	1.75	0.52
1:T:2588:SER:HB2	1:T:2623:VAL:HG13	1.92	0.52
1:T:1044:LYS:NZ	1:T:2514:VAL:O	2.40	0.52
1:T:1116:ASN:O	1:T:1120:LEU:CB	2.58	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:3371:ILE:HG22	1:T:3393:ILE:HG21	1.91	0.52
1:T:3614:PHE:HE2	1:T:3667:ILE:HG23	1.75	0.52
1:T:2090:LEU:HD23	1:T:2093:ARG:HH11	1.75	0.51
1:T:1641:GLU:OE2	1:T:1680:ASN:ND2	2.43	0.51
1:T:1879:ILE:HD12	1:T:1882:ILE:HG13	1.92	0.51
1:T:1995:LEU:O	1:T:2041:LYS:NZ	2.43	0.51
1:T:2280:LYS:O	1:T:2284:LYS:N	2.42	0.51
1:T:3473:GLU:O	1:T:3477:LYS:CB	2.57	0.51
1:T:3261:ASN:OD1	1:T:3267:ARG:NH1	2.43	0.51
1:T:3211:LEU:O	1:T:3215:LEU:CB	2.57	0.51
1:T:2996:MET:HG2	1:T:3032:LYS:HE3	1.91	0.51
1:T:611:TYR:OH	1:T:1585:ARG:NH2	2.36	0.51
1:T:920:VAL:HG12	1:T:923:ASP:HB2	1.93	0.51
1:T:2181:MET:HE2	1:T:2226:ILE:HD11	1.93	0.51
1:T:2094:GLU:O	1:T:2098:ALA:CB	2.58	0.51
1:T:3309:THR:O	1:T:3313:ARG:CB	2.59	0.51
1:T:1437:ARG:HA	1:T:1440:ILE:HG12	1.93	0.51
1:T:695:ASN:HA	1:T:698:PHE:HB3	1.92	0.50
1:T:848:THR:OG1	1:T:849:ALA:N	2.37	0.50
1:T:3659:LEU:O	1:T:3663:LEU:HB2	2.11	0.50
1:T:1203:ASP:O	1:T:1209:LYS:NZ	2.42	0.50
1:T:3067:ARG:HH11	1:T:3077:PHE:HZ	1.59	0.50
1:T:1423:LEU:HD12	1:T:1440:ILE:HD11	1.93	0.50
1:T:1757:LYS:HZ2	1:T:1805:ASN:HB3	1.76	0.50
1:T:2240:THR:HG22	1:T:2256:GLY:HA2	1.94	0.50
1:T:793:LEU:HB3	1:T:831:ILE:HD11	1.94	0.50
1:T:2232:GLY:O	1:T:2235:PHE:HB3	2.11	0.50
1:T:1473:LEU:HD21	1:T:1477:LEU:HB3	1.94	0.50
1:T:2837:PRO:O	1:T:2840:LYS:HB3	2.12	0.50
1:T:4:THR:HG22	1:T:7:ILE:HD12	1.94	0.50
1:T:1804:LYS:HE2	1:T:1863:GLU:HB2	1.94	0.50
1:T:2022:SER:OG	1:T:2023:ASP:N	2.44	0.50
1:T:3643:VAL:O	1:T:3647:THR:OG1	2.24	0.49
1:T:1649:ASP:O	1:T:1653:SER:CB	2.60	0.49
1:T:2373:ALA:HA	1:T:2415:ARG:HH21	1.77	0.49
1:T:3289:ALA:HA	1:T:3293:ARG:HH21	1.77	0.49
1:T:1036:PRO:HG2	1:T:1039:TYR:HB2	1.94	0.49
1:T:2376:LEU:HD12	1:T:2379:MET:HG3	1.95	0.49
1:T:24:ARG:HA	1:T:28:LEU:HD23	1.93	0.49
1:T:152:PRO:HA	1:T:155:ILE:HG12	1.94	0.49
1:T:232:VAL:O	1:T:236:SER:OG	2.29	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:1340:LYS:NZ	1:T:1344:ALA:O	2.45	0.49
1:T:1932:ARG:HE	1:T:1933:SER:H	1.59	0.49
1:T:602:LYS:HB3	1:T:624:ARG:HH21	1.77	0.49
1:T:3620:VAL:HG11	1:T:3733:LEU:HD23	1.95	0.49
1:T:776:PHE:O	1:T:778:ASN:N	2.43	0.49
1:T:1237:LEU:HD13	1:T:1267:LEU:HD11	1.95	0.49
1:T:1861:ARG:HH12	1:T:1896:LEU:HG	1.78	0.49
1:T:13:ARG:HH22	1:T:30:GLU:HA	1.78	0.49
1:T:2877:ILE:O	1:T:2881:LEU:HB3	2.12	0.49
1:T:1286:GLU:OE2	1:T:1328:HIS:NE2	2.46	0.49
1:T:485:ILE:HG23	1:T:579:PRO:HB2	1.94	0.48
1:T:944:ASN:OD1	1:T:947:ARG:NH2	2.42	0.48
1:T:407:GLN:N	1:T:410:GLU:OE2	2.45	0.48
1:T:2244:THR:HA	1:T:2253:VAL:HG23	1.94	0.48
1:T:3082:ILE:O	1:T:3086:LEU:HB2	2.13	0.48
1:T:983:ASN:ND2	1:T:2480:PHE:O	2.45	0.48
1:T:1914:SER:HA	1:T:1952:VAL:HG21	1.95	0.48
1:T:2303:GLU:O	1:T:2307:THR:OG1	2.21	0.48
1:T:732:THR:HB	1:T:735:ASN:HD22	1.79	0.48
1:T:952:LEU:HB2	1:T:955:ARG:HB2	1.95	0.48
1:T:1062:ASP:O	1:T:3320:ARG:NH1	2.46	0.48
1:T:2240:THR:HA	1:T:2243:ILE:HG22	1.94	0.48
1:T:3234:ASN:OD1	1:T:3452:SER:OG	2.30	0.48
1:T:1702:THR:HA	1:T:1705:THR:HG22	1.96	0.48
1:T:1767:PHE:HA	1:T:1770:ILE:HD12	1.94	0.48
1:T:2862:LEU:HD13	1:T:2865:THR:HB	1.96	0.48
1:T:13:ARG:HH12	1:T:30:GLU:HB2	1.77	0.48
1:T:2347:ASN:O	1:T:2351:LYS:NZ	2.47	0.48
1:T:2608:ASP:O	1:T:2611:SER:OG	2.30	0.48
1:T:1779:GLN:HA	1:T:1782:PHE:HD2	1.79	0.48
1:T:1128:THR:HG21	1:T:3291:TYR:HB2	1.95	0.48
1:T:1246:LYS:HA	1:T:1303:VAL:HG21	1.96	0.48
1:T:1796:LEU:HB3	1:T:1799:ARG:HB2	1.96	0.48
1:T:2175:LYS:HG2	1:T:2179:TRP:HB3	1.96	0.48
1:T:1519:GLY:O	1:T:1523:LEU:HB2	2.14	0.48
1:T:1670:VAL:O	1:T:1674:ASN:HB2	2.14	0.48
1:T:770:PHE:HE1	1:T:784:LEU:HD21	1.77	0.48
1:T:2184:LEU:HA	1:T:2187:ILE:HG22	1.95	0.48
1:T:486:MET:HB2	1:T:486:MET:HE2	1.81	0.47
1:T:1837:LEU:HD21	1:T:1886:ILE:HD11	1.95	0.47
1:T:2273:PRO:HB2	1:T:2274:LEU:HD12	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:3491:ASP:O	1:T:3495:ALA:CB	2.62	0.47
1:T:1482:LEU:HB2	1:T:1486:LEU:HD13	1.96	0.47
1:T:2621:HIS:CE1	1:T:2661:ALA:HB3	2.49	0.47
1:T:3131:TRP:CD1	1:T:3365:ASN:HD22	2.32	0.47
1:T:1116:ASN:O	1:T:1120:LEU:HB3	2.14	0.47
1:T:776:PHE:HB3	1:T:779:ILE:HG12	1.96	0.47
1:T:1056:GLY:N	1:T:2506:GLU:OE1	2.47	0.47
1:T:1120:LEU:HD22	1:T:2500:LEU:HD11	1.97	0.47
1:T:2877:ILE:O	1:T:2881:LEU:CB	2.62	0.47
1:T:327:ASP:O	1:T:331:ARG:CB	2.63	0.47
1:T:1649:ASP:O	1:T:1653:SER:HB3	2.14	0.47
1:T:2998:GLU:O	1:T:3002:GLY:N	2.48	0.47
1:T:132:ILE:HD13	1:T:134:GLN:HG2	1.96	0.47
1:T:2276:THR:O	1:T:2279:MET:HB3	2.14	0.47
1:T:2962:VAL:O	1:T:2966:GLN:N	2.47	0.47
1:T:345:LYS:HG2	1:T:387:LEU:HD11	1.96	0.47
1:T:740:LEU:HD12	1:T:769:SER:HB3	1.96	0.47
1:T:3003:LEU:HD12	1:T:3026:LYS:HB2	1.97	0.47
1:T:1355:ASP:HA	1:T:1358:THR:HG23	1.97	0.47
1:T:110:GLU:HG2	1:T:154:LEU:HD21	1.96	0.47
1:T:2950:PHE:HA	1:T:2953:VAL:HG12	1.96	0.47
1:T:2980:GLU:O	1:T:2984:LYS:CB	2.63	0.47
