



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:59 PM UTC

PDB ID : 9EUW / pdb_00009euw
EMDB ID : EMD-19988
Title : Lymphostatin, conformation 2 (composite structure)
Authors : Griessmann, M.; Rasmussen, T.; Bottcher, B.
Deposited on : 2024-03-28
Resolution : 2.80 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

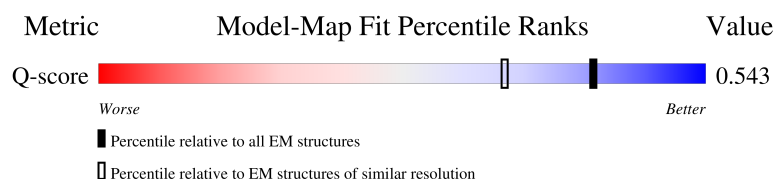
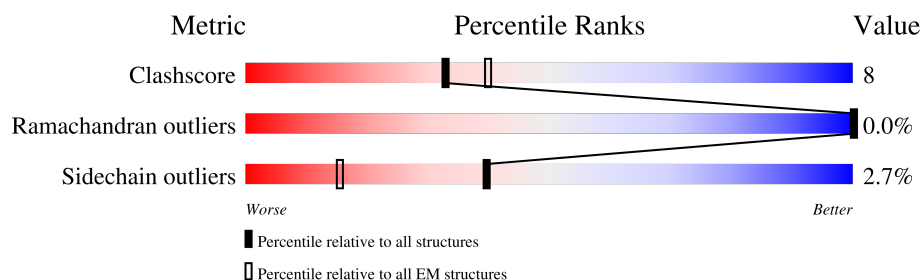
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	11806 (2.30 - 3.30)

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	3229	68% 18% 13%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22338 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.

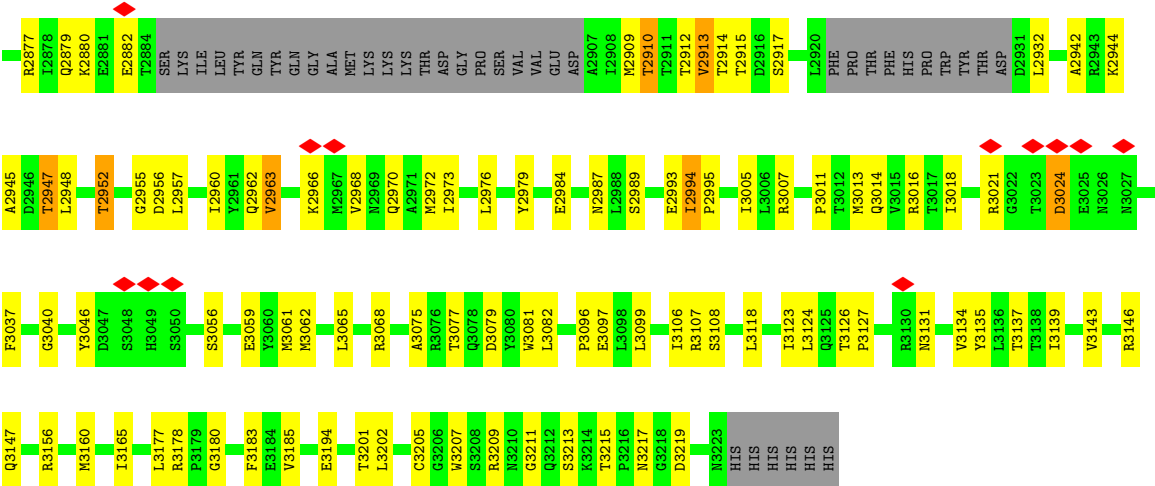
- Molecule 1 is a protein called Efa1/LifA protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2803	22338	14119	3874	4269	76	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3224	HIS	-	expression tag	UNP B7UI23
A	3225	HIS	-	expression tag	UNP B7UI23
A	3226	HIS	-	expression tag	UNP B7UI23
A	3227	HIS	-	expression tag	UNP B7UI23
A	3228	HIS	-	expression tag	UNP B7UI23
A	3229	HIS	-	expression tag	UNP B7UI23





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	182000	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 ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	68.256	Depositor
Minimum map value	-34.889	Depositor
Average map value	-0.007	Depositor
Map value standard deviation	1.109	Depositor
Recommended contour level	6.5	Depositor
Map size (Å)	378.4, 378.4, 378.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.946, 0.946, 0.946	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	0.19	0/22775	0.32	2/30861 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2188	ARG	CB-CA-C	-5.24	110.51	116.54
1	A	2647	VAL	N-CA-C	-5.02	108.38	113.20

