Full wwPDB EM Validation Report ⓘ

Jun 8, 2024 – 09:02 AM EDT

PDB ID	:	8EHQ
EMDB ID	:	EMD-28149
Title	:	Mycobacterium tuberculosis paused transcription complex with Bacillus subtilis NusG
Authors	:	Vishwakarma, R.K.; Murakami, K.S.
Deposited on	:	2022-09-14
Resolution	:	3.00 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:

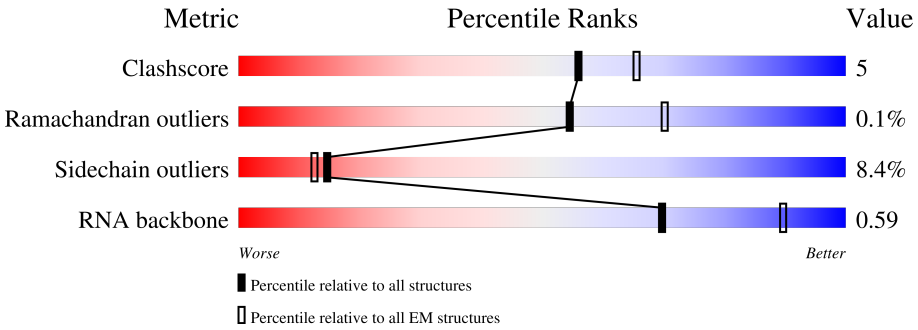
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	347	54% 10% • 35%
1	B	347	56% 11% • 32%
2	C	1178	79% 15% • 5%
3	D	1316	78% 17% • •
4	E	110	64% 11% • 25%
5	G	177	• 46% 14% • 38%
6	T	40	5% 55% 40% 5%

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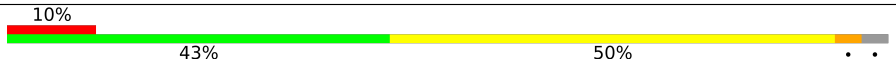
Mol	Chain	Length	Quality of chain
7	N	40	
8	R	30	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 25828 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-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	226	Total	C	N	O	S	0	0
			1724	1085	297	339	3		
1	B	237	Total	C	N	O	S	0	0
			1765	1115	301	346	3		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1122	Total	C	N	O	S	0	0
			8689	5440	1526	1684	39		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1273	Total	C	N	O	S	0	0
			9953	6229	1811	1872	41		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	83	Total	C	N	O	0	0
			649	414	108	127		

- Molecule 5 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	110	Total	C	N	O	S	1	0
			878	563	147	165	3		

- Molecule 6 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	38	Total 772	C 365	N 142	O 227	P 38	0	0

- Molecule 7 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	38	Total 770	C 366	N 132	O 234	P 38	0	0

- Molecule 8 is a RNA chain called RNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	29	Total 625	C 278	N 116	O 202	P 29	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	D	1	Total 1	Mg 1	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

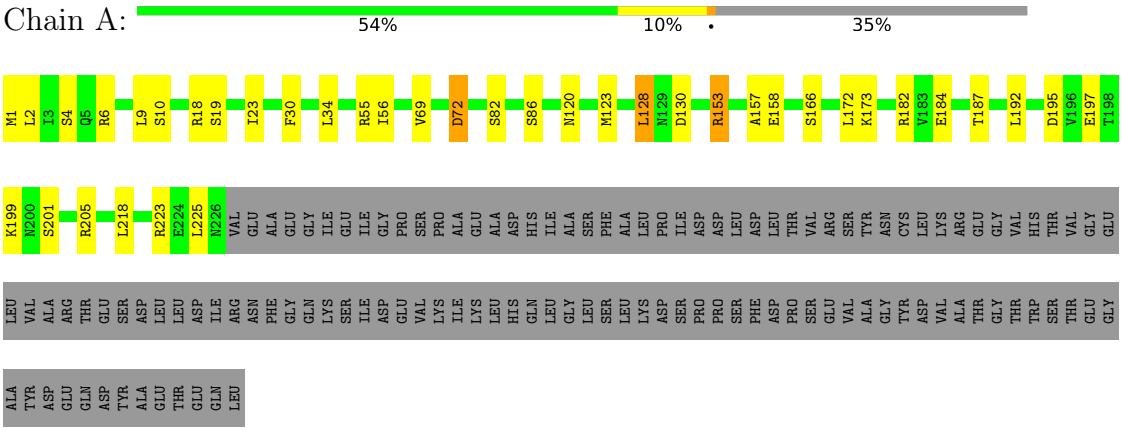
Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total 2	Zn 2	0

3 Residue-property plots (i)

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.

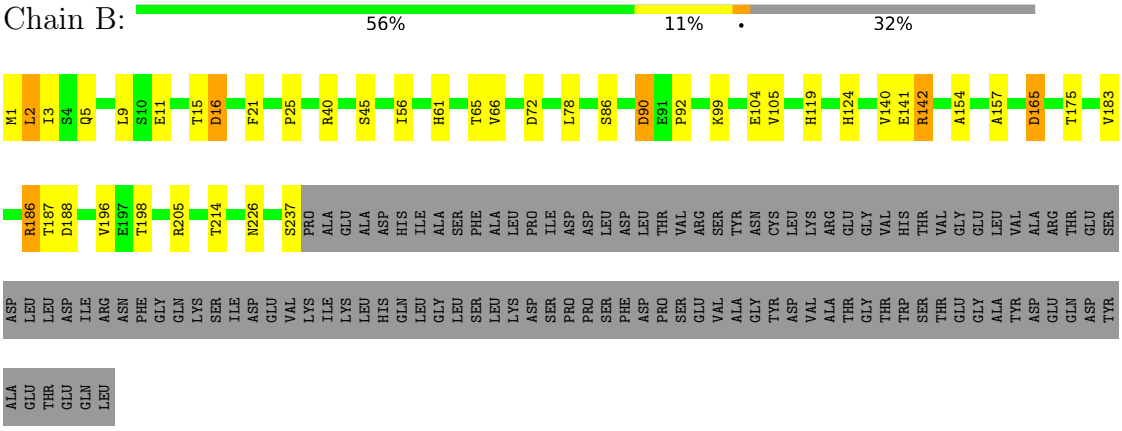
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



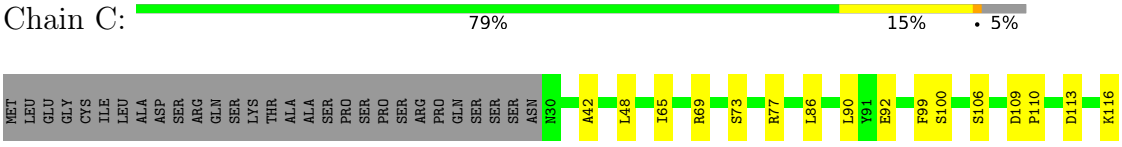
• Molecule 1: DNA-directed RNA polymerase subunit alpha

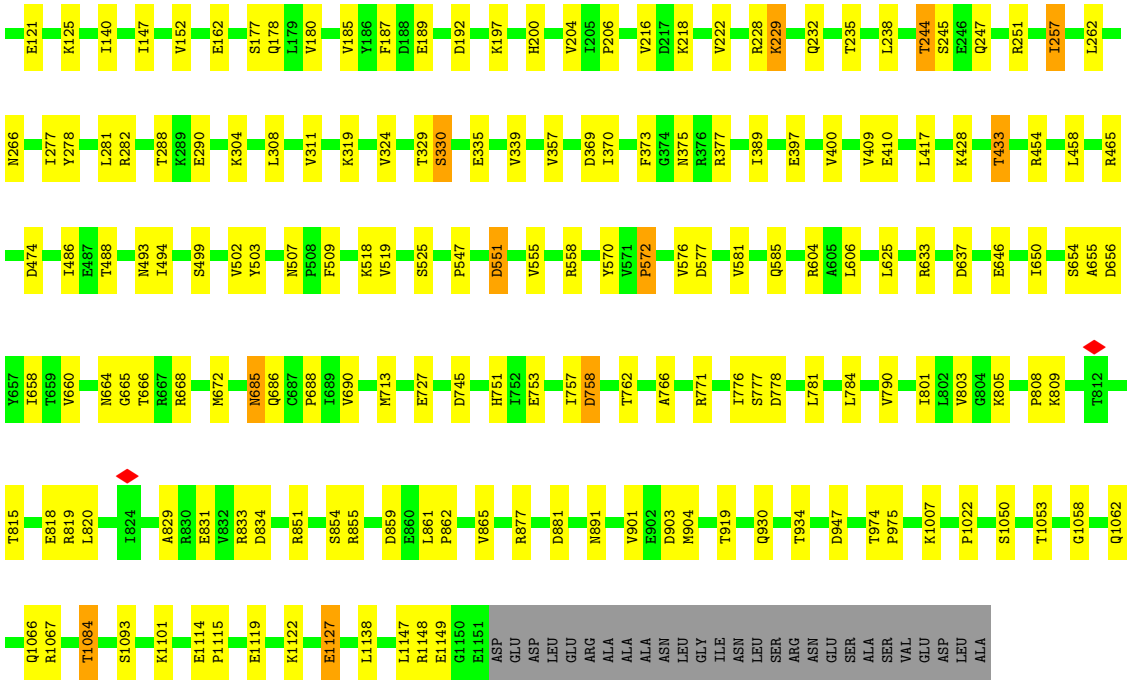
Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta

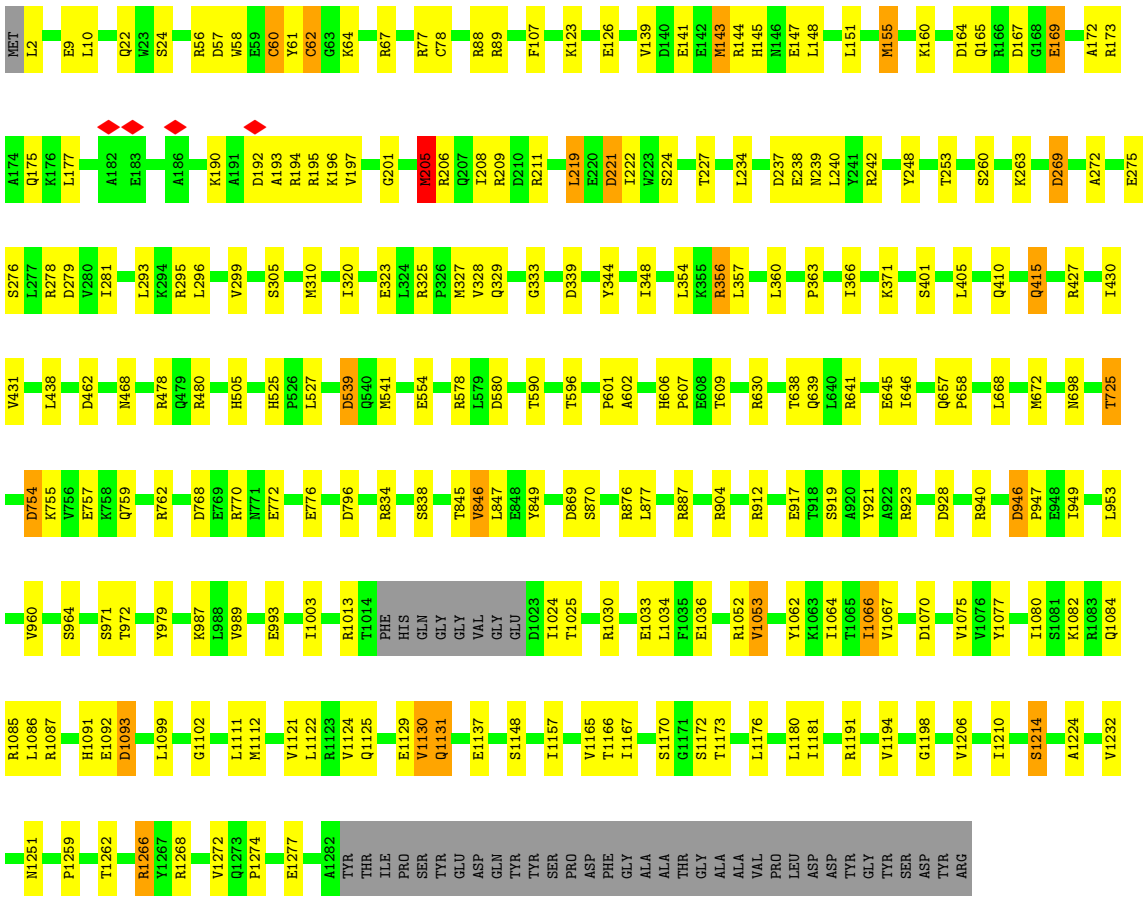
Chain C:





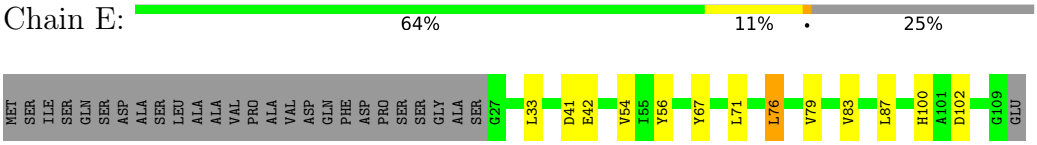
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:



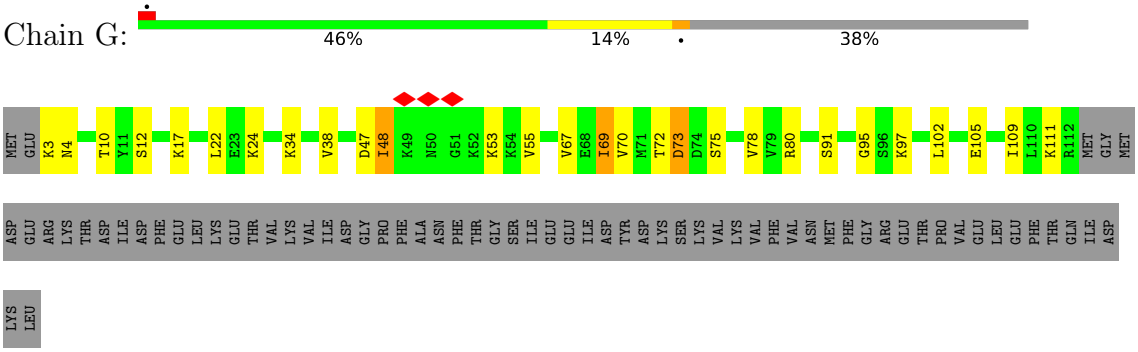
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



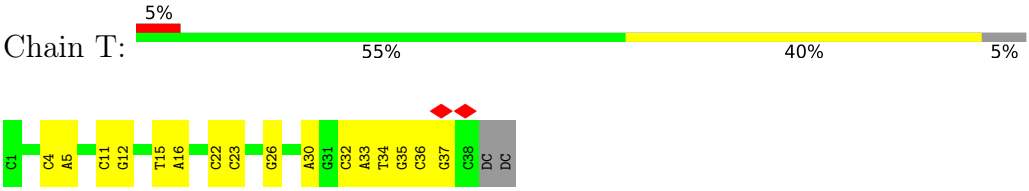
• Molecule 5: Transcription termination/antitermination protein NusG

Chain G:



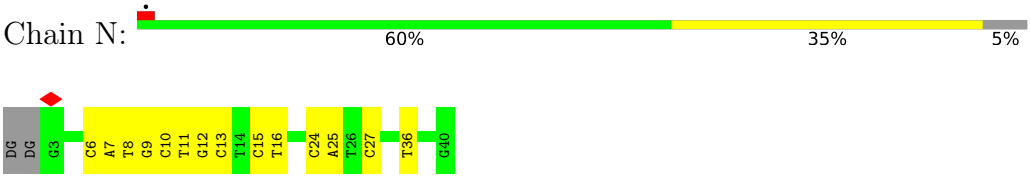
• Molecule 6: DNA (38-MER)

Chain T:



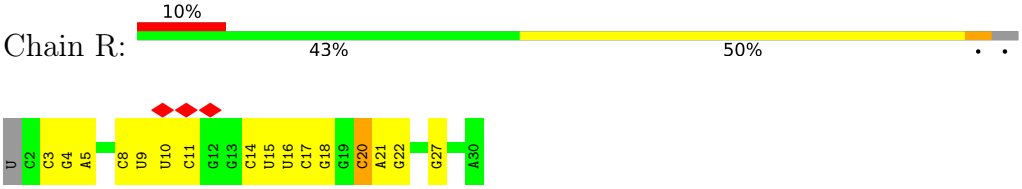
• Molecule 7: DNA (38-MER)

Chain N:



• Molecule 8: RNA (29-MER)

Chain R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110849	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 ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.101	Depositor
Minimum map value	-0.718	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.238	Depositor
Map size (Å)	348.0, 348.0, 348.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.27	0/1750	0.53	0/2380
1	B	0.26	0/1792	0.51	0/2442
2	C	0.28	0/8848	0.53	1/11996 (0.0%)
3	D	0.27	0/10119	0.54	2/13679 (0.0%)
4	E	0.28	0/662	0.48	0/901
5	G	0.26	0/896	0.45	0/1209
6	T	0.54	0/864	0.87	0/1329
7	N	0.51	0/859	0.93	0/1322
8	R	0.25	0/699	0.75	0/1089
All	All	0.30	0/26489	0.57	3/36347 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	572	PRO	CA-N-CD	-9.82	97.75	111.50
3	D	601	PRO	CA-N-CD	-6.06	103.02	111.50
3	D	205	MET	CA-CB-CG	5.05	121.89	113.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1724	0	1768	14	0
1	B	1765	0	1794	19	0
2	C	8689	0	8621	87	0
3	D	9953	0	10020	109	0
4	E	649	0	645	5	0
5	G	878	0	896	12	0
6	T	772	0	425	11	0
7	N	770	0	429	12	0
8	R	625	0	314	13	0
9	D	1	0	0	0	0
10	D	2	0	0	0	0
All	All	25828	0	24912	262	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 5.