1:T:3587:LEU:HA	1:T:3588:PRO:HD3	1.75	0.47
1:T:3623:ARG:NH2	1:T:3744:PHE:O	2.47	0.47
1:T:48:LEU:HA	1:T:51:VAL:HG22	1.97	0.46
1:T:1079:PHE:HD2	1:T:1144:LEU:HD11	1.80	0.46
1:T:3241:THR:HB	1:T:3288:LEU:HD22	1.97	0.46
1:T:1535:LEU:HA	1:T:1538:LEU:HD23	1.96	0.46
1:T:1884:LYS:HA	1:T:1887:ILE:HD12	1.98	0.46
1:T:2481:ASN:O	1:T:2538:SER:OG	2.32	0.46
1:T:24:ARG:NH2	1:T:69:HIS:O	2.36	0.46
1:T:742:ARG:HH21	1:T:1545:GLU:H	1.61	0.46
1:T:1342:LEU:HB3	1:T:1377:LEU:HD12	1.96	0.46
1:T:1535:LEU:HD12	1:T:1584:LEU:HD21	1.97	0.46
1:T:1805:ASN:O	1:T:1809:SER:OG	2.28	0.46
1:T:790:ASP:O	1:T:794:ASN:CB	2.64	0.46
1:T:2851:GLU:OE1	1:T:2884:TRP:NE1	2.49	0.46
1:T:1519:GLY:O	1:T:1523:LEU:HB3	2.16	0.46
1:T:1902:LYS:O	1:T:1906:TYR:CB	2.55	0.46
1:T:2676:TYR:HB3	1:T:2680:ARG:HH21	1.81	0.46
1:T:2979:GLN:HG3	1:T:2982:PHE:HD2	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:3106:TRP:HE3	1:T:3107:LEU:HD22	1.80	0.46
1:T:791:LEU:O	1:T:795:SER:CB	2.64	0.45
1:T:122:LEU:O	1:T:126:PHE:CB	2.64	0.45
1:T:232:VAL:O	1:T:236:SER:CB	2.64	0.45
1:T:2373:ALA:O	1:T:2415:ARG:NH2	2.48	0.45
1:T:3354:ILE:HD13	1:T:3401:HIS:CE1	2.51	0.45
1:T:628:TYR:CG	1:T:1622:LEU:HD21	2.51	0.45
1:T:685:TYR:O	1:T:689:MET:CB	2.62	0.45
1:T:1789:PHE:O	1:T:1792:SER:OG	2.34	0.45
1:T:1941:LEU:HD13	1:T:1944:GLN:HE21	1.81	0.45
1:T:588:ARG:O	1:T:592:SER:HB2	2.17	0.45
1:T:2989:ALA:HB2	1:T:3006:ILE:HG21	1.99	0.45
1:T:709:VAL:HG12	1:T:713:MET:HE3	1.98	0.45
1:T:1667:THR:HG21	1:T:1717:GLN:HB2	1.99	0.45
1:T:1787:THR:HG21	1:T:1833:TRP:HB2	1.99	0.45
1:T:2399:LEU:HD12	1:T:2438:ILE:HD11	1.98	0.45
1:T:3288:LEU:HD11	1:T:3292:ILE:HG12	1.99	0.45
1:T:3467:LEU:HD22	1:T:3527:LEU:HD11	1.99	0.45
1:T:2377:THR:HG23	1:T:2415:ARG:HH22	1.82	0.45
1:T:3054:ALA:O	1:T:3058:ALA:N	2.49	0.45
1:T:3294:PRO:O	1:T:3298:ALA:HB2	2.16	0.45
1:T:1770:ILE:HG23	1:T:1810:THR:HA	1.99	0.45
1:T:1087:PHE:CG	1:T:1153:LEU:HD11	2.52	0.45
1:T:1840:LYS:HE2	1:T:1864:LEU:HD12	1.99	0.45
1:T:1905:ALA:HA	1:T:1908:VAL:HG22	1.98	0.45
1:T:3551:GLN:O	1:T:3555:PHE:N	2.50	0.44
1:T:154:LEU:HD22	1:T:214:LEU:HD13	1.98	0.44
1:T:1946:LEU:HD23	1:T:1989:LEU:HD22	1.99	0.44
1:T:2257:VAL:O	1:T:2261:TRP:CB	2.64	0.44
1:T:2278:LEU:O	1:T:2281:THR:HB	2.17	0.44
1:T:3103:ARG:HG3	1:T:3107:LEU:HD23	1.99	0.44
1:T:845:MET:HE3	1:T:845:MET:HB3	1.92	0.44
1:T:3019:LYS:HB2	1:T:3049:ILE:HG21	1.98	0.44
1:T:1800:ILE:HA	1:T:1803:LEU:HB2	2.00	0.44
1:T:2858:ILE:HD11	1:T:2877:ILE:HD13	1.98	0.44
1:T:3416:GLU:HG2	1:T:3586:MET:H	1.81	0.44
1:T:730:GLU:OE1	1:T:732:THR:OG1	2.31	0.44
1:T:1241:LEU:HD23	1:T:1241:LEU:HA	1.84	0.44
1:T:1378:LEU:HD12	1:T:1415:CYS:SG	2.57	0.44
1:T:1379:GLN:NE2	1:T:1439:ARG:HD3	2.33	0.44
1:T:413:LYS:HA	1:T:416:LYS:HG2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:2643:ILE:O	1:T:2647:THR:N	2.44	0.44
1:T:3112:ASP:HA	1:T:3113:ALA:HA	1.59	0.44
1:T:3522:VAL:HG11	1:T:3743:TRP:HD1	1.83	0.44
1:T:901:LEU:HD12	1:T:948:ILE:HD13	1.99	0.44
1:T:1129:PHE:HB3	1:T:1131:ILE:HG12	1.99	0.44
1:T:2351:LYS:O	1:T:2355:MET:HB2	2.17	0.44
1:T:2985:LEU:HD12	1:T:3006:ILE:HG23	2.00	0.44
1:T:3054:ALA:HB3	1:T:3092:TYR:HB2	2.00	0.44
1:T:307:TYR:HE1	1:T:346:GLU:HB2	1.82	0.44
1:T:2334:SER:O	1:T:2338:LEU:HB2	2.18	0.44
1:T:2869:ASN:ND2	1:T:2872:SER:OG	2.51	0.44
1:T:3280:LEU:HA	1:T:3283:PHE:HB2	1.99	0.44
1:T:749:LYS:HA	1:T:798:TYR:CE2	2.53	0.44
1:T:1275:VAL:HG23	1:T:1280:LEU:HB2	2.00	0.43
1:T:1726:GLN:NE2	1:T:1758:ALA:O	2.51	0.43
1:T:2772:ASP:HB2	1:T:2775:ALA:HB3	1.99	0.43
1:T:3322:GLU:OE2	1:T:3382:ARG:NH2	2.51	0.43
1:T:984:GLY:HA3	1:T:2447:ILE:HG22	2.00	0.43
1:T:988:ASP:OD1	1:T:988:ASP:N	2.49	0.43
1:T:2644:GLN:NE2	1:T:3634:ASP:OD2	2.51	0.43
1:T:977:ILE:HA	1:T:992:SER:HA	2.00	0.43
1:T:1173:GLU:O	1:T:1177:LEU:CB	2.60	0.43
1:T:1649:ASP:O	1:T:1653:SER:OG	2.36	0.43
1:T:2748:GLU:O	1:T:2752:HIS:ND1	2.50	0.43
1:T:3240:THR:HG23	1:T:3242:ASP:H	1.81	0.43
1:T:964:THR:HA	1:T:3578:SER:HB3	2.00	0.43
1:T:1302:LYS:O	1:T:1306:ALA:HB2	2.19	0.43
1:T:1841:ILE:HD11	1:T:1886:ILE:HD13	2.01	0.43
1:T:2661:ALA:HA	1:T:2664:GLU:HG3	2.00	0.43
1:T:2684:LYS:HB3	1:T:2719:LEU:HD13	2.00	0.43
1:T:1885:ASP:HA	1:T:1888:LYS:HG2	1.99	0.43
1:T:2460:TRP:HE1	1:T:2462:PHE:HD1	1.67	0.43
1:T:2680:ARG:HH12	1:T:2693:SER:HB3	1.83	0.43
1:T:3025:LEU:HA	1:T:3028:MET:HG2	2.01	0.43
1:T:217:SER:HA	1:T:304:PHE:HD2	1.83	0.43
1:T:445:ARG:O	1:T:449:LEU:CB	2.67	0.43
1:T:1090:THR:HG21	1:T:1163:VAL:HG11	2.00	0.43
1:T:3111:ASP:HA	1:T:3117:LEU:HD22	2.01	0.43
1:T:2673:ASP:HB3	1:T:3640:ILE:HG12	2.01	0.43
1:T:2793:MET:HE3	1:T:2848:GLN:HE22	1.84	0.43
1:T:613:VAL:HG12	1:T:615:ASN:H	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:2855:ALA:HA	1:T:2858:ILE:HG22	1.99	0.43
1:T:3575:ASP:OD2	1:T:3577:THR:OG1	2.35	0.43
1:T:897:GLY:O	1:T:901:LEU:HB2	2.18	0.43
1:T:2621:HIS:CE1	1:T:2658:ASN:HA	2.54	0.43
1:T:3018:GLN:HG3	1:T:3021:GLU:HB3	2.01	0.43
1:T:3144:LEU:HD11	1:T:3207:TYR:HB2	2.01	0.43
1:T:3448:ALA:HA	1:T:3458:MET:HB3	2.01	0.43