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	22338	0	22342	373	0
All	All	22338	0	22342	373	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 (373) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1857:LEU:HB3	1:A:1943:ARG:HH12	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1853:MET:O	1:A:1857:LEU:HB2	1.84	0.77
1:A:1812:ASN:HB3	1:A:1826:GLN:H	1.51	0.75
1:A:2380:LEU:HD22	1:A:2425:MET:HG3	1.67	0.75
1:A:1683:ALA:HB2	1:A:1746:THR:HG21	1.69	0.75
1:A:615:ASP:O	1:A:619:ASN:ND2	2.20	0.75
1:A:2791:ARG:HH22	1:A:2800:ARG:HH21	1.35	0.75
1:A:867:THR:HG21	1:A:912:ASP:HB2	1.69	0.74
1:A:1122:LYS:H	1:A:1122:LYS:HD2	1.52	0.74
1:A:2507:GLN:NE2	1:A:2529:MET:SD	2.61	0.74
1:A:1754:ARG:HG2	1:A:1978:ILE:HD13	1.71	0.73
1:A:1489:GLN:HG2	1:A:1654:LEU:HD13	1.71	0.72
1:A:1842:GLU:OE2	1:A:1842:GLU:N	2.21	0.71
1:A:1965:GLU:N	1:A:1965:GLU:OE2	2.21	0.70
1:A:2805:ARG:NH1	1:A:2807:GLN:OE1	2.25	0.69
1:A:795:THR:HA	1:A:801:TYR:HA	1.75	0.68
1:A:2699:ILE:HD12	1:A:2702:LEU:HD11	1.76	0.67
1:A:2525:ARG:NH1	1:A:2554:ASP:OD2	2.27	0.67
1:A:1210:HIS:O	1:A:1210:HIS:ND1	2.26	0.67
1:A:1930:GLU:OE2	1:A:1930:GLU:N	2.22	0.66
1:A:2948:LEU:HB3	1:A:2960:ILE:HB	1.77	0.66
1:A:342:GLU:OE2	1:A:639:LYS:NZ	2.27	0.66
1:A:689:GLN:OE1	1:A:692:ARG:NH1	2.29	0.65
1:A:575:GLN:HE21	1:A:627:GLU:HG2	1.59	0.65
1:A:792:VAL:HG23	1:A:807:GLU:HB2	1.78	0.65
1:A:653:ARG:HD2	1:A:792:VAL:HG12	1.78	0.64
1:A:2731:LEU:HD22	1:A:2749:GLN:HE21	1.60	0.64
1:A:1309:MET:HE1	1:A:1350:GLN:HE21	1.63	0.64
1:A:2440:ILE:HD13	1:A:2466:LEU:HD13	1.80	0.64
1:A:2532:VAL:HG13	1:A:2533:THR:HG23	1.81	0.64
1:A:1738:ASP:OD1	1:A:1741:ARG:NH2	2.30	0.63
1:A:340:TYR:O	1:A:505:ARG:NH2	2.32	0.63
1:A:2473:LEU:HD12	1:A:2477:VAL:HG21	1.80	0.62
1:A:765:LEU:HD12	1:A:779:ILE:HD12	1.82	0.62
1:A:2116:ARG:NH1	1:A:2122:ALA:O	2.33	0.61
1:A:2773:ILE:HD11	1:A:2783:LEU:HD23	1.82	0.61
1:A:1317:GLN:NE2	1:A:1321:GLN:OE1	2.33	0.61
1:A:3134:VAL:HG21	1:A:3160:MET:HE1	1.83	0.61
1:A:571:LYS:HA	1:A:574:MET:HE3	1.83	0.60
1:A:2605:GLN:HB2	1:A:2635:VAL:HG23	1.84	0.60
1:A:446:ASN:ND2	1:A:848:GLU:OE2	2.33	0.60
1:A:1323:LEU:HD12	1:A:1332:LEU:HG	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1822:ARG:HH12	1:A:1837:SER:HA	1.68	0.59
1:A:2226:THR:HG23	1:A:2293:LEU:HD21	1.84	0.59
1:A:907:MET:HE3	1:A:916:LYS:HG2	1.83	0.59
1:A:2375:LEU:HB3	1:A:2378:THR:HB	1.84	0.59
1:A:2944:LYS:HB2	1:A:2962:GLN:HB2	1.83	0.59
1:A:3096:PRO:HA	1:A:3099:LEU:HD23	1.85	0.59
1:A:494:ILE:HG12	1:A:508:ILE:HG13	1.84	0.59
1:A:1178:ARG:NH1	1:A:1192:GLU:OE2	2.34	0.59
1:A:1214:ASP:OD1	1:A:1214:ASP:N	2.34	0.58
1:A:2106:HIS:CE1	1:A:2108:PRO:HG3	2.38	0.58
1:A:2909:MET:HE2	1:A:2972:MET:HB3	1.85	0.58
1:A:2588:SER:OG	1:A:2589:GLY:N	2.36	0.57
1:A:2751:HIS:NE2	1:A:2816:THR:OG1	2.27	0.57
1:A:1182:HIS:CD2	1:A:1266:MET:HE1	2.40	0.57
1:A:769:ARG:HH12	1:A:782:ARG:HA	1.69	0.57
1:A:1401:SER:OG	1:A:1416:ASP:OD2	2.20	0.57
1:A:677:SER:HB3	1:A:680:ILE:HG13	1.87	0.57
1:A:244:GLU:O	1:A:248:ILE:HD12	2.05	0.56
1:A:2857:LEU:HD13	1:A:2869:ALA:HB2	1.88	0.56
1:A:2546:ASP:OD2	1:A:2549:HIS:ND1	2.38	0.56
1:A:2651:LEU:HB2	1:A:2720:VAL:HB	1.88	0.56
1:A:1350:GLN:HE22	1:A:1358:HIS:CE1	2.23	0.56
1:A:1822:ARG:HH22	1:A:1837:SER:HA	1.70	0.56
1:A:3024:ASP:OD1	1:A:3024:ASP:N	2.27	0.56
1:A:2910:THR:HA	1:A:2973:ILE:HG13	1.88	0.55
1:A:1301:ASP:OD2	1:A:1328:SER:OG	2.23	0.55
1:A:2619:ASP:OD1	1:A:2620:ASN:N	2.39	0.55
1:A:2955:GLY:O	1:A:2979:TYR:N	2.39	0.55
1:A:1248:PRO:HD2	1:A:1251:GLU:HG3	1.88	0.55
1:A:245:ILE:HA	1:A:248:ILE:HD12	1.88	0.55
1:A:245:ILE:O	1:A:249:LYS:HG2	2.06	0.55
1:A:3068:ARG:HD3	1:A:3075:ALA:HB1	1.88	0.55
1:A:443:ASN:ND2	1:A:848:GLU:OE1	2.31	0.55
1:A:871:LEU:HD22	1:A:906:ILE:HG23	1.88	0.55
1:A:1988:GLU:N	1:A:1988:GLU:OE2	2.39	0.55
1:A:2947:THR:HG23	1:A:3046:TYR:HB3	1.89	0.55
1:A:375:ILE:HD13	1:A:428:MET:HE3	1.89	0.54
1:A:2661:VAL:HG22	1:A:2713:ILE:HD13	1.90	0.54
1:A:2689:ALA:HB3	1:A:2692:GLU:HB3	1.89	0.54
1:A:3107:ARG:HH12	1:A:3147:GLN:HB3	1.73	0.54
1:A:2404:PRO:HG3	1:A:2410:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1488:LEU:HD11	1:A:1573:ARG:HB3	1.89	0.54
1:A:2354:ARG:HD2	1:A:2377:GLU:HB3	1.87	0.54
1:A:2367:ASN:OD1	1:A:2367:ASN:N	2.30	0.54
1:A:2516:THR:HB	1:A:2539:THR:HG23	1.88	0.54
1:A:409:ASN:O	1:A:413:GLU:HG2	2.08	0.53
1:A:1816:ALA:HB2	1:A:1824:ASN:HD21	1.73	0.53
1:A:2987:ASN:HA	1:A:3007:ARG:HH22	1.73	0.53
1:A:248:ILE:HG13	1:A:276:LEU:HD13	1.90	0.53
1:A:566:LYS:HD2	1:A:804:LEU:HD13	1.90	0.53
1:A:1807:HIS:O	1:A:1829:ASP:HA	2.08	0.53
1:A:288:GLU:HA	1:A:291:PHE:HD2	1.74	0.53
1:A:1447:ARG:NH2	1:A:1784:GLN:OE1	2.32	0.53
1:A:2187:SER:HB2	1:A:2188:ARG:HH21	1.73	0.53
1:A:255:TYR:OH	1:A:304:GLU:OE2	2.25	0.53
1:A:2942:ALA:HB1	1:A:2995:PRO:HD3	1.91	0.53
1:A:2603:GLN:HB2	1:A:2606:ASP:HB3	1.89	0.53
1:A:2628:ARG:HG2	1:A:2630:GLY:H	1.73	0.53
1:A:2819:ASP:OD1	1:A:2850:ASN:ND2	2.41	0.53
1:A:2910:THR:HG23	1:A:2973:ILE:HD11	1.89	0.53
1:A:614:SER:OG	1:A:617:ASP:OD1	2.26	0.53
1:A:984:PHE:CE2	1:A:1121:PHE:HA	2.44	0.53
1:A:2932:LEU:HD11	1:A:3016:ARG:HH21	1.73	0.53
1:A:3005:ILE:HD13	1:A:3018:ILE:HD12	1.90	0.53
1:A:1898:ASP:H	1:A:1901:GLN:HE21	1.57	0.53
1:A:2327:ASP:HA	1:A:2345:GLY:H	1.75	0.52
1:A:2594:LEU:HD22	1:A:2610:LEU:HD21	1.91	0.52
1:A:2733:ILE:HD12	1:A:2739:MET:SD	2.50	0.52
1:A:2423:ASP:HA	1:A:2451:VAL:HG21	1.91	0.52
1:A:3106:ILE:HD11	1:A:3134:VAL:HG12	1.91	0.52
1:A:575:GLN:NE2	1:A:627:GLU:HG2	2.24	0.52
1:A:734:SER:O	1:A:734:SER:OG	2.26	0.52
1:A:2101:ASP:OD1	1:A:2135:TYR:OH	2.23	0.52
1:A:3123:ILE:HD12	1:A:3124:LEU:H	1.74	0.52
1:A:544:ARG:HG3	1:A:545:MET:HE2	1.92	0.52
1:A:1860:SER:HB3	1:A:2035:ASN:HD22	1.73	0.52
1:A:1862:ILE:HD12	1:A:1862:ILE:O	2.09	0.52
1:A:2502:ARG:NH2	1:A:3194:GLU:O	2.43	0.52
1:A:334:LYS:HG2	1:A:501:PHE:HE2	1.75	0.51
1:A:1151:ASP:OD1	1:A:1151:ASP:N	2.41	0.51