All (262) 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)
3:D:194:ARG:HH21	3:D:197:VAL:HG21	1.45	0.81
3:D:1194:VAL:HA	3:D:1198:GLY:HA2	1.68	0.76
3:D:917:GLU:HA	3:D:921:TYR:HD2	1.49	0.75
6:T:30:DA:H61	7:N:11:DT:H3	1.34	0.75
1:B:3:ILE:HG22	1:B:5:GLN:H	1.55	0.71
8:R:20:C:O2	8:R:21:A:N6	2.25	0.70
3:D:238:GLU:OE2	3:D:242:ARG:NH1	2.25	0.69
3:D:1167:ILE:HD11	3:D:1181:ILE:HD11	1.75	0.69
3:D:1251:ASN:HD22	3:D:1259:PRO:HD3	1.56	0.69
3:D:1124:VAL:HG12	3:D:1125:GLN:HG3	1.75	0.68
2:C:465:ARG:NH2	8:R:27:G:OP2	2.26	0.68
2:C:1058:GLY:O	2:C:1062:GLN:NE2	2.26	0.68
7:N:15:DC:H2"	7:N:16:DT:H5'	1.77	0.67
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.76	0.67
3:D:123:LYS:NZ	7:N:36:DT:OP2	2.27	0.67
1:A:18:ARG:HG2	1:A:197:GLU:HG3	1.76	0.66
3:D:155:MET:HB3	3:D:219:LEU:HD11	1.78	0.66
3:D:62:CYS:HB3	3:D:78:CYS:SG	2.35	0.66
2:C:558:ARG:HA	2:C:572:PRO:HA	1.79	0.65
2:C:572:PRO:HD2	2:C:572:PRO:O	1.95	0.65
7:N:24:DC:H1'	7:N:25:DA:C8	2.32	0.65
3:D:64:LYS:HB2	3:D:77:ARG:HH21	1.62	0.64
3:D:641:ARG:HA	3:D:657:GLN:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:877:LEU:HD22	3:D:1157:ILE:HD13	1.78	0.64
2:C:369:ASP:O	2:C:375:ASN:ND2	2.31	0.64
2:C:86:LEU:HD21	2:C:389:ILE:HD13	1.80	0.63
2:C:278:TYR:OH	2:C:282:ARG:NH1	2.32	0.63
2:C:1122:LYS:NZ	2:C:1149:GLU:OE2	2.33	0.61
5:G:72:THR:HG23	5:G:75:SER:H	1.65	0.61
3:D:1093:ASP:N	3:D:1093:ASP:OD1	2.32	0.61
2:C:1119:GLU:OE2	3:D:89:ARG:NH2	2.26	0.61
3:D:1003:ILE:HD12	3:D:1157:ILE:HD12	1.82	0.60
2:C:178:GLN:NE2	2:C:458:LEU:O	2.35	0.59
6:T:26:DG:H1	7:N:16:DT:H3	1.51	0.59
3:D:757:GLU:OE2	3:D:770:ARG:NH1	2.34	0.59
2:C:400:VAL:HG23	2:C:417:LEU:HB3	1.85	0.58
3:D:165:GLN:O	3:D:169:GLU:HG2	2.03	0.58
3:D:946:ASP:OD2	3:D:947:PRO:HD3	2.04	0.58
1:A:69:VAL:HG22	1:A:128:LEU:HD23	1.85	0.58
3:D:638:THR:HG22	3:D:639:GLN:HG2	1.85	0.58
3:D:190:LYS:HD2	3:D:193:ALA:H	1.69	0.57
2:C:551:ASP:OD1	2:C:551:ASP:N	2.29	0.57
6:T:4:DC:H2"	6:T:5:DA:C8	2.40	0.57
3:D:143:MET:O	3:D:147:GLU:HB3	2.05	0.57
1:A:23:ILE:HD12	1:A:192:LEU:HD23	1.87	0.57
3:D:876:ARG:NH1	3:D:1036:GLU:OE2	2.38	0.57
4:E:67:TYR:HD1	4:E:76:LEU:HD11	1.70	0.56
3:D:979:TYR:HD2	3:D:989:VAL:HG21	1.71	0.56
3:D:430:ILE:HG21	3:D:541:MET:HG3	1.88	0.56
1:B:5:GLN:HE21	1:B:183:VAL:HG13	1.70	0.56
2:C:433:THR:O	2:C:433:THR:OG1	2.23	0.56
5:G:3:LYS:HG3	5:G:70:VAL:HG23	1.88	0.55
2:C:758:ASP:O	2:C:805:LYS:NZ	2.29	0.55
2:C:235:THR:HG21	2:C:262:LEU:HA	1.88	0.55
1:B:104:GLU:OE1	1:B:124:HIS:ND1	2.32	0.55
3:D:141:GLU:OE2	3:D:144:ARG:NH1	2.40	0.55
3:D:1274:PRO:HG3	4:E:79:VAL:HG21	1.89	0.55
1:A:172:LEU:HG	1:A:199:LYS:HG2	1.88	0.55
2:C:654:SER:OG	2:C:655:ALA:N	2.40	0.54
5:G:48:ILE:HG13	5:G:53:LYS:HD2	1.89	0.54
2:C:855:ARG:NH2	2:C:865:VAL:O	2.40	0.54
1:B:187:THR:HG22	1:B:188:ASP:H	1.72	0.54
1:A:82:SER:HB2	1:A:123:MET:HE1	1.89	0.53
1:B:56:ILE:HD11	1:B:66:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:518:LYS:NZ	2:C:577:ASP:OD1	2.42	0.53
3:D:1052:ARG:O	3:D:1067:VAL:N	2.42	0.53
2:C:809:LYS:HE2	8:R:18:G:H5"	1.90	0.53
3:D:1030:ARG:NH1	3:D:1033:GLU:OE2	2.41	0.53
3:D:1166:THR:HG22	3:D:1180:LEU:HD23	1.90	0.52
6:T:15:DT:H2'	6:T:16:DA:C8	2.45	0.52
3:D:1052:ARG:HH21	3:D:1102:GLY:HA2	1.74	0.52
2:C:90:LEU:HD12	2:C:110:PRO:HG3	1.92	0.52
8:R:4:G:H2'	8:R:5:A:H8	1.73	0.52
3:D:144:ARG:NH2	3:D:227:THR:O	2.42	0.52
3:D:275:GLU:OE2	3:D:278:ARG:NH2	2.40	0.52
8:R:17:C:H2'	8:R:18:G:H8	1.74	0.51
6:T:32:DC:H2"	6:T:33:DA:C8	2.45	0.51
3:D:1053:VAL:HA	3:D:1066:ILE:HA	1.93	0.51
2:C:229:LYS:HD2	2:C:281:LEU:HD23	1.91	0.51
3:D:525:HIS:HD2	3:D:527:LEU:HB2	1.75	0.51
2:C:633:ARG:NH2	2:C:637:ASP:OD2	2.33	0.51
2:C:757:ILE:HG21	2:C:803:VAL:HG21	1.92	0.51
2:C:829:ALA:HB1	2:C:831:GLU:OE1	2.11	0.51
3:D:845:THR:HG22	3:D:846:VAL:H	1.76	0.50
1:A:72:ASP:OD1	1:A:72:ASP:N	2.30	0.50
5:G:72:THR:OG1	5:G:73:ASP:N	2.44	0.50
1:A:153:ARG:NH2	1:A:157:ALA:O	2.44	0.50
8:R:17:C:H2'	8:R:18:G:C8	2.47	0.50
2:C:42:ALA:HB2	2:C:975:PRO:HG2	1.93	0.50
2:C:1084:THR:OG1	3:D:554:GLU:OE1	2.30	0.50
6:T:26:DG:H22	7:N:16:DT:H3	1.60	0.50
8:R:4:G:H2'	8:R:5:A:C8	2.47	0.50
2:C:519:VAL:HG21	2:C:576:VAL:HG23	1.93	0.49
3:D:208:ILE:O	3:D:211:ARG:HG2	2.11	0.49
3:D:144:ARG:O	3:D:148:LEU:HG	2.11	0.49
3:D:363:PRO:HG2	3:D:366:ILE:HD12	1.93	0.49
1:B:154:ALA:HB1	1:B:157:ALA:HB3	1.95	0.49
2:C:465:ARG:HE	2:C:493:ASN:HD21	1.60	0.49
2:C:751:HIS:HD2	2:C:877:ARG:HG3	1.78	0.49
3:D:776:GLU:HA	3:D:776:GLU:OE2	2.13	0.49
3:D:602:ALA:HB1	3:D:606:HIS:CD2	2.48	0.49
2:C:1007:LYS:HB3	2:C:1022:PRO:HB2	1.94	0.48
1:A:2:LEU:HD23	1:A:2:LEU:H	1.78	0.48
1:A:9:LEU:HD12	1:A:23:ILE:HG12	1.94	0.48
2:C:185:VAL:HG23	2:C:204:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:121:GLU:O	2:C:125:LYS:HG2	2.14	0.48
2:C:288:THR:HG22	2:C:290:GLU:OE2	2.13	0.48
3:D:1131:GLN:H	3:D:1131:GLN:HG2	1.47	0.48
6:T:34:DT:H2"	6:T:35:DG:C8	2.48	0.48
1:B:72:ASP:OD1	1:B:72:ASP:N	2.43	0.48
3:D:754:ASP:OD1	3:D:755:LYS:N	2.46	0.48
2:C:206:PRO:HA	2:C:308:LEU:HD23	1.96	0.48
3:D:657:GLN:N	3:D:658:PRO:HD2	2.29	0.48
6:T:36:DC:H2"	6:T:37:DG:C8	2.49	0.48
3:D:1084:GLN:HG2	3:D:1112:MET:HE2	1.95	0.48
2:C:1127:GLU:OE1	3:D:405:LEU:HD12	2.14	0.48
3:D:979:TYR:CD2	3:D:989:VAL:HG21	2.48	0.48
3:D:354:LEU:HD21	3:D:371:LYS:HG2	1.96	0.47
2:C:502:VAL:HG23	2:C:503:TYR:CD2	2.50	0.47
1:B:86:SER:HB3	1:B:119:HIS:HE1	1.80	0.47
3:D:645:GLU:HG2	3:D:646:ILE:N	2.28	0.47
3:D:1034:LEU:HD11	3:D:1137:GLU:HB3	1.97	0.47
6:T:22:DC:H2"	6:T:23:DC:H5'	1.96	0.47
2:C:861:LEU:HD22	2:C:862:PRO:HD2	1.96	0.47
3:D:668:LEU:O	3:D:672:MET:HG3	2.14	0.47
3:D:190:LYS:HD2	3:D:193:ALA:N	2.30	0.47
3:D:237:ASP:HB3	3:D:240:LEU:HD13	1.96	0.47
3:D:1210:ILE:O	3:D:1214:SER:OG	2.31	0.47
3:D:554:GLU:HG3	4:E:54:VAL:HG11	1.96	0.46
3:D:151:LEU:O	3:D:155:MET:HG3	2.14	0.46
7:N:6:DC:H2"	7:N:7:DA:C8	2.50	0.46
2:C:650:ILE:HD13	2:C:660:VAL:HG22	1.95	0.46
5:G:69:ILE:HG12	5:G:70:VAL:N	2.30	0.46
2:C:664:ASN:OD1	2:C:665:GLY:N	2.48	0.46
2:C:851:ARG:HA	2:C:851:ARG:HD2	1.72	0.46
3:D:1125:GLN:HB3	3:D:1129:GLU:HG3	1.96	0.46
2:C:1101:LYS:HB2	2:C:1101:LYS:HE2	1.74	0.46
7:N:9:DG:H2"	7:N:10:DC:C5	2.51	0.46
2:C:189:GLU:OE1	2:C:200:HIS:NE2	2.49	0.46
3:D:295:ARG:O	3:D:299:VAL:HG23	2.16	0.46
2:C:581:VAL:HB	2:C:585:GLN:HE21	1.81	0.46
6:T:11:DC:H2'	6:T:12:DG:C8	2.50	0.46
3:D:224:SER:O	3:D:227:THR:OG1	2.32	0.46
7:N:15:DC:C6	7:N:16:DT:H72	2.51	0.46
2:C:861:LEU:HD13	2:C:865:VAL:HG23	1.97	0.46
7:N:8:DT:H2"	7:N:9:DG:C8	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:547:PRO:HB2	2:C:555:VAL:HB	1.99	0.45
2:C:815:THR:O	2:C:819:ARG:HG2	2.17	0.45
5:G:91:SER:HB2	5:G:95:GLY:HA2	1.97	0.45
1:B:2:LEU:HD23	1:B:2:LEU:HA	1.83	0.45
2:C:1050:SER:HB3	2:C:1053:THR:O	2.17	0.45
3:D:1077:TYR:HB2	3:D:1080:ILE:HD11	1.99	0.45
1:A:182:ARG:HA	1:A:182:ARG:HD3	1.82	0.45
1:B:165:ASP:OD1	1:B:165:ASP:N	2.50	0.45
2:C:187:PHE:CD1	2:C:319:LYS:HE2	2.52	0.45
2:C:335:GLU:O	2:C:339:VAL:HG23	2.17	0.45
2:C:1147:LEU:HD12	3:D:2:LEU:HD13	1.97	0.45
3:D:1086:LEU:HD23	3:D:1099:LEU:HB3	1.99	0.45
5:G:75:SER:HA	5:G:78:VAL:HG12	1.99	0.45
3:D:173:ARG:HH11	3:D:177:LEU:HD12	1.81	0.44
2:C:776:ILE:HD11	2:C:781:LEU:HD21	1.98	0.44
2:C:69:ARG:HH12	2:C:73:SER:HB2	1.82	0.44
2:C:244:THR:HG23	2:C:247:GLN:HB2	1.99	0.44
2:C:815:THR:HG23	2:C:818:GLU:H	1.82	0.44
2:C:1066:GLN:HE22	3:D:427:ARG:HD2	1.82	0.44
1:A:225:LEU:HD13	1:B:205:ARG:HG2	1.99	0.44
2:C:216:VAL:HG22	2:C:222:VAL:HG12	1.99	0.44
1:B:186:ARG:HG3	1:B:187:THR:O	2.16	0.44
2:C:257:ILE:H	2:C:257:ILE:HG13	1.40	0.44
5:G:22:LEU:HD23	5:G:38:VAL:HG11	2.00	0.44
1:A:1:MET:N	1:B:142:ARG:O	2.43	0.44
2:C:930:GLN:O	2:C:934:THR:HG23	2.18	0.44
3:D:356:ARG:HD2	3:D:357:LEU:HD12	1.99	0.43
3:D:1087:ARG:HB2	3:D:1111:LEU:O	2.17	0.43
3:D:1122:LEU:HG	3:D:1130:VAL:HG21	1.99	0.43
8:R:8:C:H2'	8:R:9:U:O4'	2.18	0.43
2:C:820:LEU:HD23	2:C:820:LEU:HA	1.81	0.43
3:D:57:ASP:HB3	3:D:58:TRP:CD1	2.53	0.43
3:D:239:ASN:HA	3:D:242:ARG:HG3	2.00	0.43
3:D:953:LEU:HD23	3:D:953:LEU:HA	1.79	0.43
1:A:187:THR:O	1:A:187:THR:HG23	2.18	0.43
3:D:1091:HIS:CG	3:D:1092:GLU:H	2.37	0.43
2:C:140:ILE:HD12	2:C:147:ILE:HG12	2.00	0.43
2:C:187:PHE:HD1	2:C:319:LYS:HE2	1.83	0.43
2:C:397:GLU:HA	2:C:400:VAL:HG12	2.01	0.43
3:D:1224:ALA:HA	3:D:1232:VAL:HG21	2.00	0.43
2:C:685:ASN:HD22	2:C:686:GLN:N	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:784:LEU:HD11	2:C:801:ILE:HG21	2.01	0.43
5:G:34:LYS:HA	5:G:34:LYS:HD3	1.80	0.43
2:C:369:ASP:OD2	2:C:370:ILE:N	2.52	0.42
2:C:409:VAL:O	2:C:410:GLU:HB2	2.19	0.42
3:D:278:ARG:HA	3:D:281:ILE:HG22	2.00	0.42
5:G:97:LYS:HA	5:G:97:LYS:HD3	1.78	0.42
2:C:232:GLN:HE22	2:C:277:ILE:HD13	1.85	0.42
2:C:833:ARG:HG2	2:C:834:ASP:H	1.84	0.42
3:D:60:CYS:SG	3:D:61:TYR:N	2.92	0.42
3:D:344:TYR:O	3:D:348:ILE:HG13	2.20	0.42
3:D:193:ALA:O	3:D:196:LYS:HG3	2.19	0.42
3:D:590:THR:O	3:D:630:ARG:HB3	2.19	0.42
5:G:105:GLU:O	5:G:109:ILE:HG12	2.20	0.42
3:D:164:ASP:HA	3:D:167:ASP:OD2	2.20	0.42
6:T:15:DT:H2'	6:T:16:DA:H8	1.84	0.42
2:C:192:ASP:HB3	2:C:197:LYS:H	1.83	0.42
2:C:604:ARG:HA	2:C:604:ARG:HD2	1.68	0.42
2:C:777:SER:OG	2:C:778:ASP:N	2.53	0.42
3:D:296:LEU:HD12	3:D:296:LEU:HA	1.92	0.42
3:D:1170:SER:O	3:D:1173:THR:OG1	2.28	0.42
4:E:67:TYR:HA	4:E:76:LEU:HD13	2.02	0.42
2:C:766:ALA:H	2:C:808:PRO:HG3	1.85	0.42
3:D:194:ARG:HA	3:D:197:VAL:HB	2.01	0.42
3:D:949:ILE:HD13	3:D:949:ILE:HA	1.84	0.42
1:B:11:GLU:HG3	1:B:21:PHE:CE2	2.55	0.42
3:D:1013:ARG:HH22	3:D:1024:ILE:HD11	1.85	0.42
8:R:14:C:H2'	8:R:15:U:H6	1.85	0.42
1:B:15:THR:HG22	1:B:16:ASP:N	2.35	0.41
3:D:221:ASP:OD2	3:D:222:ILE:N	2.53	0.41
2:C:1138:LEU:HB2	3:D:9:GLU:HB2	2.02	0.41
3:D:67:ARG:NH1	8:R:16:U:OP1	2.53	0.41
3:D:293:LEU:HA	3:D:293:LEU:HD23	1.73	0.41
3:D:928:ASP:OD1	3:D:940:ARG:N	2.53	0.41
2:C:685:ASN:HD22	2:C:686:GLN:H	1.68	0.41
2:C:751:HIS:CD2	2:C:877:ARG:HG3	2.55	0.41
3:D:759:GLN:HG2	3:D:762:ARG:HH21	1.85	0.41
3:D:208:ILE:HA	3:D:211:ARG:HE	1.85	0.41
2:C:486:ILE:HD11	3:D:849:TYR:HE2	1.85	0.41
2:C:854:SER:O	2:C:859:ASP:HB2	2.19	0.41
3:D:320:ILE:HG22	3:D:325:ARG:HE	1.85	0.41
1:B:90:ASP:OD1	1:B:90:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:539:ASP:OD1	3:D:539:ASP:N	2.54	0.41
2:C:244:THR:OG1	2:C:245:SER:N	2.53	0.41
3:D:88:ARG:HB3	3:D:323:GLU:HG3	2.02	0.41
3:D:1266:ARG:H	3:D:1266:ARG:HG3	1.61	0.41
8:R:3:C:H2'	8:R:4:G:H8	1.86	0.41
3:D:172:ALA:O	3:D:175:GLN:HG3	2.20	0.41
3:D:607:PRO:O	3:D:609:THR:HG23	2.20	0.41
1:B:40:ARG:HE	1:B:40:ARG:HB2	1.62	0.41
3:D:263:LYS:HE3	3:D:263:LYS:HB2	1.86	0.41
3:D:410:GLN:HA	3:D:415:GLN:HG3	2.03	0.41
5:G:47:ASP:HB3	5:G:55:VAL:HA	2.02	0.41
1:A:55:ARG:HH22	1:A:158:GLU:HB3	1.85	0.41
2:C:329:THR:O	2:C:330:SER:HB2	2.21	0.41
2:C:727:GLU:H	3:D:725:THR:HG21	1.86	0.41
3:D:329:GLN:NE2	3:D:333:GLY:O	2.43	0.41
1:B:92:PRO:HB3	1:B:141:GLU:HG3	2.03	0.40
2:C:656:ASP:OD1	2:C:656:ASP:N	2.54	0.40
2:C:228:ARG:NH2	7:N:27:DC:OP2	2.54	0.40
3:D:206:ARG:HA	3:D:209:ARG:NE	2.37	0.40
3:D:1062:TYR:CZ	3:D:1082:LYS:HE2	2.57	0.40
7:N:12:DG:H1'	7:N:13:DC:H5'	2.03	0.40
2:C:488:THR:HG22	2:C:606:LEU:HD11	2.02	0.40
2:C:518:LYS:O	2:C:525:SER:OG	2.26	0.40
2:C:1114:GLU:HA	2:C:1115:PRO:HD3	1.95	0.40
3:D:190:LYS:NZ	3:D:193:ALA:HB2	2.37	0.40
3:D:1277:GLU:H	3:D:1277:GLU:HG3	1.69	0.40
2:C:507:ASN:HB3	2:C:509:PHE:H	1.87	0.40
3:D:525:HIS:CD2	3:D:527:LEU:HB2	2.54	0.40
8:R:16:U:H2'	8:R:17:C:C6	2.57	0.40
1:B:61:HIS:CD2	1:B:61:HIS:H	2.39	0.40
3:D:201:GLY:O	3:D:205:MET:SD	2.80	0.40
3:D:269:ASP:OD2	3:D:272:ALA:HB3	2.21	0.40
4:E:42:GLU:OE1	4:E:100:HIS:NE2	2.54	0.40
8:R:16:U:H2'	8:R:17:C:H6	1.86	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	224/347 (65%)	211 (94%)	13 (6%)	0	100 100
1	B	235/347 (68%)	220 (94%)	15 (6%)	0	100 100
2	C	1120/1178 (95%)	1073 (96%)	46 (4%)	1 (0%)	51 85
3	D	1269/1316 (96%)	1211 (95%)	57 (4%)	1 (0%)	51 85
4	E	81/110 (74%)	81 (100%)	0	0	100 100
5	G	109/177 (62%)	101 (93%)	8 (7%)	0	100 100
All	All	3038/3475 (87%)	2897 (95%)	139 (5%)	2 (0%)	54 85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	1066	ILE
2	C	330	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	195/297 (66%)	174 (89%)	21 (11%)	6 26
1	B	195/297 (66%)	174 (89%)	21 (11%)	6 26
2	C	945/998 (95%)	883 (93%)	62 (7%)	16 49
3	D	1054/1095 (96%)	963 (91%)	91 (9%)	10 37
4	E	69/90 (77%)	61 (88%)	8 (12%)	5 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	G	98/159 (62%)	86 (88%)	12 (12%)	5 21
All	All	2556/2936 (87%)	2341 (92%)	215 (8%)	14 38