1:T:695:ASN:HB3	1:T:732:THR:HG21	2.01	0.42
1:T:3099:GLU:HG3	1:T:3661:THR:HG21	2.01	0.42
1:T:3466:THR:HG22	1:T:3573:HIS:CD2	2.54	0.42
1:T:1116:ASN:HD22	1:T:2500:LEU:HD12	1.84	0.42
1:T:1685:LEU:HD22	1:T:1685:LEU:HA	1.84	0.42
1:T:1722:ILE:HD13	1:T:1754:ASN:HD22	1.84	0.42
1:T:2037:TYR:O	1:T:2041:LYS:N	2.53	0.42
1:T:2372:LYS:O	1:T:2376:LEU:CB	2.61	0.42
1:T:79:MET:HA	1:T:82:ILE:HD12	2.00	0.42
1:T:1026:LEU:HD21	1:T:1102:LEU:HD21	2.00	0.42
1:T:1584:LEU:HB2	1:T:1586:LEU:HD23	2.00	0.42
1:T:2610:ILE:HD12	1:T:2616:LEU:HD11	2.01	0.42
1:T:840:GLN:HE22	1:T:878:PHE:C	2.28	0.42
1:T:1355:ASP:O	1:T:1358:THR:OG1	2.29	0.42
1:T:1864:LEU:HD13	1:T:1864:LEU:HA	1.84	0.42
1:T:2222:VAL:HG11	1:T:2229:GLU:HB3	2.01	0.42
1:T:2658:ASN:O	1:T:2662:LEU:HB2	2.20	0.42
1:T:327:ASP:O	1:T:331:ARG:HB2	2.19	0.42
1:T:396:ALA:HB1	1:T:438:LEU:HG	2.00	0.42
1:T:459:ARG:O	1:T:463:LEU:HB2	2.18	0.42
1:T:588:ARG:O	1:T:592:SER:CB	2.67	0.42
1:T:1379:GLN:NE2	1:T:1439:ARG:O	2.53	0.42
1:T:2242:VAL:O	1:T:2245:GLN:HB2	2.20	0.42
1:T:491:ARG:O	1:T:495:HIS:ND1	2.35	0.42
1:T:2870:LEU:HD12	1:T:2938:ARG:HG3	2.02	0.42
1:T:1927:PHE:HZ	1:T:1966:TRP:HB2	1.84	0.42
1:T:2191:LEU:HD22	1:T:2194:CYS:HB2	2.01	0.42
1:T:3244:ASP:O	1:T:3248:LEU:HB2	2.20	0.42
1:T:2877:ILE:HG21	1:T:2940:TYR:HE1	1.85	0.42
1:T:3240:THR:HG23	1:T:3243:GLU:H	1.85	0.42
1:T:1727:ALA:O	1:T:1731:ARG:HB2	2.20	0.41
1:T:1838:HIS:HE2	1:T:1882:ILE:HD12	1.85	0.41
1:T:1974:MET:HE1	1:T:1990:ILE:HG12	2.01	0.41
1:T:2308:THR:HA	1:T:2311:LEU:HD23	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:2906:GLN:HG2	1:T:2943:ILE:HG23	2.02	0.41
1:T:3549:ALA:HA	1:T:3632:ILE:HD11	2.01	0.41
1:T:3613:ILE:H	1:T:3613:ILE:HG13	1.64	0.41
1:T:408:LEU:HD23	1:T:459:ARG:HH21	1.83	0.41
1:T:727:LEU:HB3	1:T:736:PHE:HD2	1.85	0.41
1:T:3419:MET:HE3	1:T:3588:PRO:HG3	2.02	0.41
1:T:63:PRO:HB2	1:T:64:ILE:HG13	2.00	0.41
1:T:1803:LEU:HA	1:T:1806:VAL:HG12	2.02	0.41
1:T:2727:ALA:HA	1:T:2730:GLU:HG2	2.02	0.41
1:T:2946:VAL:O	1:T:2950:PHE:CB	2.68	0.41
1:T:3321:LEU:HD22	1:T:3321:LEU:HA	1.92	0.41
1:T:1392:LEU:HD22	1:T:1396:ILE:HA	2.02	0.41
1:T:2519:LEU:HA	1:T:2522:PHE:HB3	2.02	0.41
1:T:3165:GLN:HE22	1:T:3353:GLU:N	2.18	0.41
1:T:3649:SER:OG	1:T:3703:VAL:O	2.39	0.41
1:T:977:ILE:HG22	1:T:2490:ASN:HD22	1.85	0.41
1:T:1608:THR:HG22	1:T:1640:PHE:HE1	1.85	0.41
1:T:3484:ASP:O	1:T:3488:PHE:HB2	2.20	0.41
1:T:3489:MET:O	1:T:3493:LEU:HB2	2.19	0.41
1:T:95:TYR:O	1:T:99:VAL:HB	2.20	0.41
1:T:1184:ALA:O	1:T:1188:SER:OG	2.28	0.41
1:T:1290:THR:O	1:T:1294:CYS:HB2	2.21	0.41
1:T:1276:LYS:HG2	1:T:1318:THR:HG21	2.02	0.41
1:T:2803:PHE:HE2	1:T:2860:ALA:HB2	1.85	0.41
1:T:3121:PHE:HZ	1:T:3155:ILE:HD11	1.86	0.41
1:T:2100:LEU:HD22	1:T:2124:LEU:HB2	2.02	0.41
1:T:2234:THR:HG22	1:T:2237:GLN:HE21	1.86	0.41
1:T:2333:LEU:HD22	1:T:2375:ILE:HG21	2.02	0.41
1:T:2447:ILE:HD13	1:T:2479:SER:HB3	2.02	0.41
1:T:2719:LEU:HA	1:T:2720:PRO:HD3	1.91	0.41
1:T:2777:GLU:HA	1:T:2780:VAL:HB	2.03	0.41
1:T:3644:ASN:O	1:T:3648:ILE:HD12	2.21	0.41
1:T:346:GLU:HA	1:T:349:HIS:HB2	2.03	0.41
1:T:1032:SER:O	1:T:1032:SER:OG	2.39	0.41
1:T:1155:TYR:HD2	1:T:1157:ILE:HG12	1.86	0.41
1:T:1402:TYR:HA	1:T:1405:SER:HB3	2.02	0.41
1:T:1861:ARG:HH11	1:T:1893:PHE:HD1	1.68	0.41
1:T:1864:LEU:O	1:T:1868:SER:CB	2.69	0.41
1:T:1931:LEU:HD22	1:T:1970:VAL:HG22	2.02	0.41
1:T:2628:ILE:HD12	1:T:2628:ILE:HA	1.83	0.41
1:T:2658:ASN:O	1:T:2662:LEU:CB	2.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:3583:THR:OG1	1:T:3586:MET:SD	2.73	0.41
1:T:3614:PHE:CE2	1:T:3667:ILE:HD12	2.56	0.41
1:T:1781:ASN:HA	1:T:1784:ASN:HD22	1.86	0.41
1:T:1931:LEU:HD11	1:T:1969:TRP:HB3	2.03	0.41
1:T:1935:HIS:ND1	1:T:1937:GLU:OE1	2.54	0.41
1:T:2102:ARG:O	1:T:2106:ALA:CB	2.68	0.41
1:T:2355:MET:HB2	1:T:2355:MET:HE3	1.99	0.41
1:T:2911:VAL:O	1:T:2915:ALA:HB3	2.20	0.41
1:T:3025:LEU:HA	1:T:3028:MET:HE3	2.02	0.41
1:T:1223:VAL:HG12	1:T:1227:SER:HB2	2.03	0.40
1:T:1787:THR:HA	1:T:1790:VAL:HG12	2.03	0.40
1:T:1903:GLN:HA	1:T:1906:TYR:HB3	2.02	0.40
1:T:2365:ILE:HG22	1:T:2367:PRO:HA	2.03	0.40
1:T:3087:GLN:HE21	1:T:3124:PHE:HD1	1.70	0.40
1:T:302:THR:O	1:T:305:LEU:HB3	2.21	0.40
1:T:587:TYR:O	1:T:591:MET:HB2	2.22	0.40
1:T:1543:LEU:O	1:T:1545:GLU:N	2.54	0.40
1:T:3202:ARG:HB3	1:T:3203:GLN:H	1.59	0.40
1:T:1382:ILE:HG22	1:T:1412:ARG:HG3	2.02	0.40
1:T:2672:GLU:OE2	1:T:3438:ARG:NH1	2.54	0.40
1:T:900:THR:HA	1:T:903:LEU:HD22	2.04	0.40
1:T:2298:ALA:HB1	1:T:2302:GLU:HG3	2.03	0.40
1:T:2847:GLN:HE21	1:T:2887:ARG:HD3	1.87	0.40
1:T:3708:HIS:CE1	1:T:3710:ASN:HB3	2.56	0.40
1:T:743:PHE:HD2	1:T:744:LEU:HD12	1.86	0.40
1:T:997:ILE:HD13	1:T:1078:LEU:HD21	2.03	0.40
1:T:1197:PHE:HB3	1:T:1216:ILE:HG23	2.03	0.40
1:T:1416:ILE:HG21	1:T:1459:THR:HG22	2.03	0.40
1:T:2121:ILE:O	1:T:2125:SER:OG	2.33	0.40
1:T:2462:PHE:CE2	1:T:2466:TYR:HB3	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	T	3443/3767 (91%)	2913 (85%)	508 (15%)	22 (1%)	21	52