1:A:2987:ASN:OD1	1:A:3007:ARG:NH2	2.42	0.51
1:A:3215:THR:OG1	1:A:3217:ASN:OD1	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:THR:OG1	1:A:1367:ASP:OD1	2.28	0.51
1:A:1324:GLU:HG3	1:A:1325:ASN:OD1	2.10	0.51
1:A:2060:ILE:HD12	1:A:2078:PHE:HB2	1.92	0.51
1:A:2406:ASP:OD1	1:A:2406:ASP:N	2.40	0.51
1:A:2829:ASP:OD1	1:A:2830:ARG:N	2.44	0.51
1:A:2945:ALA:HA	1:A:2994:ILE:HD12	1.92	0.51
1:A:397:TYR:HD2	1:A:407:TYR:HB2	1.75	0.51
1:A:2318:ALA:HB1	1:A:2357:LYS:HE2	1.92	0.51
1:A:238:LYS:H	1:A:238:LYS:HD2	1.76	0.51
1:A:415:TYR:HB2	1:A:731:LEU:HB3	1.93	0.51
1:A:481:LYS:NZ	1:A:485:ASP:OD2	2.44	0.51
1:A:794:LYS:HD3	1:A:807:GLU:HG2	1.93	0.51
1:A:1857:LEU:HD23	1:A:1943:ARG:NH1	2.26	0.50
1:A:2644:LEU:HB3	1:A:3040:GLY:HA3	1.91	0.50
1:A:2220:ASP:N	1:A:2220:ASP:OD1	2.43	0.50
1:A:2754:VAL:HG12	1:A:2756:PRO:HD3	1.94	0.50
1:A:271:GLN:HA	1:A:774:LEU:HD23	1.94	0.50
1:A:2816:THR:HG21	1:A:2818:ARG:HH11	1.77	0.50
1:A:1815:LEU:HA	1:A:1823:PHE:HA	1.92	0.50
1:A:2365:SER:O	1:A:2368:SER:OG	2.24	0.50
1:A:312:ILE:HD13	1:A:672:LEU:HD23	1.94	0.50
1:A:1956:ALA:O	1:A:1960:GLU:HG3	2.12	0.50
1:A:2485:GLN:OE1	1:A:2500:GLN:NE2	2.45	0.50
1:A:976:SER:OG	1:A:1151:ASP:OD1	2.26	0.50
1:A:3021:ARG:HG2	1:A:3024:ASP:O	2.12	0.50
1:A:575:GLN:OE1	1:A:575:GLN:N	2.45	0.50
1:A:1808:LEU:HD23	1:A:1902:LEU:HD12	1.94	0.50
1:A:2107:ARG:NH2	1:A:2109:ASP:OD2	2.44	0.49
1:A:649:MET:HG3	1:A:673:SER:HB2	1.94	0.49
1:A:718:ASP:HB3	1:A:721:LYS:HG3	1.94	0.49
1:A:1831:GLU:HB2	1:A:1833:LEU:HD11	1.94	0.49
1:A:243:ASN:N	1:A:243:ASN:OD1	2.43	0.49
1:A:2432:ARG:NH2	1:A:2472:SER:OG	2.39	0.49
1:A:281:MET:HE3	1:A:281:MET:C	2.37	0.49
1:A:1746:THR:HG23	1:A:1747:GLN:HG2	1.94	0.49
1:A:2957:LEU:HB3	1:A:2976:LEU:HB2	1.94	0.49
1:A:3082:LEU:HD23	1:A:3137:THR:HG22	1.95	0.49
1:A:1559:GLN:NE2	1:A:1615:GLU:OE1	2.44	0.49
1:A:3217:ASN:ND2	1:A:3219:ASP:OD2	2.44	0.49
1:A:1427:SER:HB2	1:A:1547:THR:HG21	1.95	0.48
1:A:3062:MET:HE3	1:A:3062:MET:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2212:VAL:HG12	1:A:2214:PRO:HD3	1.95	0.48
1:A:733:GLY:O	1:A:828:ARG:NH2	2.47	0.48
1:A:1988:GLU:H	1:A:1988:GLU:CD	2.20	0.48
1:A:2564:GLU:HB3	1:A:2623:TRP:HE3	1.79	0.48
1:A:3056:SER:HB3	1:A:3059:GLU:HG3	1.96	0.48
1:A:894:LYS:NZ	1:A:894:LYS:HB3	2.29	0.48
1:A:1814:GLU:O	1:A:1824:ASN:N	2.35	0.48
1:A:2960:ILE:CD1	1:A:2973:ILE:HG22	2.43	0.48
1:A:1674:ALA:HB2	1:A:1690:LYS:HD2	1.94	0.48
1:A:2820:PHE:HA	1:A:2853:TYR:CD2	2.49	0.48
1:A:1592:TYR:CE2	1:A:1607:PRO:HG3	2.49	0.48
1:A:979:THR:O	1:A:983:ILE:HG13	2.14	0.48
1:A:1141:GLU:OE1	1:A:1141:GLU:N	2.40	0.48
1:A:1356:HIS:HE1	1:A:1368:ALA:HB2	1.79	0.48
1:A:2544:ALA:N	1:A:2551:GLU:OE2	2.42	0.48
1:A:326:PRO:HB3	1:A:493:LEU:HB2	1.95	0.47
1:A:1833:LEU:O	1:A:1834:HIS:ND1	2.47	0.47
1:A:572:ILE:HG21	1:A:583:LEU:HD21	1.96	0.47
1:A:2291:VAL:HB	1:A:2303:MET:HB3	1.97	0.47
1:A:2520:GLY:HA3	1:A:2526:TYR:OH	2.14	0.47
1:A:837:ASP:OD2	1:A:839:SER:OG	2.28	0.47
1:A:1182:HIS:CE1	1:A:1282:SER:HB2	2.50	0.47
1:A:1479:ARG:HH22	1:A:1577:SER:HB3	1.78	0.47
1:A:1553:HIS:NE2	1:A:1645:GLU:OE1	2.41	0.47
1:A:2867:ASN:OD1	1:A:2870:ASP:N	2.44	0.47
1:A:3207:TRP:CD2	1:A:3209:ARG:HD3	2.49	0.47
1:A:846:LEU:HD23	1:A:849:LEU:HD13	1.96	0.47
1:A:1802:ARG:NE	1:A:1807:HIS:H	2.13	0.47
1:A:2651:LEU:HD11	1:A:2662:LEU:HB2	1.97	0.47
1:A:599:TYR:OH	1:A:633:GLU:OE2	2.27	0.47
1:A:2484:THR:HG22	1:A:2499:LEU:HA	1.96	0.47
1:A:2879:GLN:OE1	1:A:2882:GLU:OE1	2.33	0.47
1:A:984:PHE:HE2	1:A:1121:PHE:HA	1.80	0.47
1:A:2966:LYS:HB2	1:A:2966:LYS:HE2	1.74	0.47
1:A:1829:ASP:HB3	1:A:1833:LEU:HD13	1.96	0.47
1:A:2795:ARG:NH2	1:A:2821:PHE:O	2.48	0.47
1:A:2957:LEU:HD23	1:A:2976:LEU:HD13	1.96	0.47
1:A:3118:LEU:HD21	1:A:3185:VAL:HG21	1.97	0.47
1:A:2207:GLU:OE1	1:A:2207:GLU:N	2.39	0.46
1:A:3123:ILE:HG23	1:A:3211:GLY:HA2	1.97	0.46
1:A:854:ILE:HG23	1:A:879:THR:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2543:LEU:HD21	1:A:2553:ILE:HD11	1.97	0.46
1:A:2914:THR:H	1:A:2917:SER:HB3	1.79	0.46
1:A:869:LYS:HE2	1:A:869:LYS:HB2	1.63	0.46
1:A:886:ILE:HD13	1:A:886:ILE:HA	1.82	0.46
1:A:265:ASN:OD1	1:A:265:ASN:N	2.49	0.46
1:A:1879:ARG:O	1:A:1883:GLN:HG3	2.16	0.46
1:A:3061:MET:HE3	1:A:3201:THR:HG21	1.97	0.46
1:A:329:ILE:HD12	1:A:558:THR:HG21	1.98	0.46
1:A:2364:LEU:HD12	1:A:2371:HIS:CE1	2.49	0.46
1:A:2493:ARG:HH21	1:A:2513:HIS:HB3	1.80	0.46
1:A:2742:SER:HB3	1:A:2745:GLN:HG3	1.97	0.46
1:A:3097:GLU:OE1	1:A:3097:GLU:N	2.47	0.46
1:A:654:ARG:HD2	1:A:656:HIS:CE1	2.51	0.46
1:A:2283:ASP:OD1	1:A:2285:SER:OG	2.31	0.46
1:A:966:ASN:O	1:A:1144:ARG:NH2	2.49	0.46
1:A:2102:ARG:HG3	1:A:2191:ARG:NH1	2.31	0.46
1:A:3068:ARG:NH1	1:A:3079:ASP:OD1	2.42	0.46
1:A:773:VAL:HA	1:A:776:GLU:HG3	1.98	0.46
1:A:2364:LEU:HB2	1:A:2404:PRO:HA	1.98	0.46
1:A:2401:ASN:O	1:A:2403:GLN:HG3	2.16	0.46
1:A:1558:ASN:O	1:A:1562:ILE:HG12	2.15	0.46
1:A:2993:GLU:N	1:A:2993:GLU:OE1	2.48	0.46
1:A:782:ARG:HH21	1:A:1214:ASP:HB2	1.80	0.45
1:A:2755:LYS:HD3	1:A:2818:ARG:HB3	1.98	0.45
1:A:2791:ARG:HH22	1:A:2800:ARG:NH2	2.08	0.45
1:A:754:ILE:H	1:A:754:ILE:HG12	1.54	0.45
1:A:1610:ALA:O	1:A:1614:ILE:HG13	2.16	0.45
1:A:2739:MET:HB2	1:A:2739:MET:HE3	1.75	0.45
1:A:2952:THR:HG23	1:A:2956:ASP:H	1.81	0.45
1:A:2354:ARG:HG3	1:A:2355:ASP:CG	2.41	0.45
1:A:1880:LEU:HD21	1:A:1963:VAL:HG11	1.99	0.45
1:A:1386:ARG:HD2	1:A:1386:ARG:HA	1.68	0.45
1:A:2913:VAL:HG22	1:A:2976:LEU:HG	1.98	0.45
1:A:568:VAL:O	1:A:572:ILE:HG12	2.17	0.45
1:A:1212:ASN:ND2	1:A:1214:ASP:OD1	2.46	0.45
1:A:277:LEU:HD12	1:A:294:ILE:HG23	1.97	0.45
1:A:575:GLN:HB3	1:A:623:LYS:HE3	1.98	0.45
1:A:342:GLU:OE1	1:A:342:GLU:N	2.43	0.44
1:A:580:ASN:HD22	1:A:800:LYS:HD2	1.82	0.44
1:A:2384:LYS:HD2	1:A:2393:ILE:HG21	2.00	0.44
1:A:2415:GLY:N	1:A:2429:ALA:O	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1773:THR:O	1:A:1777:ARG:HG3	2.17	0.44
1:A:2379:THR:OG1	1:A:2423:ASP:OD2	2.29	0.44