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	6	ARG
1	A	10	SER
1	A	19	SER
1	A	30	PHE
1	A	34	LEU
1	A	56	ILE
1	A	72	ASP
1	A	86	SER
1	A	120	ASN
1	A	128	LEU
1	A	130	ASP
1	A	153	ARG
1	A	166	SER
1	A	173	LYS
1	A	184	GLU
1	A	195	ASP
1	A	201	SER
1	A	205	ARG
1	A	218	LEU
1	A	223	ARG
1	B	1	MET
1	B	2	LEU
1	B	9	LEU
1	B	16	ASP
1	B	25	PRO
1	B	45	SER
1	B	65	THR
1	B	78	LEU
1	B	90	ASP
1	B	99	LYS
1	B	105	VAL
1	B	140	VAL
1	B	142	ARG
1	B	165	ASP
1	B	175	THR

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Mol	Chain	Res	Type
1	B	186	ARG
1	B	196	VAL
1	B	198	THR
1	B	214	THR
1	B	226	ASN
1	B	237	SER
2	C	48	LEU
2	C	65	ILE
2	C	77	ARG
2	C	92	GLU
2	C	99	PHE
2	C	100	SER
2	C	106	SER
2	C	109	ASP
2	C	113	ASP
2	C	116	LYS
2	C	152	VAL
2	C	162	GLU
2	C	177	SER
2	C	180	VAL
2	C	218	LYS
2	C	229	LYS
2	C	238	LEU
2	C	244	THR
2	C	251	ARG
2	C	257	ILE
2	C	266	ASN
2	C	304	LYS
2	C	311	VAL
2	C	324	VAL
2	C	357	VAL
2	C	373	PHE
2	C	377	ARG
2	C	428	LYS
2	C	433	THR
2	C	454	ARG
2	C	474	ASP
2	C	494	ILE
2	C	499	SER
2	C	551	ASP
2	C	570	TYR
2	C	625	LEU