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	T	1544	ALA
1	T	2889	PRO
1	T	1158	PRO
1	T	1157	ILE
1	T	3655	PRO
1	T	777	PRO
1	T	849	ALA
1	T	852	PRO
1	T	2223	SER
1	T	228	PRO
1	T	247	PRO
1	T	510	ASN
1	T	1206	TYR
1	T	1341	PRO
1	T	3657	ASN
1	T	695	ASN
1	T	1543	LEU
1	T	2620	PRO
1	T	2621	HIS
1	T	63	PRO
1	T	2619	PRO
1	T	2226	ILE

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	T	3181/3474 (92%)	3114 (98%)	67 (2%)	47	64

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	37	LEU
1	T	38	LEU
1	T	114	ASN
1	T	132	ILE
1	T	133	LEU
1	T	246	LEU
1	T	253	ILE
1	T	340	LEU
1	T	399	ILE
1	T	433	ILE
1	T	440	LEU
1	T	446	ILE
1	T	463	LEU
1	T	580	ILE
1	T	594	LEU
1	T	694	ASP
1	T	783	VAL
1	T	788	LEU
1	T	794	ASN
1	T	876	LEU
1	T	917	ILE
1	T	920	VAL
1	T	991	LEU
1	T	994	THR
1	T	1066	THR
1	T	1082	LEU
1	T	1119	LEU
1	T	1137	ASN
1	T	1275	VAL
1	T	1345	LEU
1	T	1366	THR
1	T	1368	LEU
1	T	1377	LEU
1	T	1503	LEU
1	T	1511	ILE
1	T	1574	LEU
1	T	1596	LEU
1	T	1685	LEU
1	T	1718	LEU
1	T	1802	VAL
1	T	1825	LEU
1	T	1864	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	1865	LEU
1	T	1907	LEU
1	T	2101	ILE
1	T	2168	LEU
1	T	2191	LEU
1	T	2278	LEU
1	T	2315	LEU
1	T	2318	LEU
1	T	2324	LEU
1	T	2481	ASN
1	T	2491	ILE
1	T	2494	LEU
1	T	2500	LEU
1	T	2527	ILE
1	T	2586	LEU
1	T	2607	LEU
1	T	2662	LEU
1	T	2678	LEU
1	T	3053	LEU
1	T	3263	LEU
1	T	3280	LEU
1	T	3321	LEU
1	T	3445	LEU
1	T	3648	ILE
1	T	3706	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	T	22	GLN
1	T	39	ASN
1	T	49	GLN
1	T	298	GLN
1	T	400	HIS
1	T	510	ASN
1	T	639	HIS
1	T	794	ASN
1	T	840	GLN
1	T	930	ASN
1	T	956	ASN
1	T	998	GLN
1	T	1002	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	1114	GLN
1	T	1130	ASN
1	T	1137	ASN
1	T	1305	ASN
1	T	1365	ASN
1	T	1379	GLN
1	T	1397	GLN
1	T	1407	GLN
1	T	1488	ASN
1	T	1601	ASN
1	T	1614	ASN
1	T	1646	ASN
1	T	1654	ASN
1	T	1690	ASN
1	T	1726	GLN
1	T	1754	ASN
1	T	1775	ASN
1	T	1781	ASN
1	T	1784	ASN
1	T	1805	ASN
1	T	1808	ASN
1	T	1839	ASN
1	T	1857	HIS
1	T	1983	ASN
1	T	2040	ASN
1	T	2122	ASN
1	T	2183	ASN
1	T	2188	GLN
1	T	2207	GLN
1	T	2237	GLN
1	T	2289	HIS
1	T	2294	GLN
1	T	2362	ASN
1	T	2406	HIS
1	T	2481	ASN
1	T	2490	ASN
1	T	2507	ASN
1	T	2551	GLN
1	T	2566	GLN
1	T	2595	GLN
1	T	2646	ASN
1	T	2670	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	2696	GLN
1	T	2811	GLN
1	T	2822	GLN
1	T	2839	HIS
1	T	2848	GLN
1	T	2861	ASN
1	T	2869	ASN
1	T	2882	GLN
1	T	2896	ASN
1	T	2899	ASN
1	T	2907	HIS
1	T	2913	ASN
1	T	2975	ASN
1	T	3010	ASN
1	T	3087	GLN
1	T	3154	HIS
1	T	3165	GLN
1	T	3250	ASN
1	T	3367	HIS
1	T	3515	ASN
1	T	3537	GLN
1	T	3547	GLN
1	T	3615	HIS
1	T	3644	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.