1:A:305:TYR:CD1	1:A:774:LEU:HG	2.52	0.44
1:A:2364:LEU:HD21	1:A:2402:VAL:HG13	1.99	0.44
1:A:1559:GLN:O	1:A:1563:THR:OG1	2.29	0.44
1:A:1858:PRO:HG3	1:A:1943:ARG:NH2	2.33	0.44
1:A:288:GLU:HG2	1:A:292:LYS:HE3	2.00	0.44
1:A:793:TYR:CE1	1:A:806:PRO:HB3	2.53	0.44
1:A:3131:ASN:HD21	1:A:3178:ARG:HH22	1.64	0.44
1:A:3146:ARG:HE	1:A:3146:ARG:HB3	1.47	0.44
1:A:599:TYR:HB2	1:A:605:ILE:HD11	1.99	0.44
1:A:1874:VAL:HG13	1:A:1911:ILE:HD13	1.98	0.44
1:A:2368:SER:HB2	1:A:2371:HIS:CE1	2.53	0.44
1:A:2619:ASP:OD1	1:A:2619:ASP:C	2.60	0.44
1:A:3201:THR:C	1:A:3202:LEU:HD23	2.43	0.44
1:A:2303:MET:HG2	1:A:2305:ILE:HD11	2.00	0.44
1:A:2312:THR:HG23	1:A:2331:THR:HB	1.99	0.44
1:A:1182:HIS:HE2	1:A:1292:SER:HG	1.62	0.43
1:A:2678:LEU:HD12	1:A:2678:LEU:HA	1.79	0.43
1:A:3123:ILE:HD12	1:A:3124:LEU:N	2.32	0.43
1:A:1854:LEU:HD23	1:A:1854:LEU:HA	1.87	0.43
1:A:2270:SER:HA	1:A:2314:VAL:HB	2.00	0.43
1:A:2461:ALA:HA	1:A:2464:ASP:OD2	2.18	0.43
1:A:3139:ILE:HD12	1:A:3139:ILE:HA	1.84	0.43
1:A:2106:HIS:HE1	1:A:2139:LYS:HE3	1.84	0.43
1:A:3065:LEU:HD23	1:A:3156:ARG:HB2	1.99	0.43
1:A:255:TYR:CZ	1:A:261:LYS:HD3	2.53	0.43
1:A:1340:LEU:HD12	1:A:1340:LEU:HA	1.90	0.43
1:A:3013:MET:HE2	1:A:3037:PHE:HE1	1.83	0.43
1:A:1614:ILE:O	1:A:1618:ILE:HG13	2.19	0.43
1:A:1797:PHE:CZ	1:A:1810:VAL:HG21	2.53	0.43
1:A:2660:GLN:HA	1:A:2660:GLN:OE1	2.19	0.43
1:A:2792:ILE:HD12	1:A:2821:PHE:CE2	2.52	0.43
1:A:2836:GLU:O	1:A:2839:PRO:HD2	2.18	0.43
1:A:349:VAL:HG21	1:A:490:VAL:HG21	2.01	0.43
1:A:1155:PHE:HB2	1:A:1158:GLN:HG2	1.99	0.43
1:A:2850:ASN:HD21	1:A:2852:ALA:HB3	1.84	0.43
1:A:3177:LEU:HD23	1:A:3177:LEU:HA	1.82	0.43
1:A:2577:ALA:HA	1:A:2582:SER:HA	2.00	0.43
1:A:2647:VAL:O	1:A:2648:MET:C	2.61	0.43
1:A:3107:ARG:HE	1:A:3107:ARG:HB3	1.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2191:ARG:H	1:A:2191:ARG:HE	1.67	0.43
1:A:2932:LEU:HD22	1:A:2989:SER:HB2	2.01	0.43
1:A:3183:PHE:HB3	1:A:3202:LEU:HD13	2.01	0.43
1:A:760:ILE:O	1:A:764:MET:HG3	2.19	0.42
1:A:907:MET:HE2	1:A:907:MET:HB3	1.79	0.42
1:A:1736:GLN:O	1:A:1740:ILE:HG12	2.19	0.42
1:A:337:LEU:O	1:A:505:ARG:NH2	2.45	0.42
1:A:1716:LEU:HD23	1:A:1716:LEU:HA	1.88	0.42
1:A:2029:ALA:O	1:A:2032:ILE:HG12	2.19	0.42
1:A:1678:GLU:C	1:A:1678:GLU:OE1	2.63	0.42
1:A:2783:LEU:HD12	1:A:2783:LEU:HA	1.68	0.42
1:A:2036:VAL:HG13	1:A:2045:GLN:HB3	2.01	0.42
1:A:2230:ILE:HD11	1:A:2295:THR:HG21	2.00	0.42
1:A:2603:GLN:OE1	1:A:2604:PRO:HD2	2.19	0.42
1:A:903:LEU:O	1:A:907:MET:HG3	2.20	0.42
1:A:1618:ILE:C	1:A:1618:ILE:HD12	2.45	0.42
1:A:1817:ASP:HB3	1:A:1822:ARG:HB2	2.00	0.42
1:A:2393:ILE:HA	1:A:2399:ASN:HB2	2.01	0.42
1:A:2432:ARG:N	1:A:2435:GLY:O	2.44	0.42
1:A:3135:TYR:CD2	1:A:3143:VAL:HG21	2.54	0.42
1:A:3207:TRP:CE2	1:A:3209:ARG:HD3	2.53	0.42
1:A:2646:GLN:CB	1:A:2648:MET:HE1	2.50	0.42
1:A:465:LEU:HD23	1:A:465:LEU:HA	1.87	0.42
1:A:500:GLN:HG2	1:A:501:PHE:CD2	2.55	0.42
1:A:908:LEU:HD23	1:A:908:LEU:HA	1.89	0.42
1:A:2041:GLU:HB3	1:A:2043:HIS:CE1	2.55	0.42
1:A:1315:ASN:HB2	1:A:1318:ASN:OD1	2.20	0.42
1:A:1990:MET:HE2	1:A:1990:MET:HB2	1.83	0.42
1:A:3127:PRO:HD3	1:A:3213:SER:HB2	2.02	0.42
1:A:516:SER:O	1:A:522:ASN:ND2	2.52	0.41
1:A:617:ASP:HA	1:A:620:ILE:HG22	2.02	0.41
1:A:976:SER:O	1:A:980:GLU:HG2	2.19	0.41
1:A:1307:VAL:HG12	1:A:1310:ARG:HH21	1.85	0.41
1:A:1615:GLU:O	1:A:1619:GLN:HB3	2.19	0.41
1:A:1928:ARG:HG3	1:A:1931:SER:HB2	2.02	0.41
1:A:2091:LEU:HD23	1:A:2091:LEU:HA	1.94	0.41
1:A:469:ILE:HD13	1:A:836:LYS:HG2	2.02	0.41
1:A:1153:VAL:HG22	1:A:1184:LEU:HD13	2.00	0.41
1:A:1801:PRO:HG2	1:A:1833:LEU:CD2	2.50	0.41
1:A:2824:VAL:HG21	1:A:2848:PHE:CG	2.55	0.41
1:A:1366:ALA:O	1:A:1369:THR:OG1	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1695:ILE:HG21	1:A:1740:ILE:HD12	2.02	0.41
1:A:2460:ASP:OD1	1:A:2461:ALA:N	2.53	0.41
1:A:2879:GLN:OE1	1:A:2879:GLN:HA	2.19	0.41
1:A:3037:PHE:O	1:A:3077:THR:HG21	2.20	0.41
1:A:595:GLY:HA3	1:A:625:LEU:HD11	2.03	0.41
1:A:966:ASN:HB2	1:A:1255:PRO:HB3	2.02	0.41
1:A:397:TYR:O	1:A:400:ASN:N	2.52	0.41
1:A:2174:ASN:OD1	1:A:2175:TRP:N	2.53	0.41
1:A:2820:PHE:HE2	1:A:2872:VAL:HG21	1.84	0.41
1:A:2963:VAL:HB	1:A:2970:GLN:O	2.20	0.41
1:A:1848:GLN:O	1:A:1852:THR:HG22	2.20	0.41
1:A:2080:LYS:HB2	1:A:2095:GLU:HG2	2.02	0.41
1:A:1408:ASN:HD21	1:A:1410:LYS:HE3	1.86	0.41
1:A:2751:HIS:CD2	1:A:2814:ARG:HG2	2.55	0.41
1:A:478:ASN:O	1:A:482:THR:HG22	2.21	0.41
1:A:1648:MET:HE3	1:A:1648:MET:HB2	1.76	0.41
1:A:2418:ARG:HB3	1:A:2418:ARG:NH1	2.36	0.41
1:A:3126:THR:HG23	1:A:3180:GLY:H	1.86	0.41
1:A:378:ASN:ND2	1:A:1646:SER:OG	2.45	0.41
1:A:565:SER:O	1:A:569:ILE:HG22	2.20	0.41
1:A:2877:ARG:NH1	1:A:2880:LYS:HD2	2.36	0.41
1:A:471:LEU:HD23	1:A:471:LEU:HA	1.86	0.40
1:A:1760:MET:SD	1:A:2003:LEU:HD11	2.61	0.40
1:A:3014:GLN:HE22	1:A:3016:ARG:HH12	1.69	0.40
1:A:396:LYS:HA	1:A:396:LYS:HD3	1.65	0.40
1:A:1327:VAL:HG23	1:A:1372:LEU:HD22	2.03	0.40
1:A:2546:ASP:C	1:A:2548:ASP:H	2.29	0.40
1:A:2698:ASN:OD1	1:A:2698:ASN:N	2.54	0.40
1:A:949:LYS:NZ	1:A:951:ASN:OD1	2.54	0.40
1:A:1690:LYS:NZ	1:A:1694:ASP:OD2	2.52	0.40
1:A:2268:THR:HA	1:A:2312:THR:HB	2.03	0.40
1:A:3011:PRO:HB3	1:A:3081:TRP:CE2	2.56	0.40
1:A:329:ILE:CD1	1:A:558:THR:HG21	2.51	0.40
1:A:400:ASN:OD1	1:A:400:ASN:C	2.64	0.40
1:A:548:LEU:HD23	1:A:548:LEU:HA	1.85	0.40
1:A:1136:LYS:HA	1:A:1147:ILE:HD13	2.03	0.40
1:A:1594:LEU:HD13	1:A:1614:ILE:HD11	2.03	0.40
1:A:2682:LYS:HE2	1:A:2682:LYS:HB3	1.80	0.40
1:A:258:LEU:HD23	1:A:258:LEU:HA	1.91	0.40
1:A:1210:HIS:CD2	1:A:1237:PRO:HG2	2.57	0.40
1:A:1906:THR:O	1:A:1910:MET:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1959:LEU:HD23	1:A:1959:LEU:HA	1.93	0.40
1:A:2484:THR:HG21	1:A:2499:LEU:HD22	2.04	0.40
1:A:2782:LYS:HG3	1:A:2874:GLU:OE1	2.22	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	2791/3229 (86%)	2708 (97%)	82 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2187	SER