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Mol	Chain	Res	Type
2	C	646	GLU
2	C	666	THR
2	C	668	ARG
2	C	672	MET
2	C	685	ASN
2	C	690	VAL
2	C	713	MET
2	C	745	ASP
2	C	753	GLU
2	C	758	ASP
2	C	762	THR
2	C	771	ARG
2	C	790	VAL
2	C	881	ASP
2	C	891	ASN
2	C	901	VAL
2	C	903	ASP
2	C	904	MET
2	C	919	THR
2	C	947	ASP
2	C	974	THR
2	C	1067	ARG
2	C	1084	THR
2	C	1093	SER
2	C	1127	GLU
2	C	1148	ARG
3	D	10	LEU
3	D	22	GLN
3	D	24	SER
3	D	56	ARG
3	D	60	CYS
3	D	62	CYS
3	D	107	PHE
3	D	126	GLU
3	D	139	VAL
3	D	143	MET
3	D	145	HIS
3	D	155	MET
3	D	160	LYS
3	D	169	GLU
3	D	192	ASP
3	D	195	ARG

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Mol	Chain	Res	Type
3	D	205	MET
3	D	219	LEU
3	D	221	ASP
3	D	234	LEU
3	D	248	TYR
3	D	253	THR
3	D	260	SER
3	D	269	ASP
3	D	276	SER
3	D	279	ASP
3	D	305	SER
3	D	310	MET
3	D	327	MET
3	D	328	VAL
3	D	339	ASP
3	D	356	ARG
3	D	360	LEU
3	D	401	SER
3	D	415	GLN
3	D	431	VAL
3	D	438	LEU
3	D	462	ASP
3	D	468	ASN
3	D	478	ARG
3	D	480	ARG
3	D	505	HIS
3	D	539	ASP
3	D	578	ARG
3	D	580	ASP
3	D	596	THR
3	D	698	ASN
3	D	725	THR
3	D	754	ASP
3	D	768	ASP
3	D	772	GLU
3	D	796	ASP
3	D	834	ARG
3	D	838	SER
3	D	846	VAL
3	D	847	LEU
3	D	869	ASP
3	D	870	SER

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Mol	Chain	Res	Type
3	D	887	ARG
3	D	904	ARG
3	D	912	ARG
3	D	919	SER
3	D	923	ARG
3	D	946	ASP
3	D	960	VAL
3	D	964	SER
3	D	971	SER
3	D	972	THR
3	D	987	LYS
3	D	993	GLU
3	D	1025	THR
3	D	1053	VAL
3	D	1064	ILE
3	D	1070	ASP
3	D	1075	VAL
3	D	1085	ARG
3	D	1093	ASP
3	D	1121	VAL
3	D	1130	VAL
3	D	1131	GLN
3	D	1148	SER
3	D	1165	VAL
3	D	1172	SER
3	D	1176	LEU
3	D	1191	ARG
3	D	1206	VAL
3	D	1214	SER
3	D	1262	THR
3	D	1266	ARG
3	D	1268	ARG
3	D	1272	VAL
4	E	33	LEU
4	E	41	ASP
4	E	56	TYR
4	E	71	LEU
4	E	76	LEU
4	E	83	VAL
4	E	87	LEU
4	E	102	ASP
5	G	4	ASN

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Mol	Chain	Res	Type
5	G	10	THR
5	G	12	SER
5	G	17	LYS
5	G	24	LYS
5	G	48	ILE
5	G	67	VAL
5	G	69	ILE
5	G	73	ASP
5	G	80	ARG
5	G	102	LEU
5	G	111	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	79	ASN
1	A	120	ASN
1	A	124	HIS
1	B	5	GLN
1	B	61	HIS
1	B	119	HIS
1	B	185	GLN
2	C	232	GLN
2	C	323	HIS
2	C	372	HIS
2	C	435	GLN
2	C	585	GLN
2	C	610	ASN
2	C	685	ASN
2	C	751	HIS
2	C	1062	GLN
2	C	1066	GLN
2	C	1077	GLN
2	C	1111	ASN
2	C	1129	GLN
3	D	5	ASN
3	D	262	GLN
3	D	352	ASN
3	D	368	ASN
3	D	396	ASN
3	D	410	GLN

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Mol	Chain	Res	Type
3	D	525	HIS
3	D	533	ASN
3	D	564	ASN
3	D	657	GLN
3	D	852	ASN
3	D	882	GLN
3	D	1001	GLN
3	D	1133	HIS
3	D	1251	ASN
3	D	1273	GLN
4	E	63	GLN
5	G	21	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	R	28/30 (93%)	4 (14%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	R	10	U
8	R	11	C
8	R	20	C
8	R	22	G

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

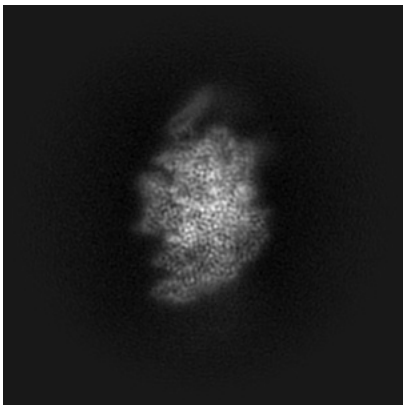
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-28149. These allow visual inspection of the internal detail of the map and identification of artifacts.

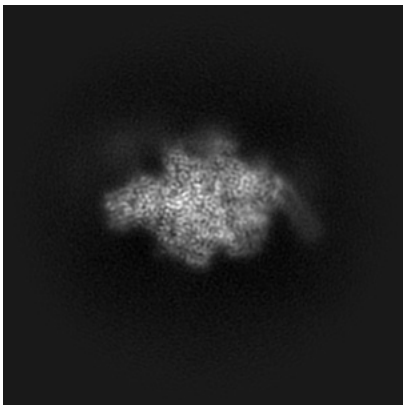
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

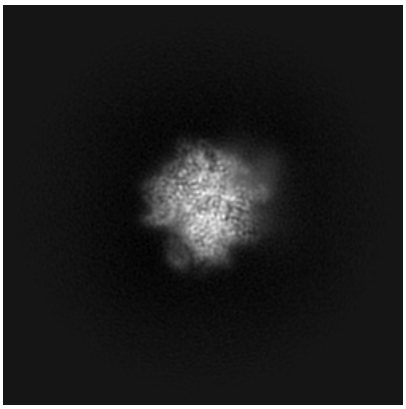
6.1.1 Primary map



X

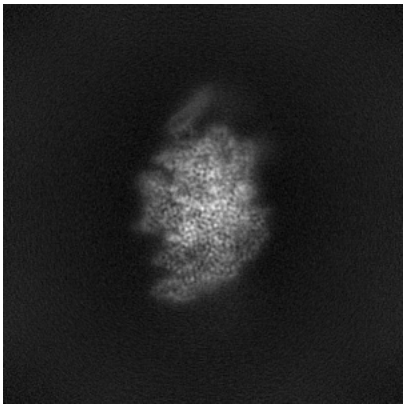


Y

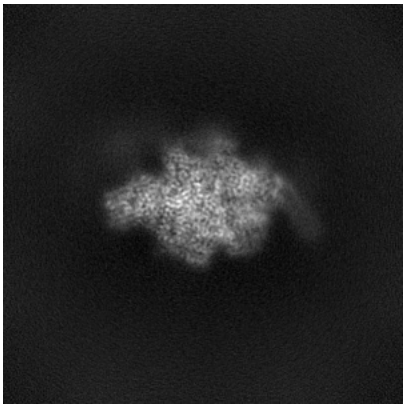


Z

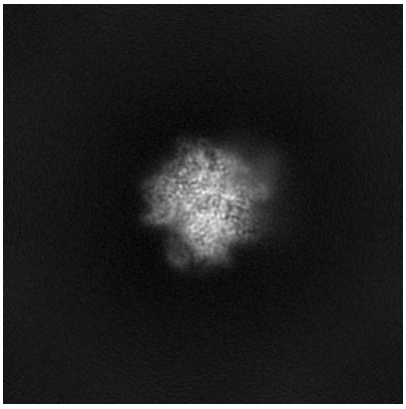
6.1.2 Raw map



X



Y

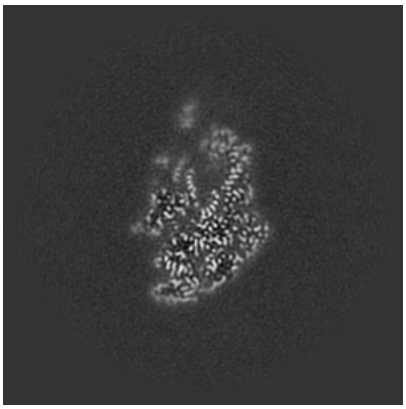


Z

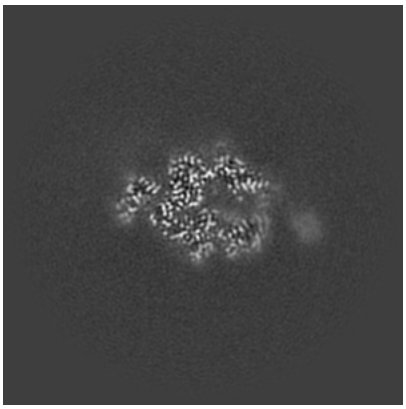
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