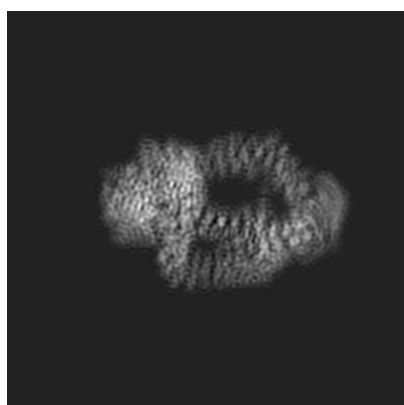
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3824. These allow visual inspection of the internal detail of the map and identification of artifacts.

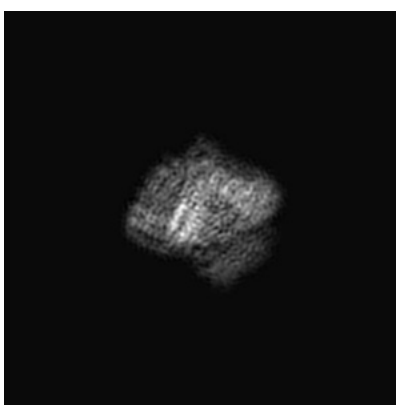
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

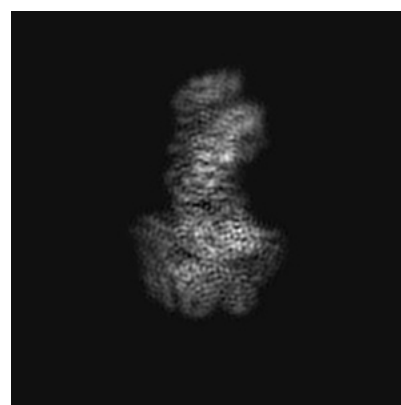
6.1.1 Primary map



X



Y

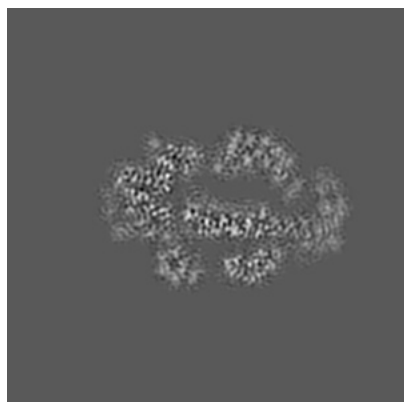


Z

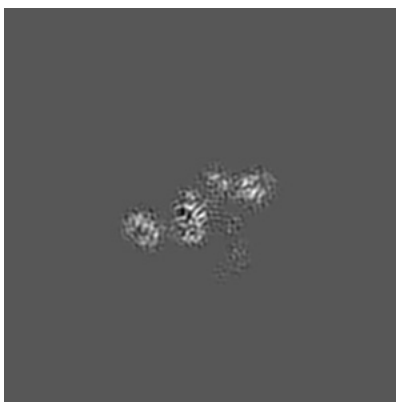
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

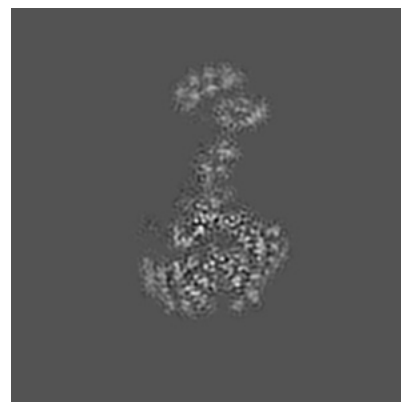
6.2.1 Primary map



X Index: 145



Y Index: 145

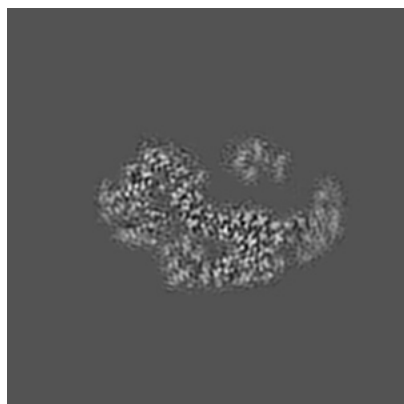


Z Index: 145

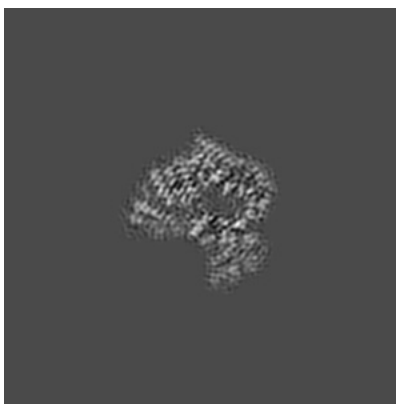
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

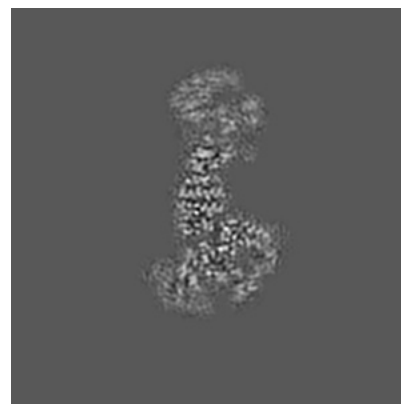
6.3.1 Primary map



X Index: 136



Y Index: 127

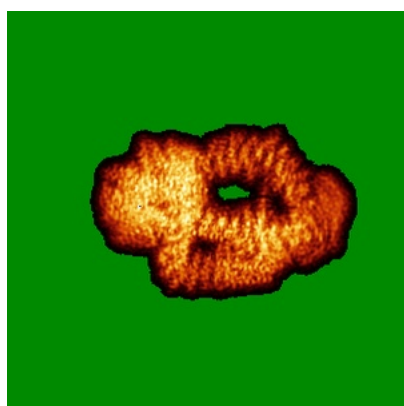


Z Index: 137

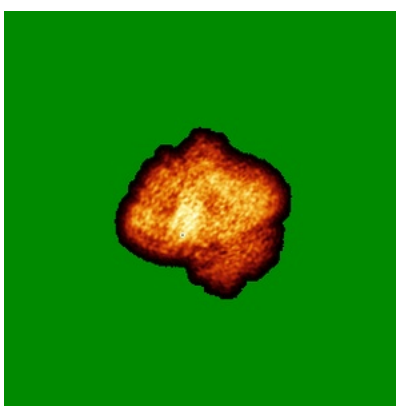
The images above show the largest variance slices of the map in three orthogonal directions.