5.3.2 Protein sidechains [i](#)

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	2490/2885 (86%)	2423 (97%)	67 (3%)	39	74

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

Mol	Chain	Res	Type
1	A	453	VAL
1	A	455	GLU
1	A	495	LEU
1	A	533	ARG
1	A	558	THR
1	A	569	ILE
1	A	575	GLN
1	A	586	LEU
1	A	606	ASP
1	A	700	ASN
1	A	754	ILE
1	A	774	LEU
1	A	804	LEU
1	A	811	VAL
1	A	854	ILE
1	A	860	PHE
1	A	862	GLN
1	A	886	ILE
1	A	1143	SER
1	A	1151	ASP
1	A	1153	VAL
1	A	1212	ASN
1	A	1214	ASP
1	A	1233	SER
1	A	1235	SER
1	A	1261	VAL
1	A	1266	MET
1	A	1328	SER
1	A	1336	SER
1	A	1578	THR
1	A	1623	THR
1	A	1631	LEU
1	A	1635	ILE
1	A	1670	THR
1	A	1689	VAL
1	A	1749	ILE
1	A	1806	ARG
1	A	1850	LEU
1	A	2002	SER
1	A	2032	ILE
1	A	2119	VAL
1	A	2153	ASP
1	A	2221	LEU

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Mol	Chain	Res	Type
1	A	2302	VAL
1	A	2367	ASN
1	A	2552	THR
1	A	2629	SER
1	A	2642	MET
1	A	2708	SER
1	A	2753	ILE
1	A	2757	ASP
1	A	2781	LEU
1	A	2796	SER
1	A	2910	THR
1	A	2912	THR
1	A	2913	VAL
1	A	2915	THR
1	A	2947	THR
1	A	2952	THR
1	A	2963	VAL
1	A	2968	VAL
1	A	2984	GLU
1	A	2994	ILE
1	A	3024	ASP
1	A	3108	SER
1	A	3165	ILE
1	A	3205	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	GLN
1	A	293	ASN
1	A	376	GLN
1	A	388	ASN
1	A	524	HIS
1	A	551	HIS
1	A	602	ASN
1	A	656	HIS
1	A	872	GLN
1	A	948	HIS
1	A	972	ASN
1	A	1242	ASN
1	A	1278	GLN
1	A	1350	GLN

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Mol	Chain	Res	Type
1	A	1358	HIS
1	A	1463	GLN
1	A	1514	ASN
1	A	1558	ASN
1	A	1636	ASN
1	A	1765	GLN
1	A	1796	HIS
1	A	1901	GLN
1	A	1912	GLN
1	A	2106	HIS
1	A	2164	GLN
1	A	2166	ASN
1	A	2200	GLN
1	A	2646	GLN
1	A	3014	GLN
1	A	3039	ASN
1	A	3067	GLN
1	A	3168	ASN
1	A	3223	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

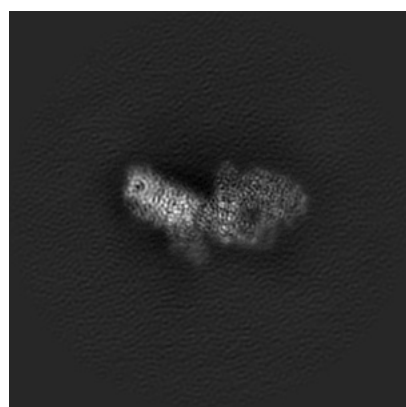
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19988. These allow visual inspection of the internal detail of the map and identification of artifacts.