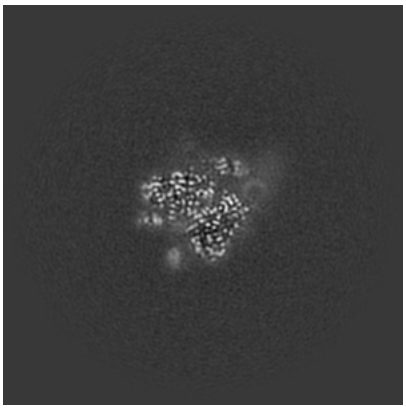
6.2.1 Primary map



X Index: 200

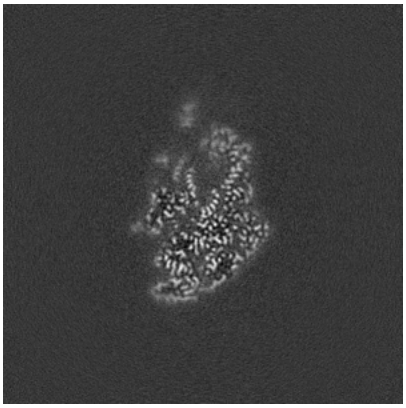


Y Index: 200

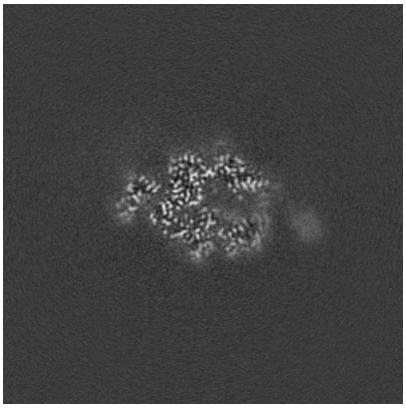


Z Index: 200

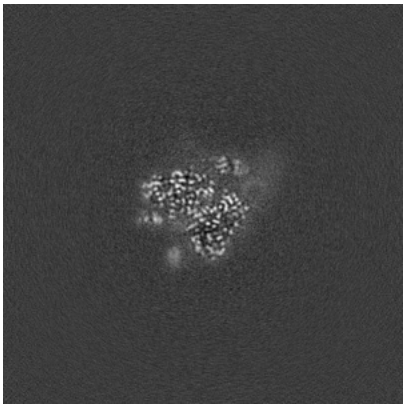
6.2.2 Raw map



X Index: 200



Y Index: 200

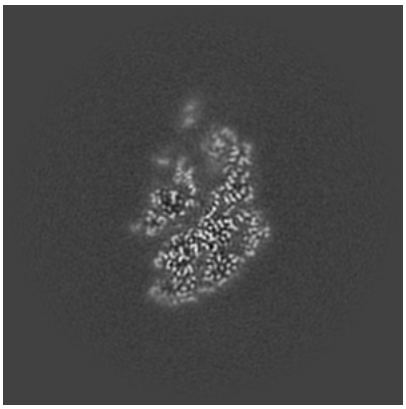


Z Index: 200

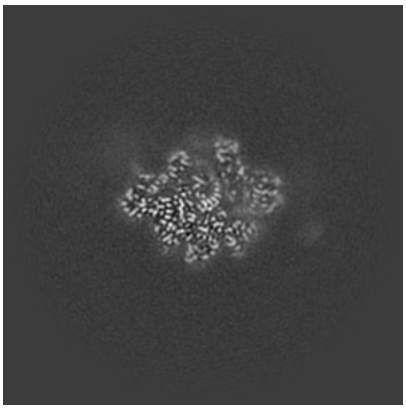
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

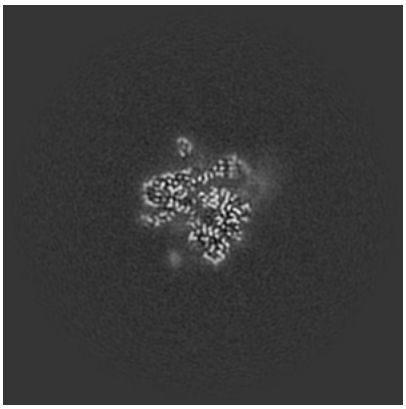
6.3.1 Primary map



X Index: 198

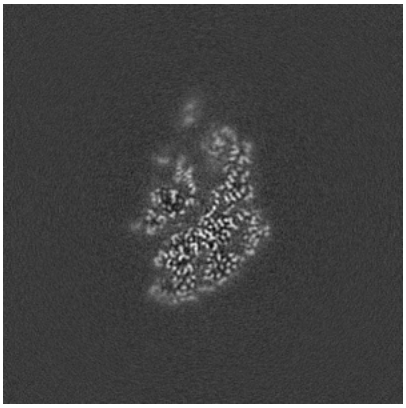


Y Index: 212

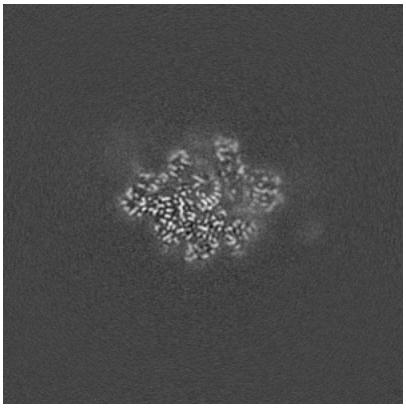


Z Index: 195

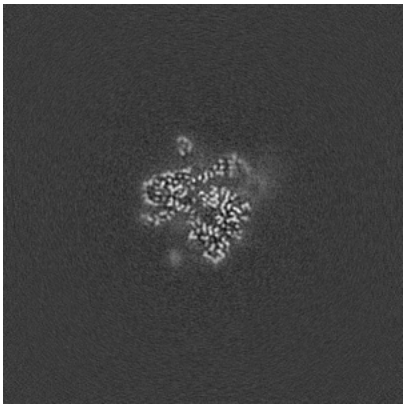
6.3.2 Raw map



X Index: 198



Y Index: 212

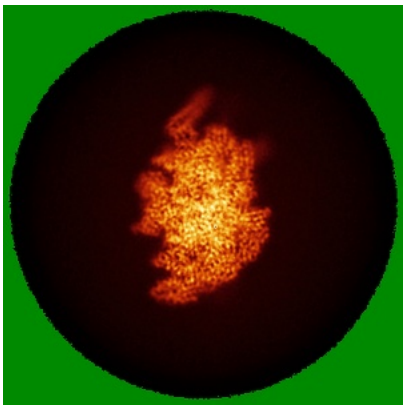


Z Index: 195

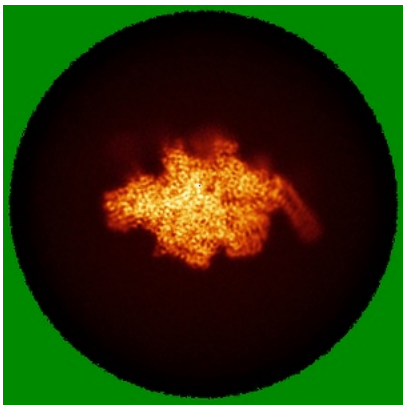
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

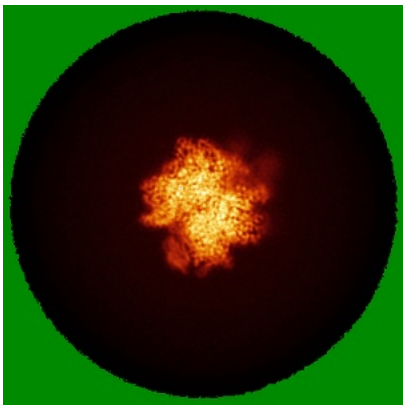
6.4.1 Primary map



X

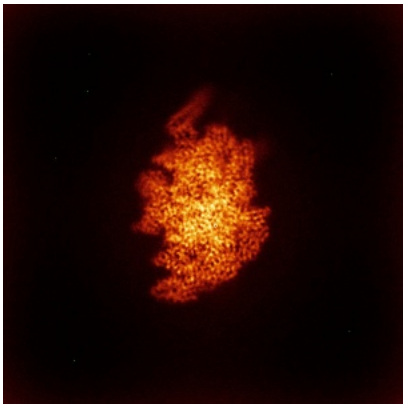


Y

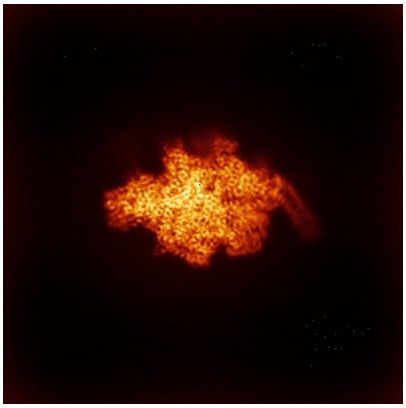


Z

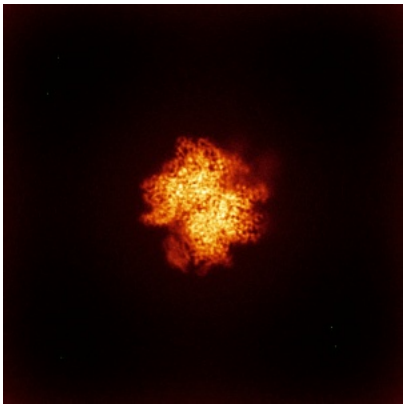
6.4.2 Raw map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.238. 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.

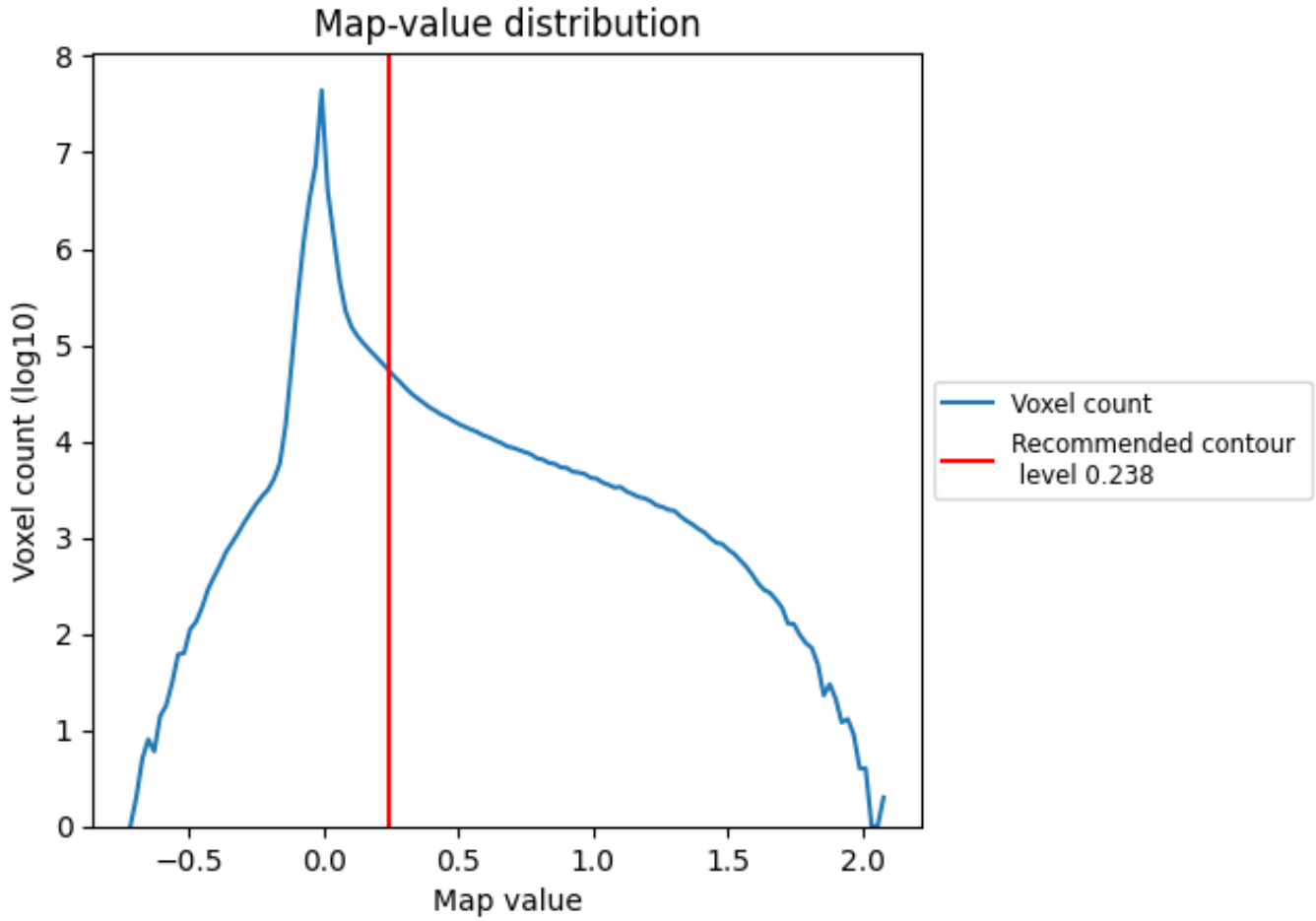
6.6 Mask visualisation (i)