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

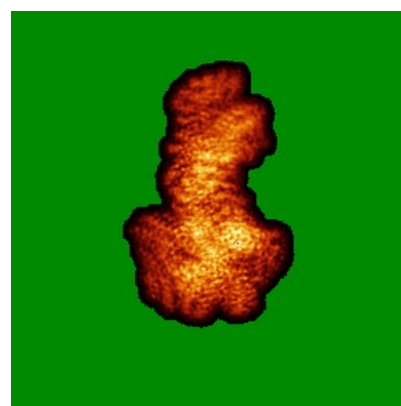
6.4.1 Primary map



X



Y

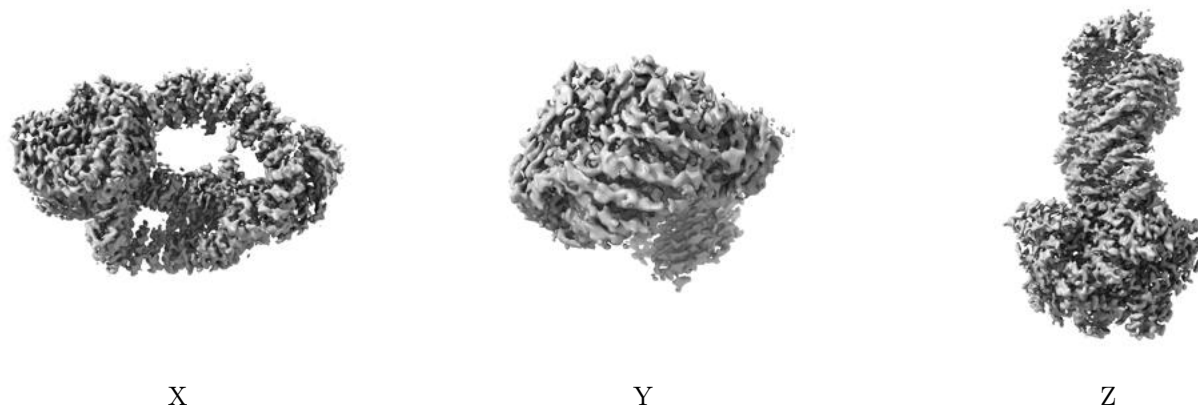


Z

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

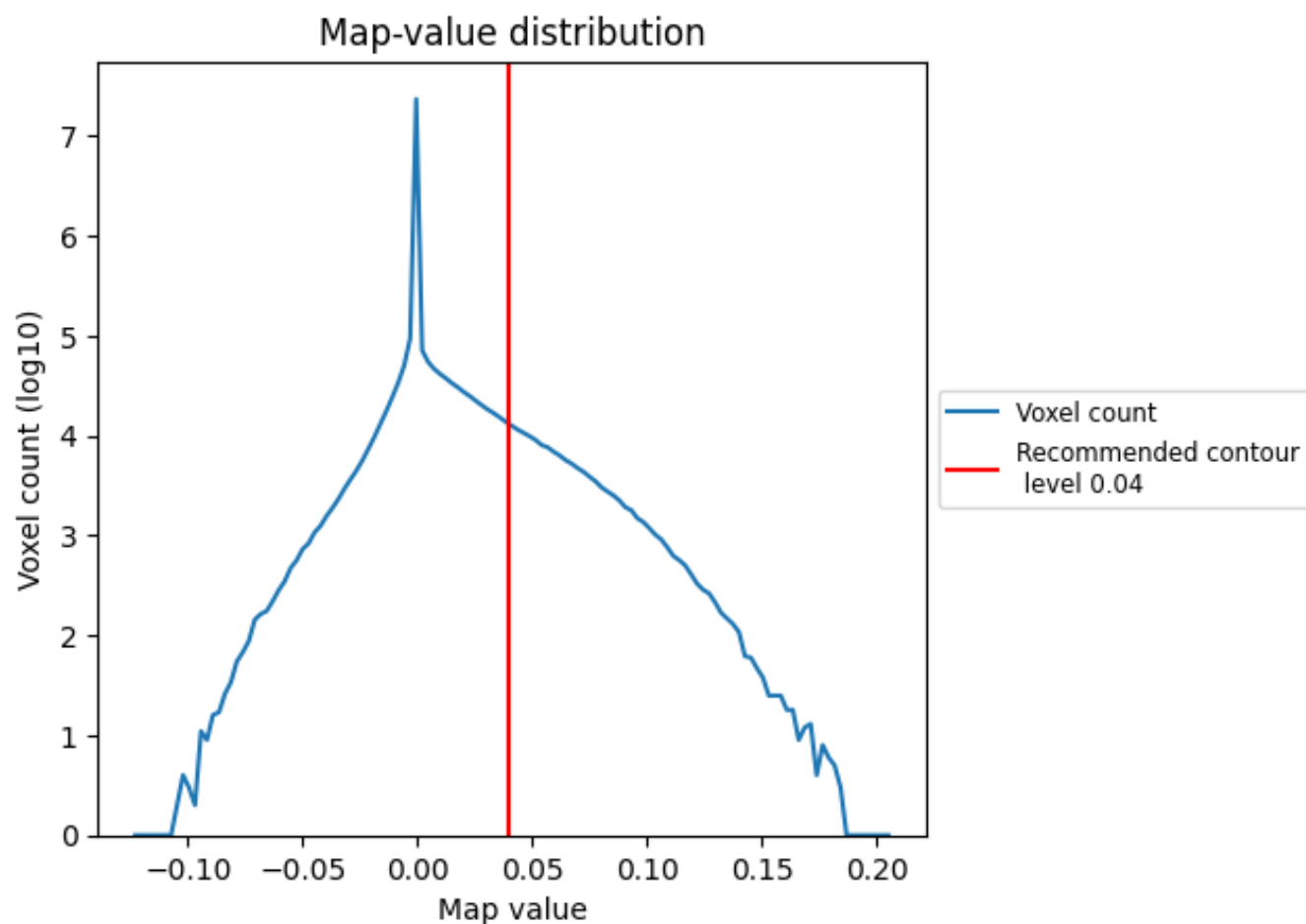
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

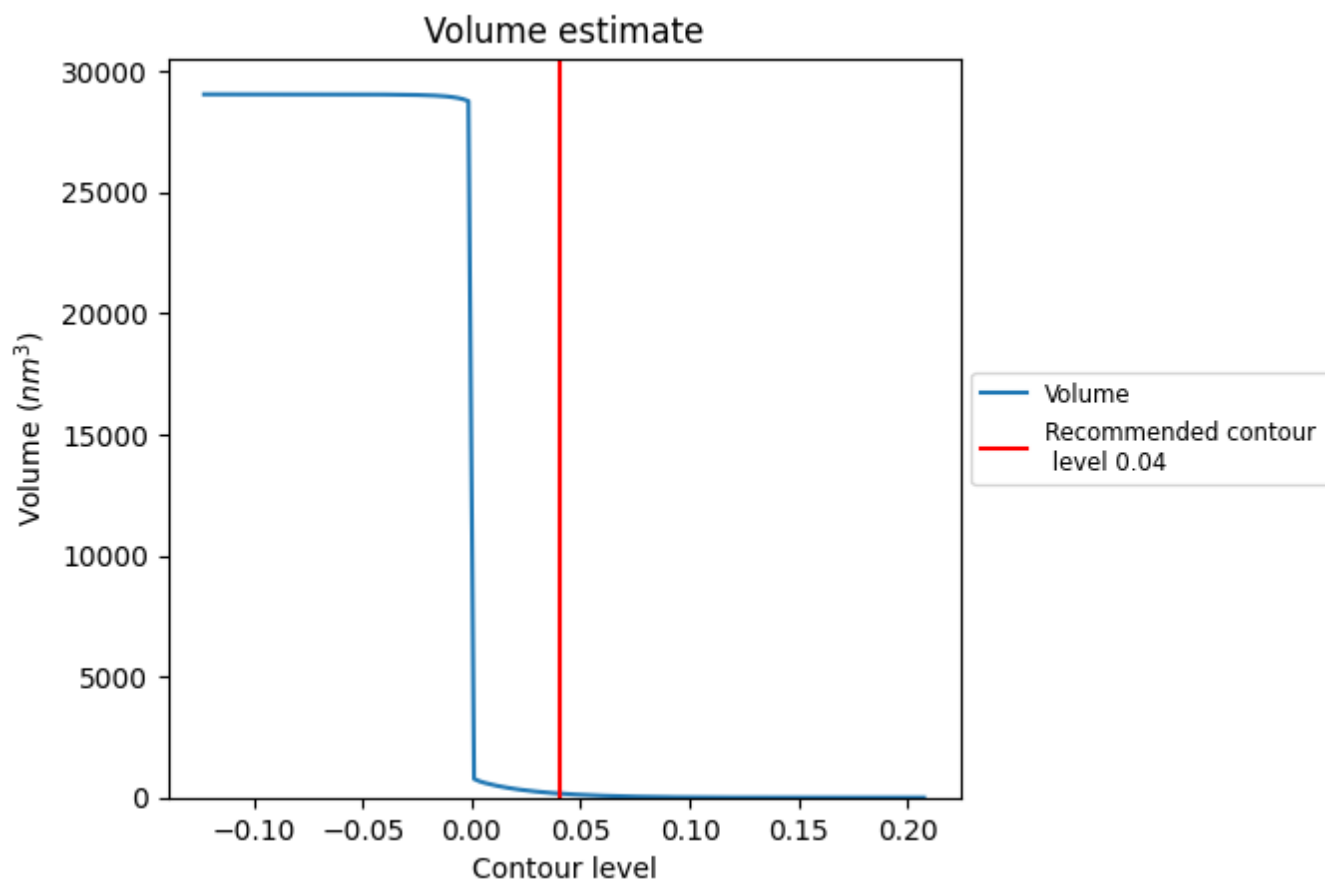
This section contains the results of statistical analysis of the map.

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.