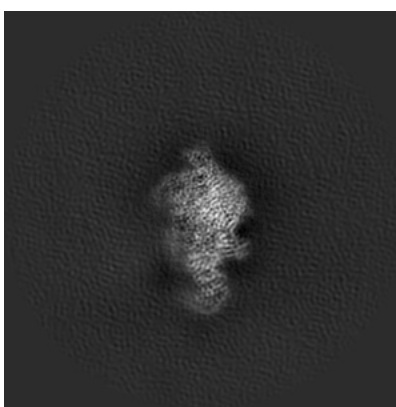
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

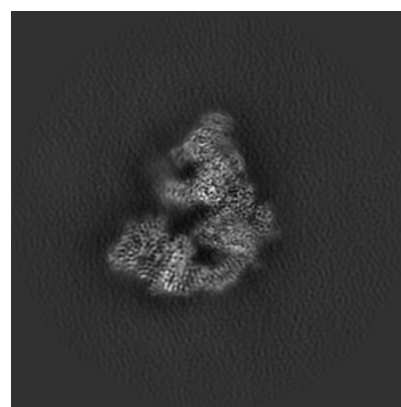
6.1.1 Primary map



X



Y

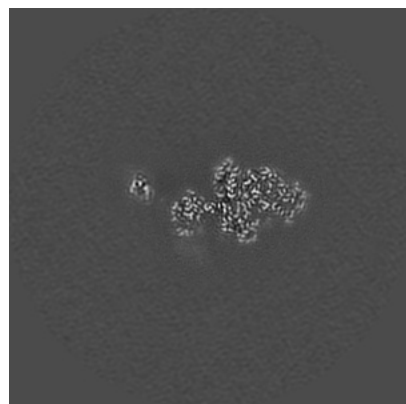


Z

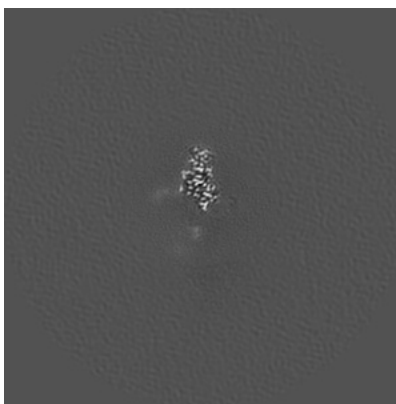
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

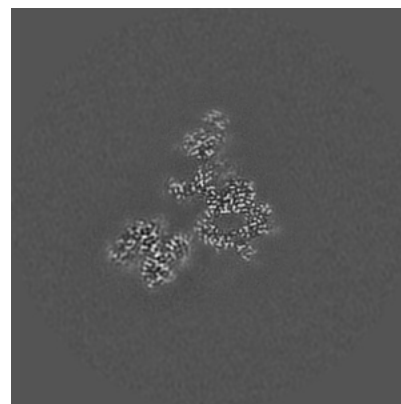
6.2.1 Primary map



X Index: 200



Y Index: 200

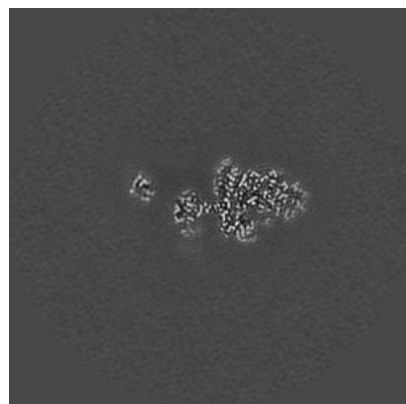


Z Index: 200

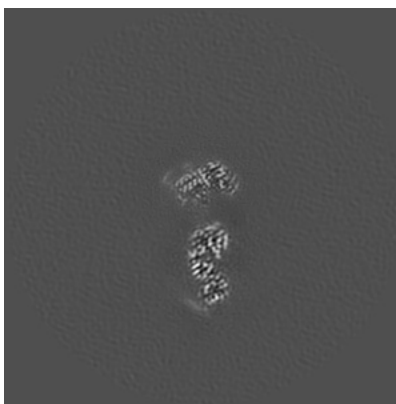
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

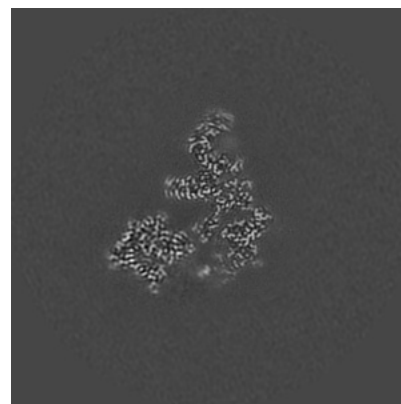
6.3.1 Primary map



X Index: 198



Y Index: 161

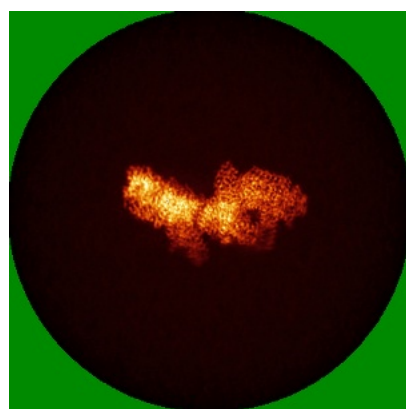


Z Index: 207

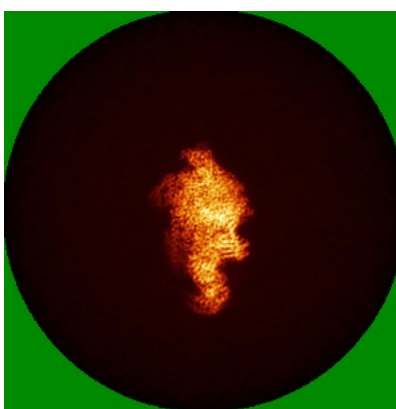
The images above show the largest variance slices of the map in three orthogonal directions.

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

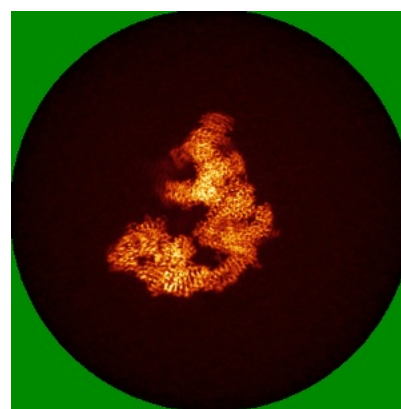
6.4.1 Primary map



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

This section was not generated.