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

7 Map analysis

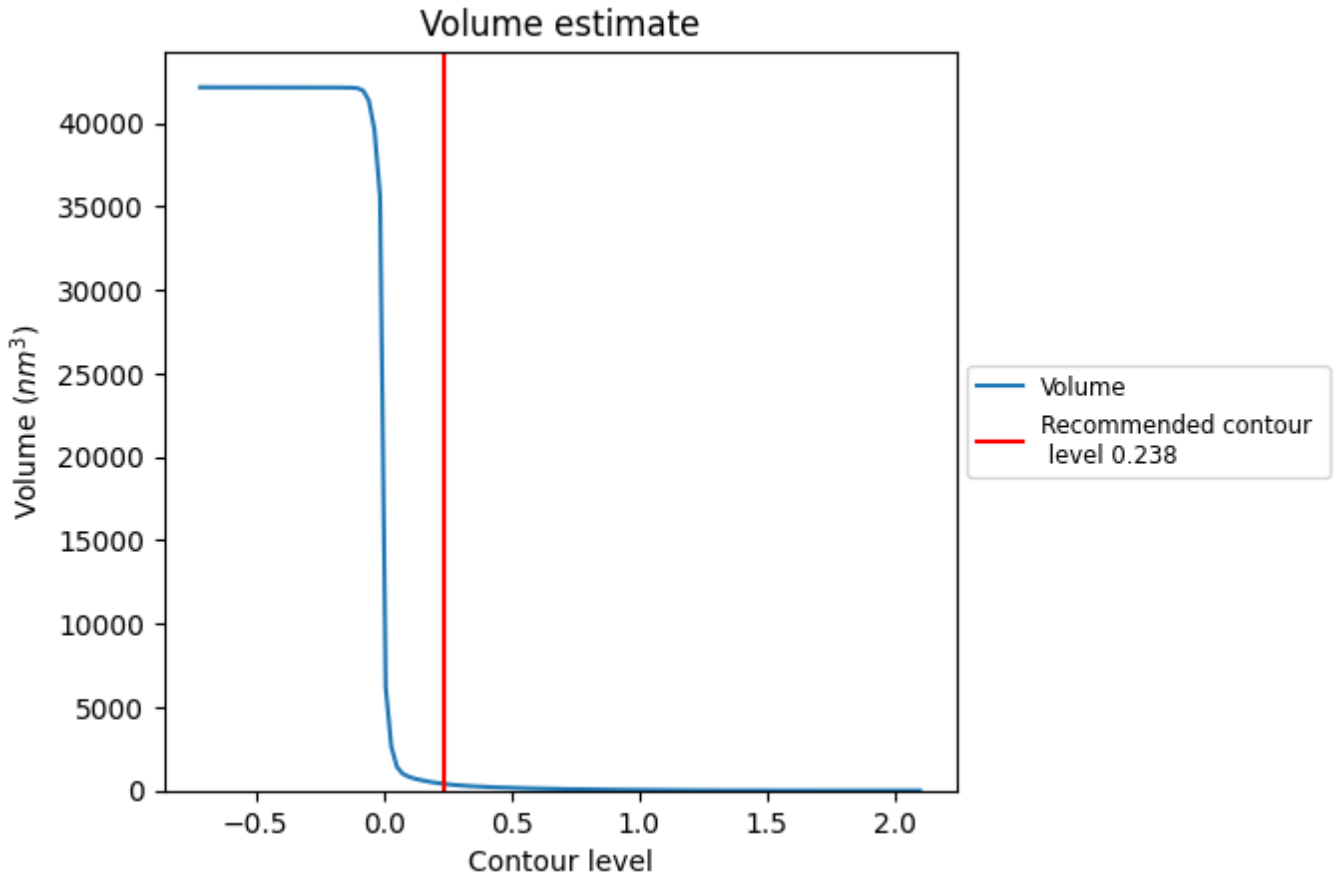
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

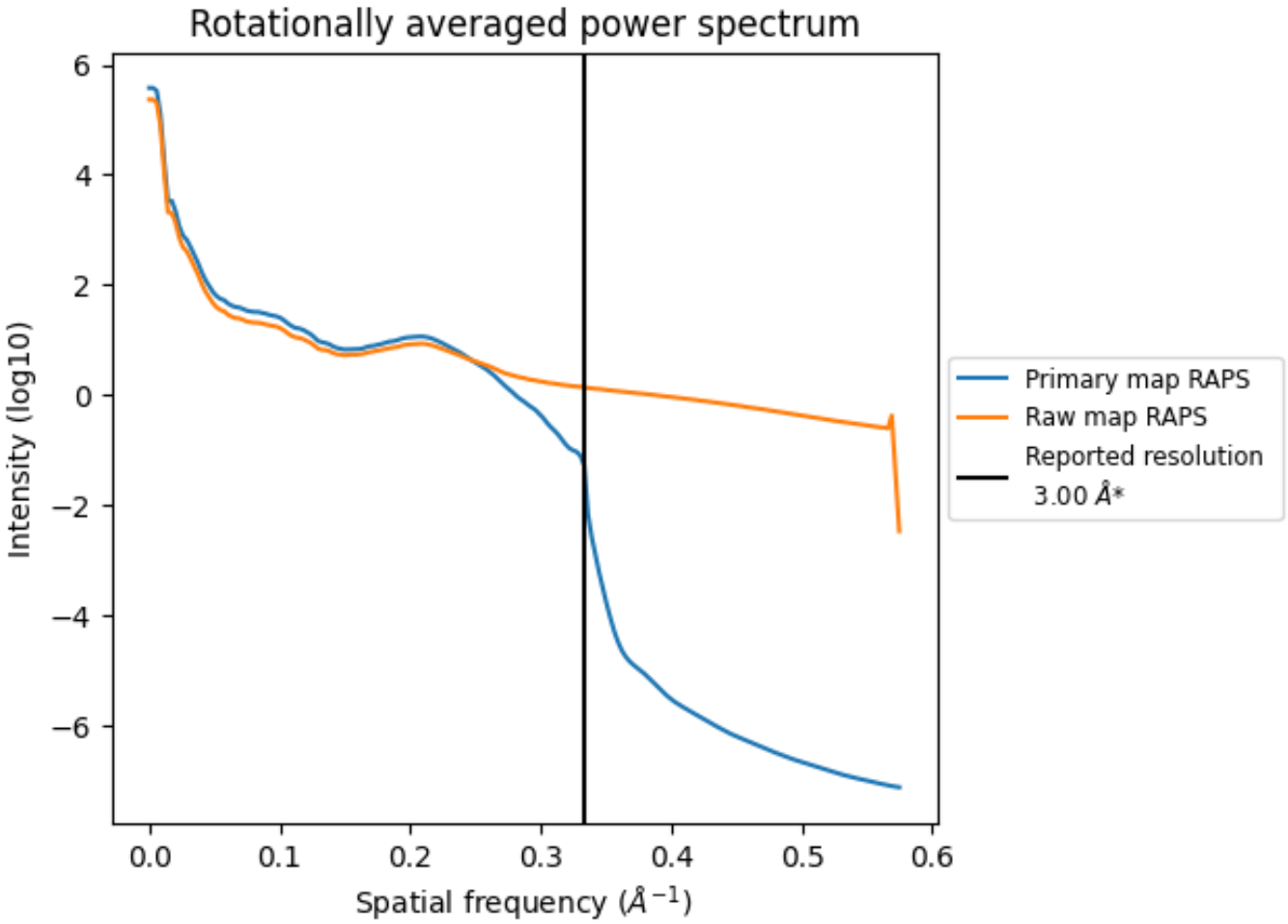
7.2 Volume estimate



The volume at the recommended contour level is 399 nm^3; this corresponds to an approximate mass of 360 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 (i)