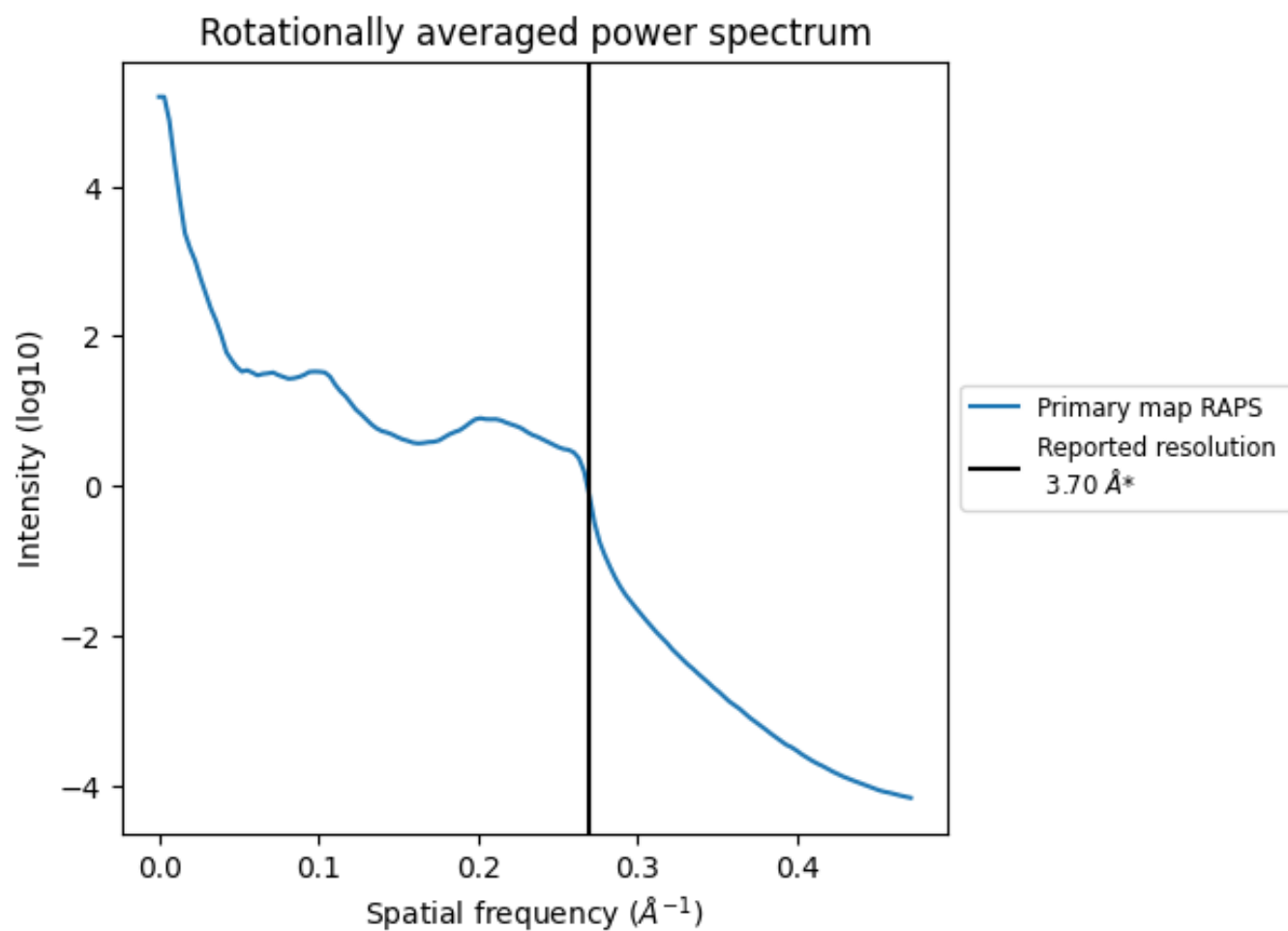
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 168 nm³; this corresponds to an approximate mass of 152 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 ⓘ

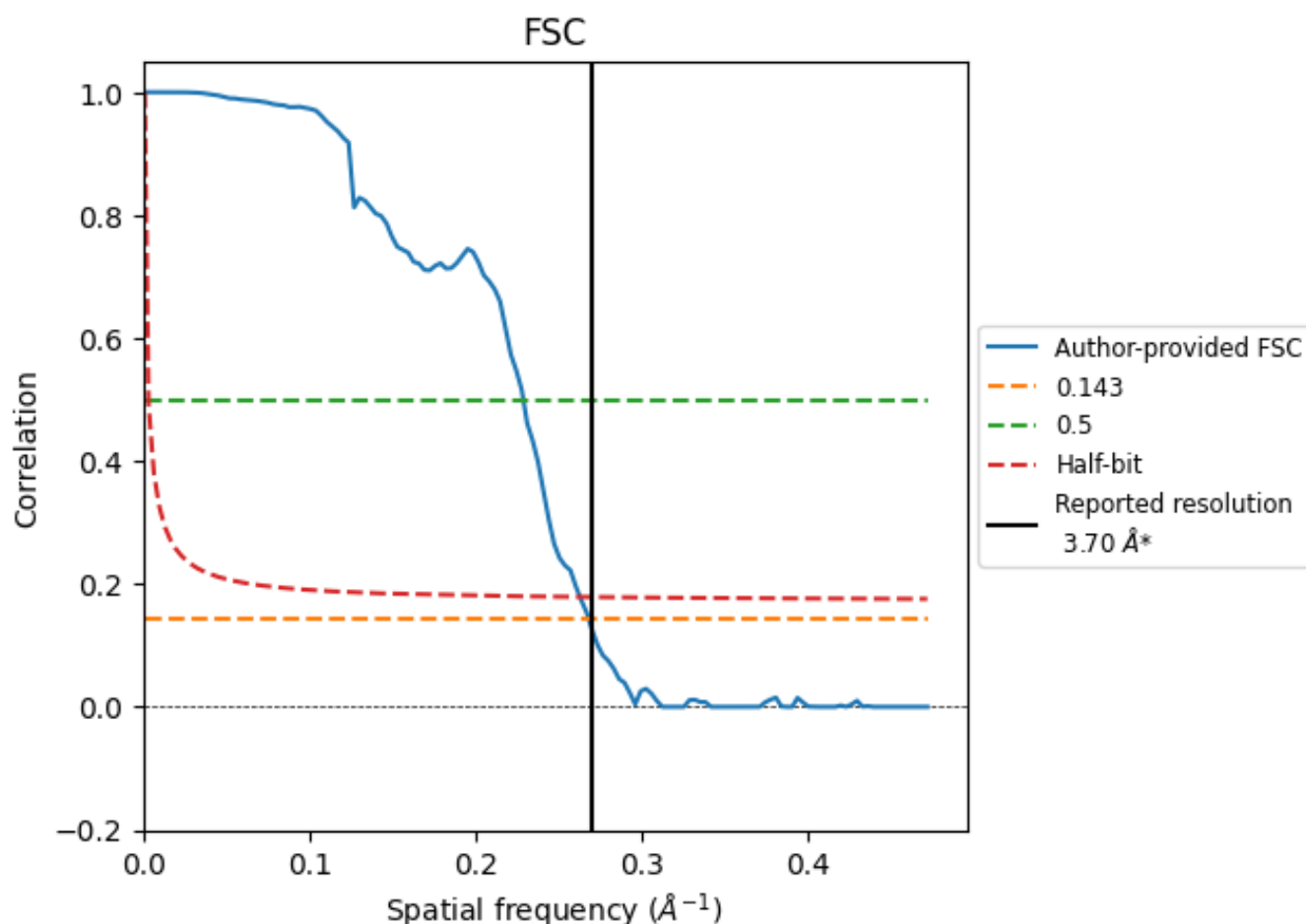


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

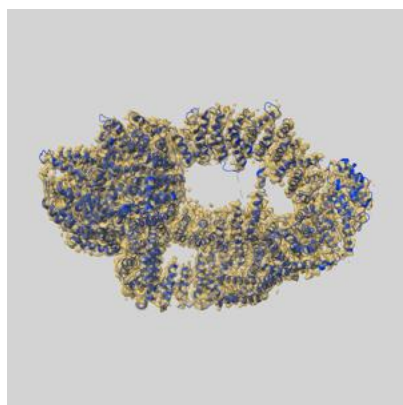
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.73	4.37	3.81
Unmasked-calculated*	-	-	-

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

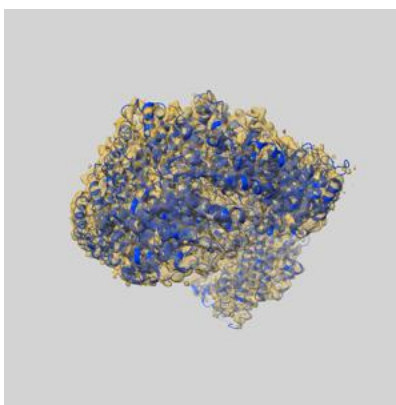
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3824 and PDB model 5OJS. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