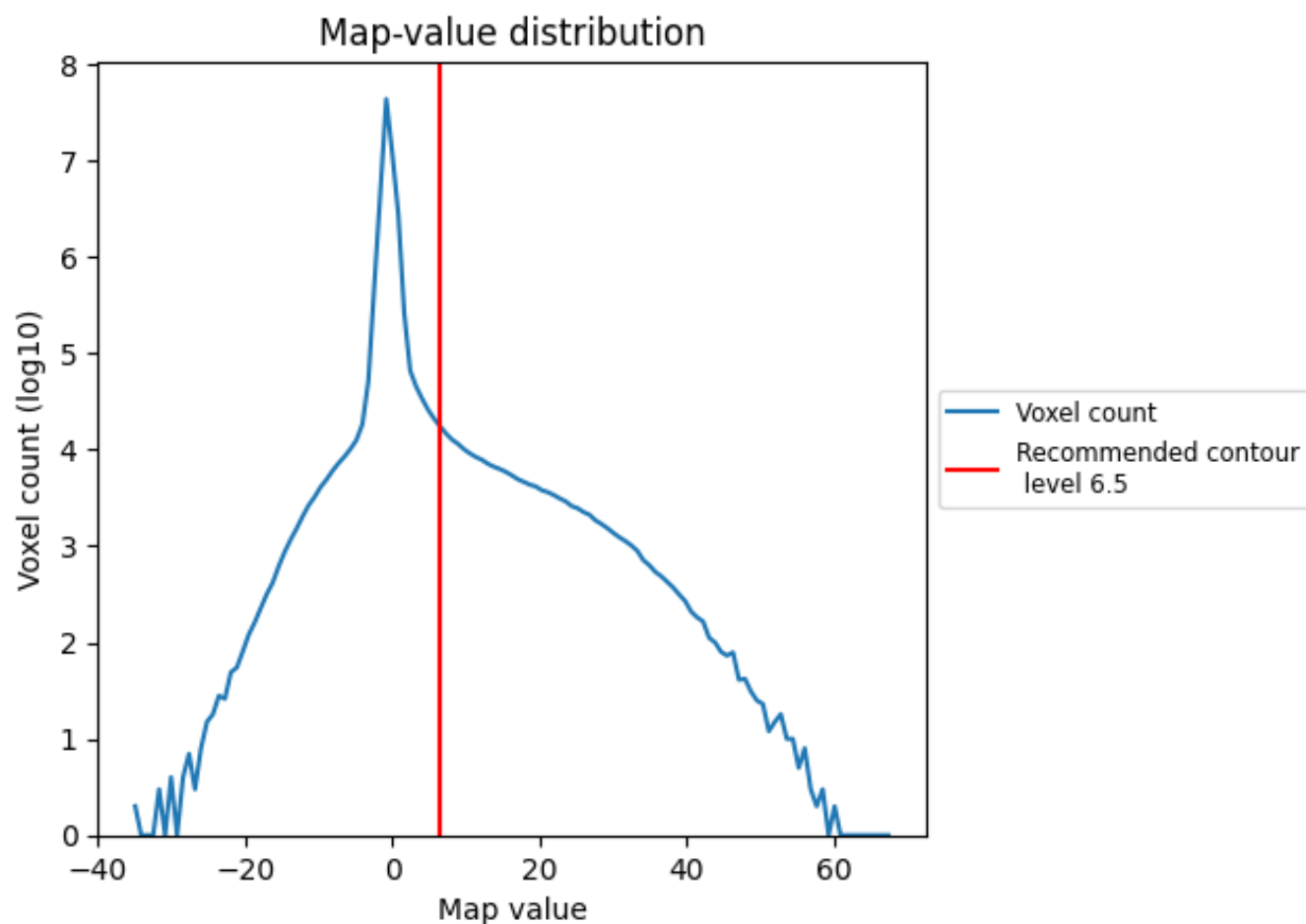
6.6 Mask visualisation

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

7 Map analysis [i](#)

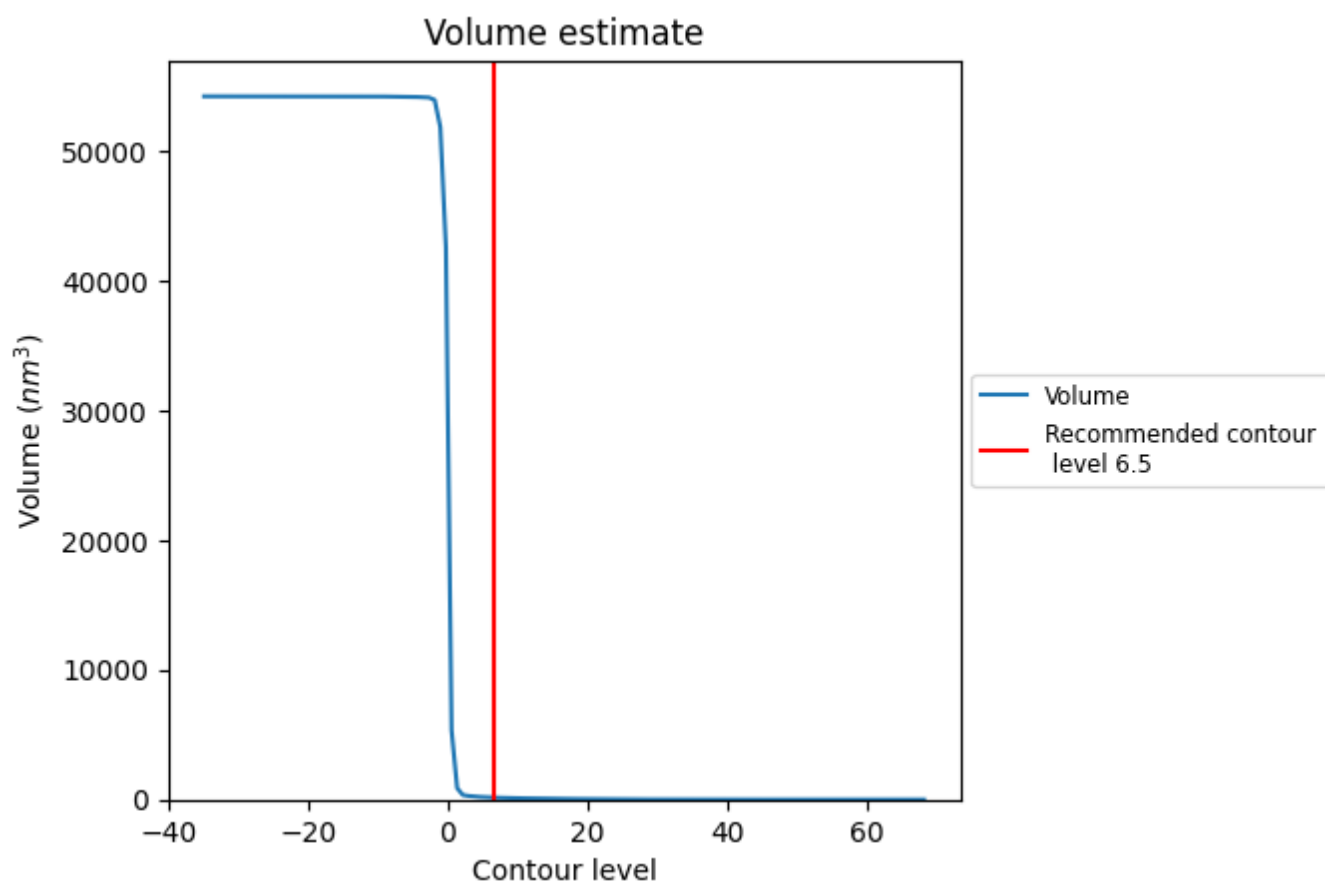
This section contains the results of statistical analysis of the map.

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.

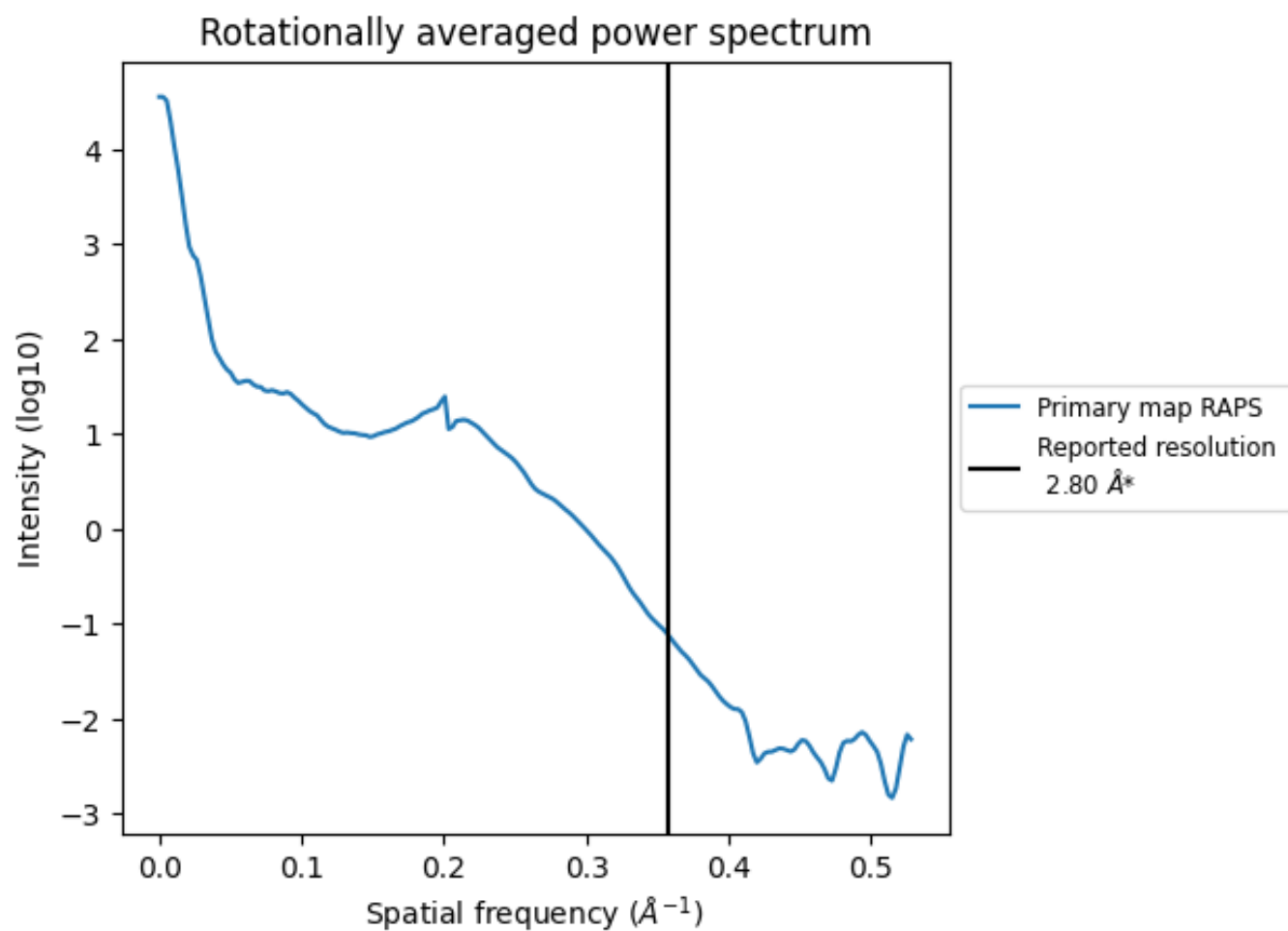
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 156 nm^3 ; this corresponds to an approximate mass of 141 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 0.357 Å⁻¹