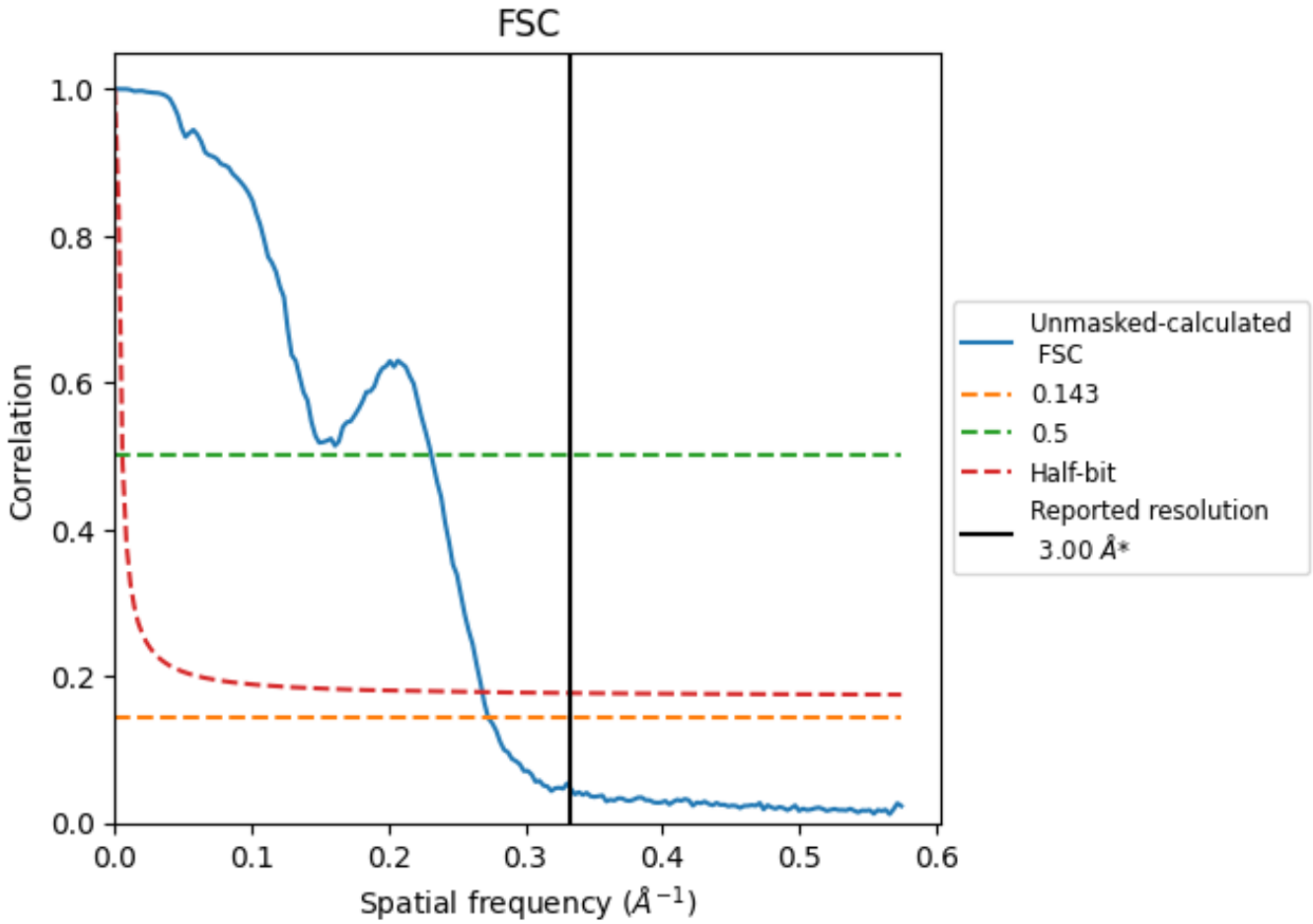


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

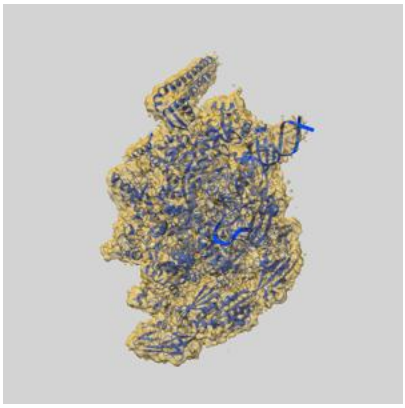
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.66	4.32	3.72

*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 3.66 differs from the reported value 3.0 by more than 10 %

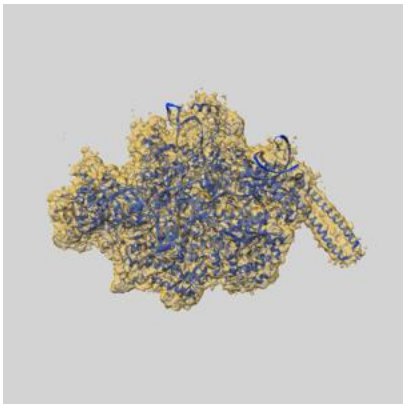
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-28149 and PDB model 8EHQ. Per-residue inclusion information can be found in section 3 on page 6.

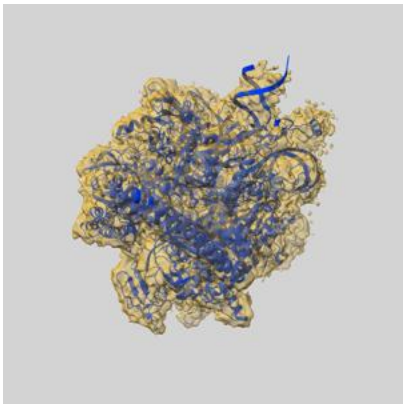
9.1 Map-model overlay



X



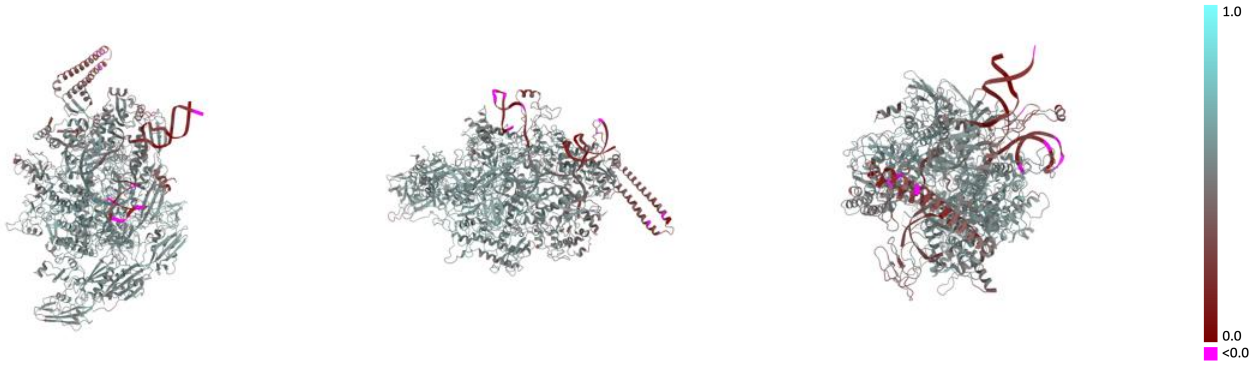
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.238 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.

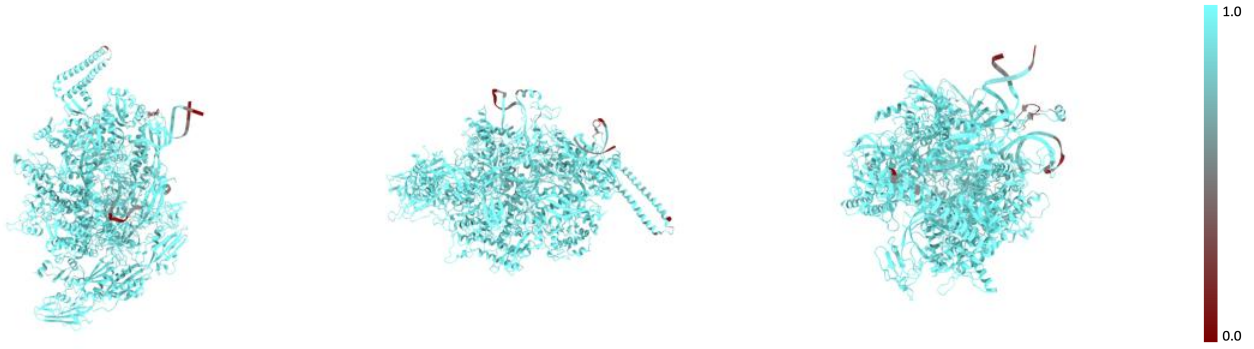
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

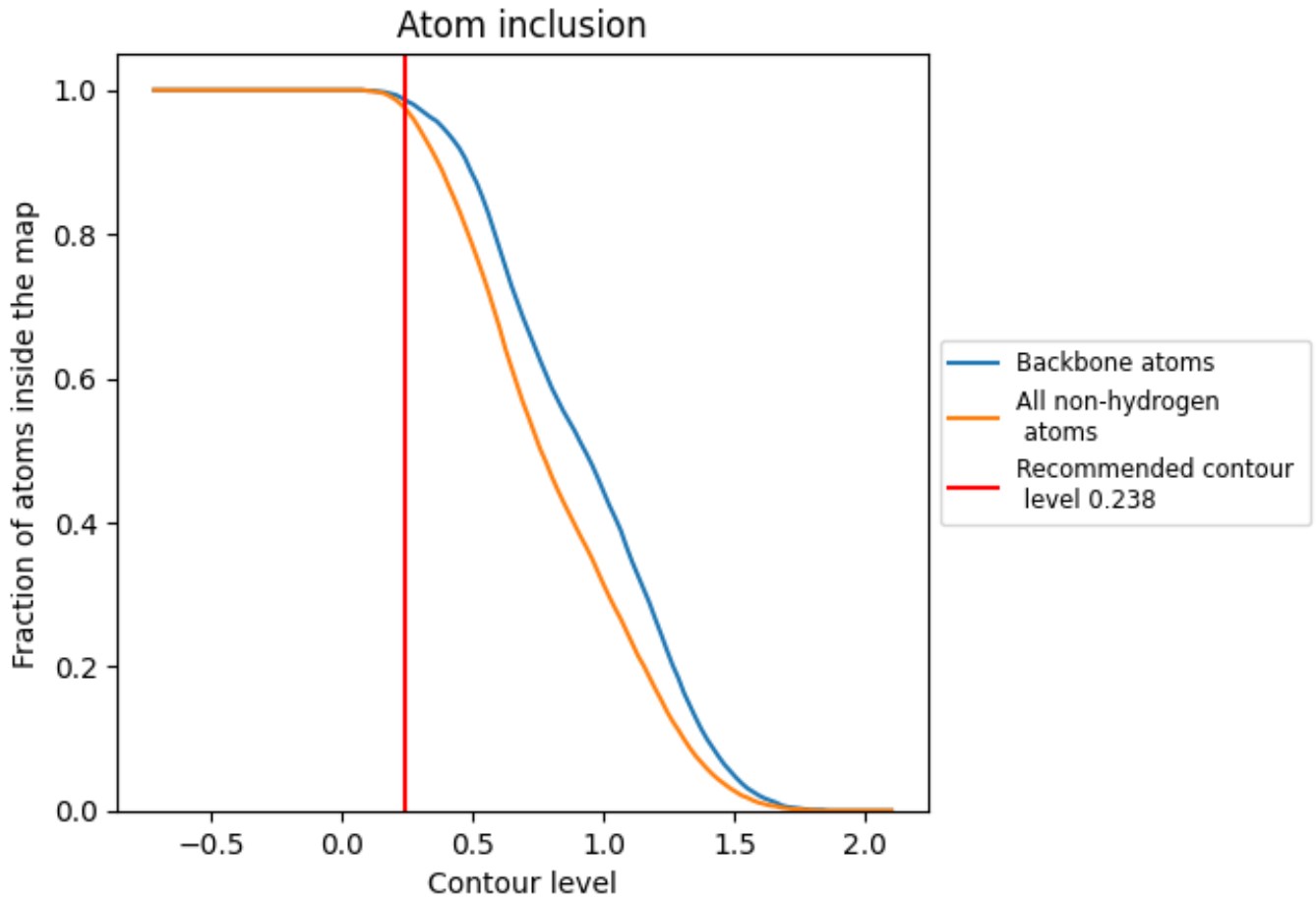
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.238).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.238) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9760	0.5060
A	0.9900	0.5380
B	0.9900	0.5220
C	0.9870	0.5370
D	0.9860	0.5120
E	0.9910	0.5400
G	0.9330	0.4470
N	0.9180	0.3210
R	0.7820	0.2650
T	0.9040	0.3700