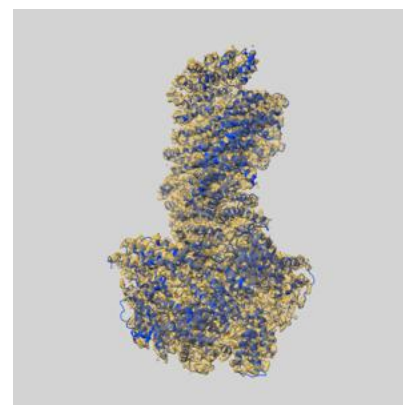
9.1 Map-model overlay [i](#)



X



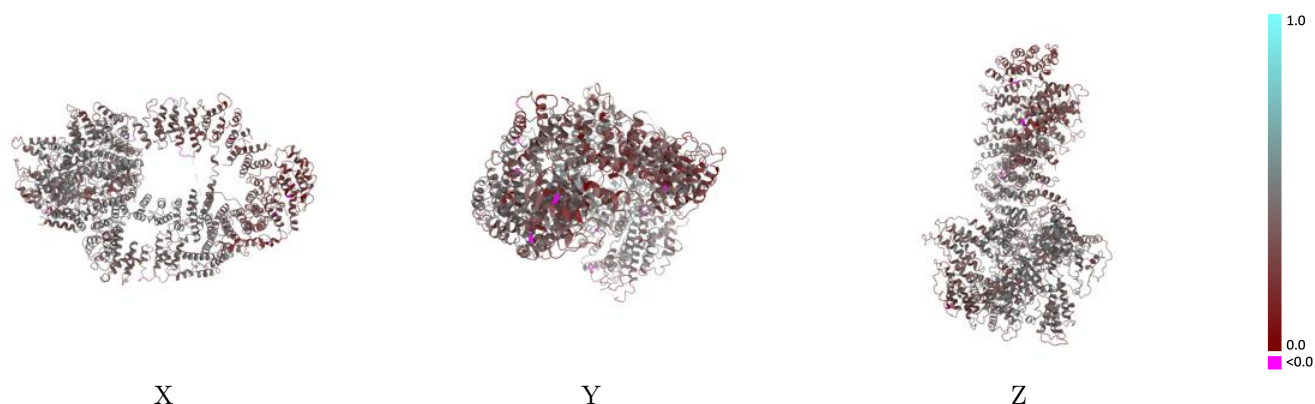
Y



Z

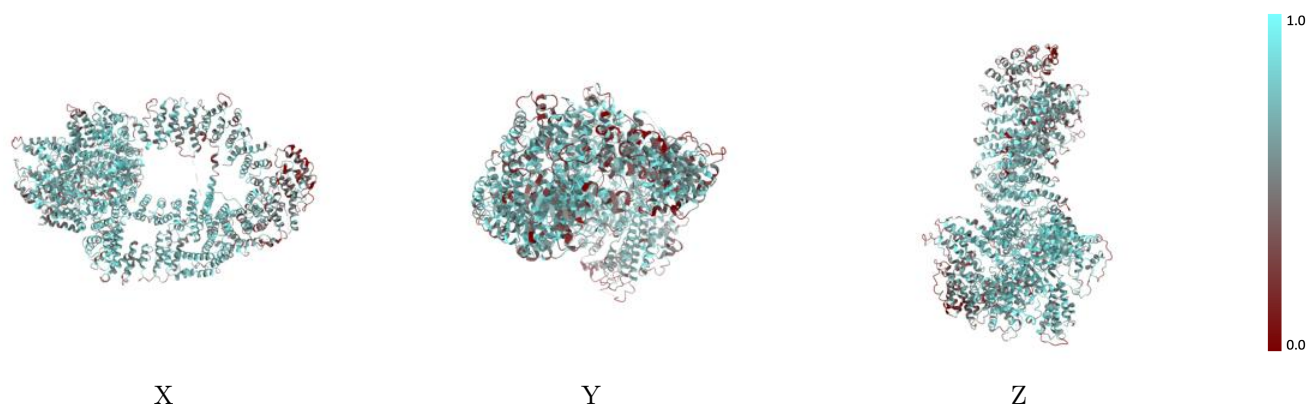
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



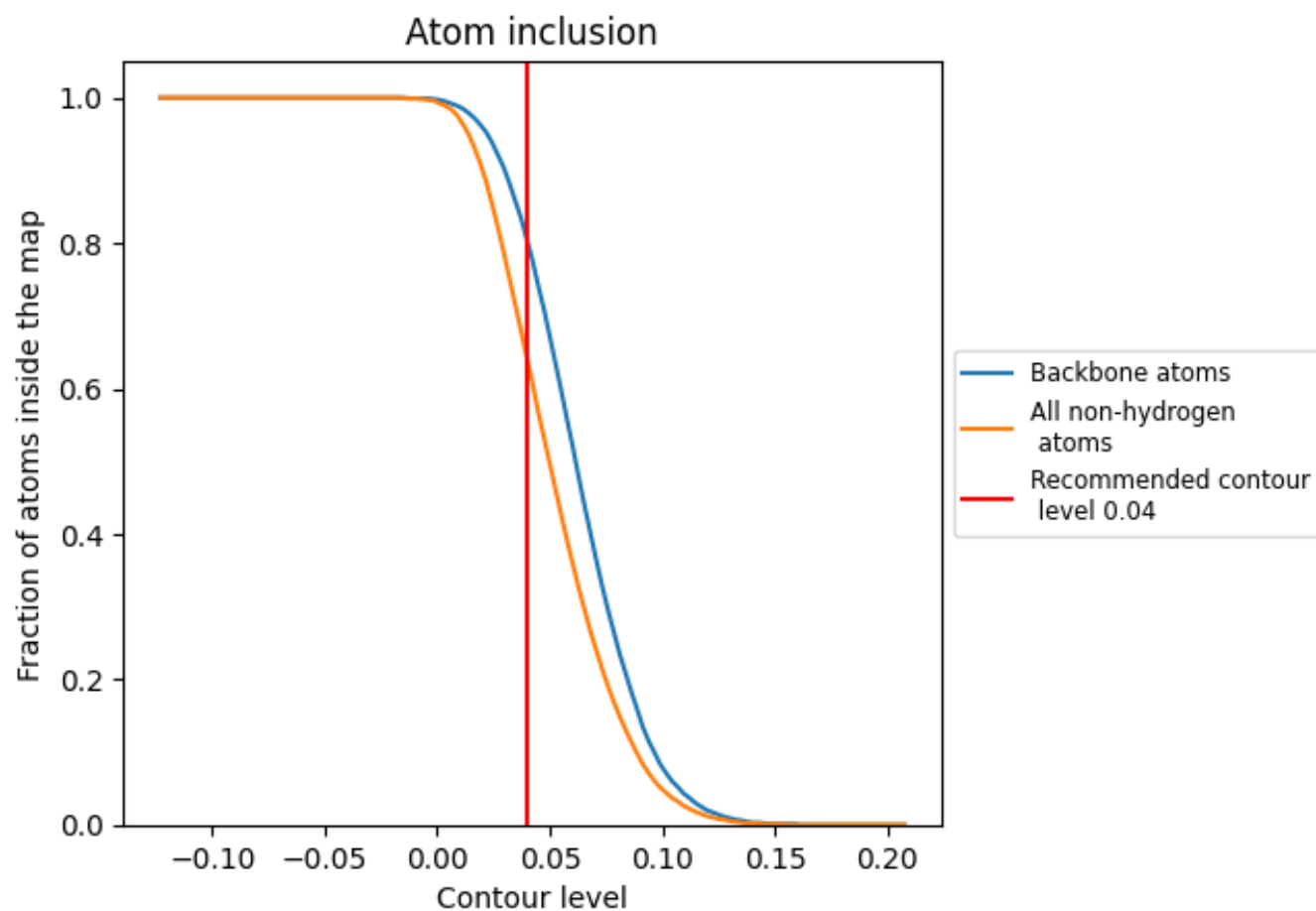
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6410	0.3870
T	0.6410	0.3870