8 Fourier-Shell correlation

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

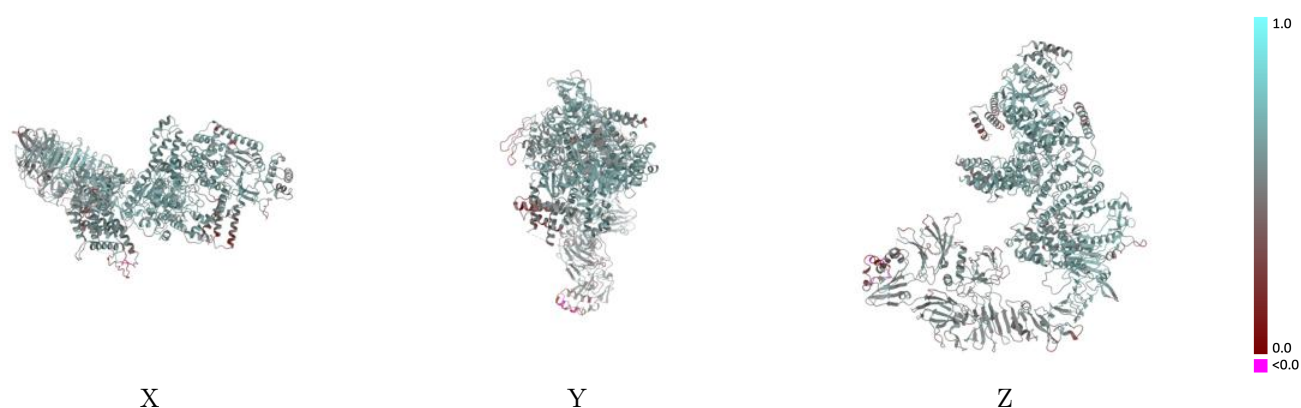
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19988 and PDB model 9EUW. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

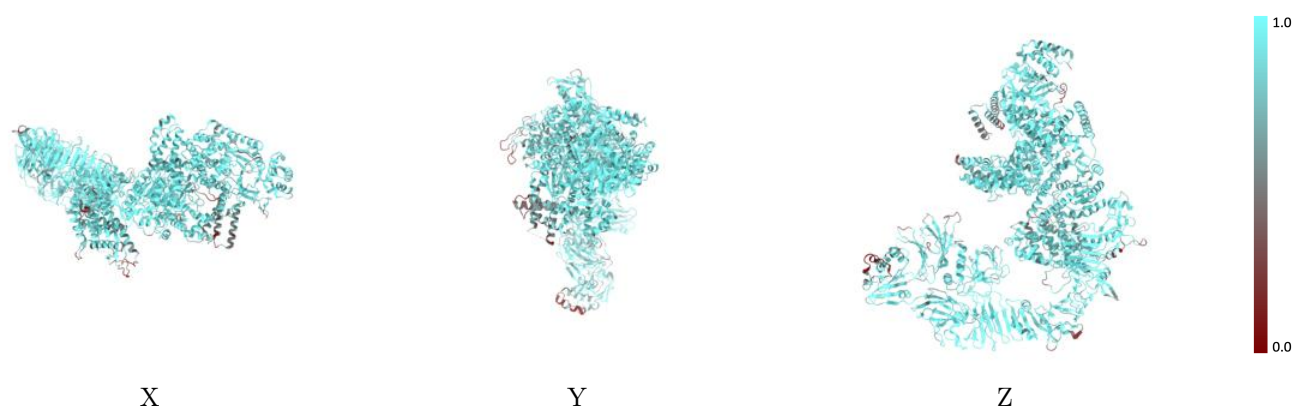
This section was not generated.

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



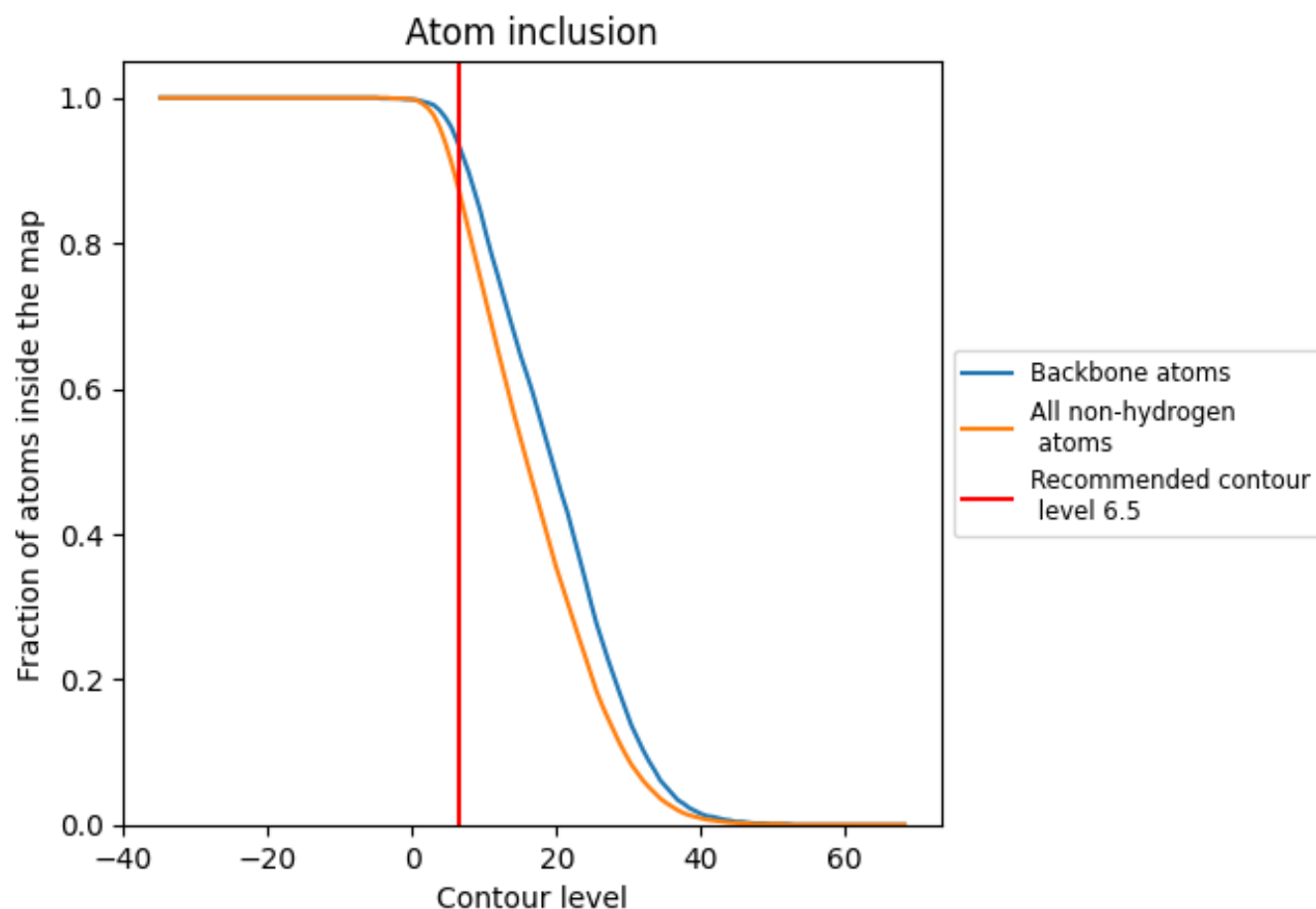
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 87% 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 (6.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8720	0.5430
A	0.8720	0.5430

