Full wwPDB EM Validation Report ⓘ

Jan 8, 2024 – 10:29 pm GMT

PDB ID	:	8RE4
EMDB ID	:	EMD-19079
Title	:	Cryo-EM structure of bacterial RNA polymerase-sigma54 initial transcribing complex - 5nt pre-translocated complex
Authors	:	Gao, F.; Zhang, X.
Deposited on	:	2023-12-10
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:

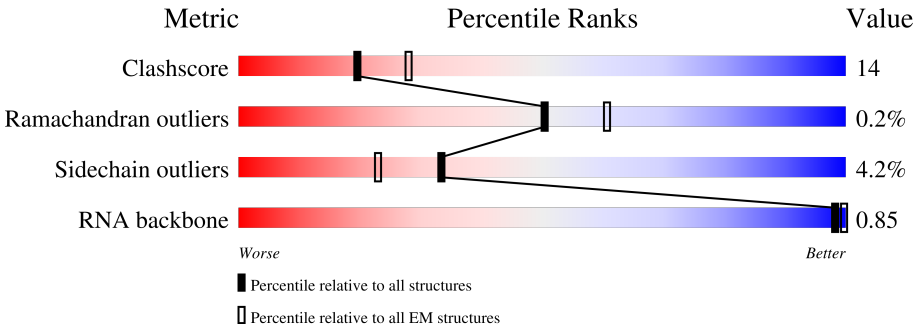
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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)
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	321	75% 18%
1	B	321	6% 50% 23% 27%
2	C	1341	7% 73% 26%
3	D	1373	9% 69% 26%
4	E	74	74% 24%
5	M	380	15% 72% 27%
6	N	47	13% 51% 45%

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Mol	Chain	Length	Quality of chain
7	R	5	100%
8	T	50	50% 50%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 29165 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	308	Total	C	N	O	S	0	0
			2365	1481	415	461	8		
1	B	234	Total	C	N	O	S	0	0
			1733	1084	304	339	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1341	Total	C	N	O	S	0	0
			10080	6328	1748	1964	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1330	Total	C	N	O	S	0	0
			9685	6088	1738	1818	41		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	74	Total	C	N	O	S	0	0
			546	337	105	103	1		

- Molecule 5 is a protein called RNA polymerase sigma-54 factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	380	Total	C	N	O	S	0	0
			2657	1670	470	511	6		

- Molecule 6 is a DNA chain called DNA (47-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	47	Total	C	N	O	P	0	0
			960	459	171	283	47		

- Molecule 7 is a RNA chain called RNA (5'-R(P*GP*CP*CP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	5	Total	C	N	O	P	0	0
			106	47	19	35	5		

- Molecule 8 is a DNA chain called DNA (50-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	50	Total	C	N	O	P	0	0
			1030	487	197	296	50		

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

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

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

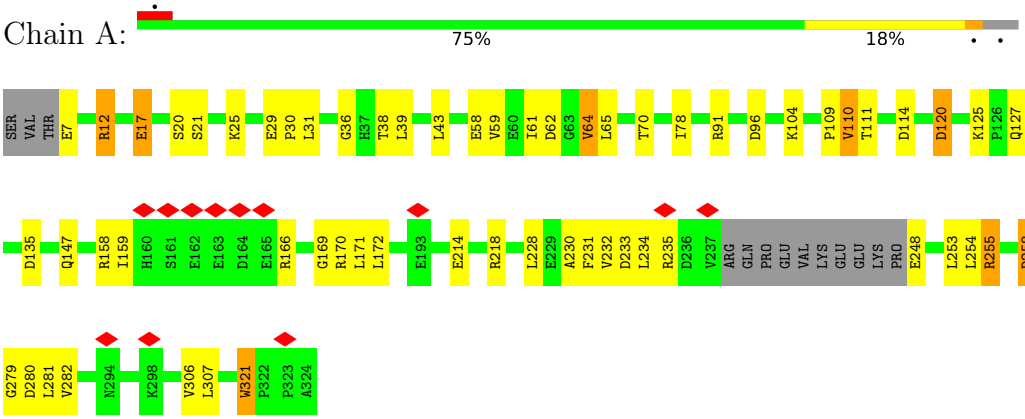
Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total	Zn	0
			2	2	

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.

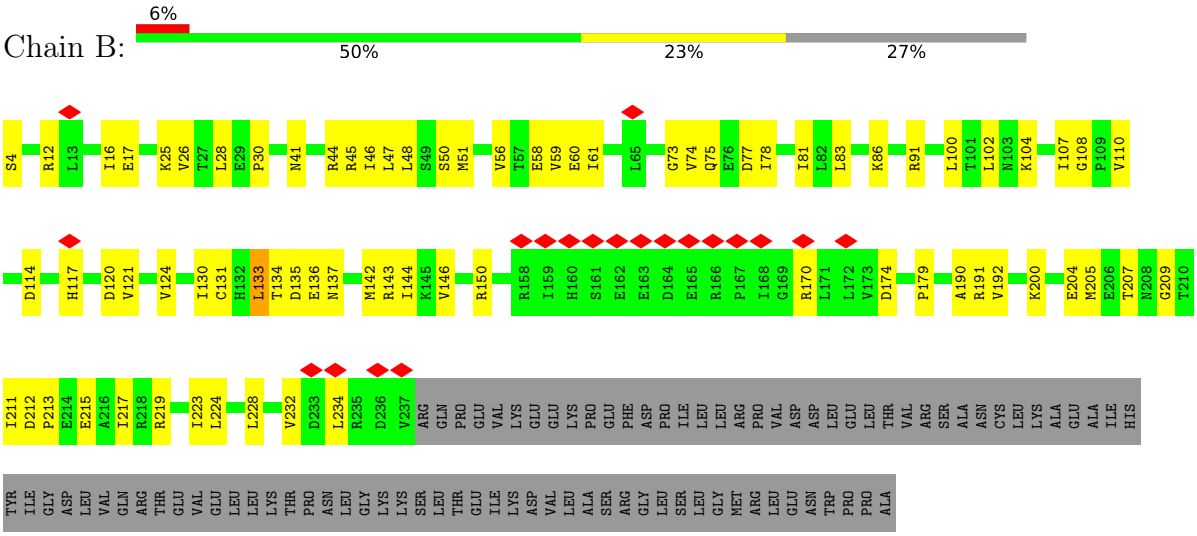
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



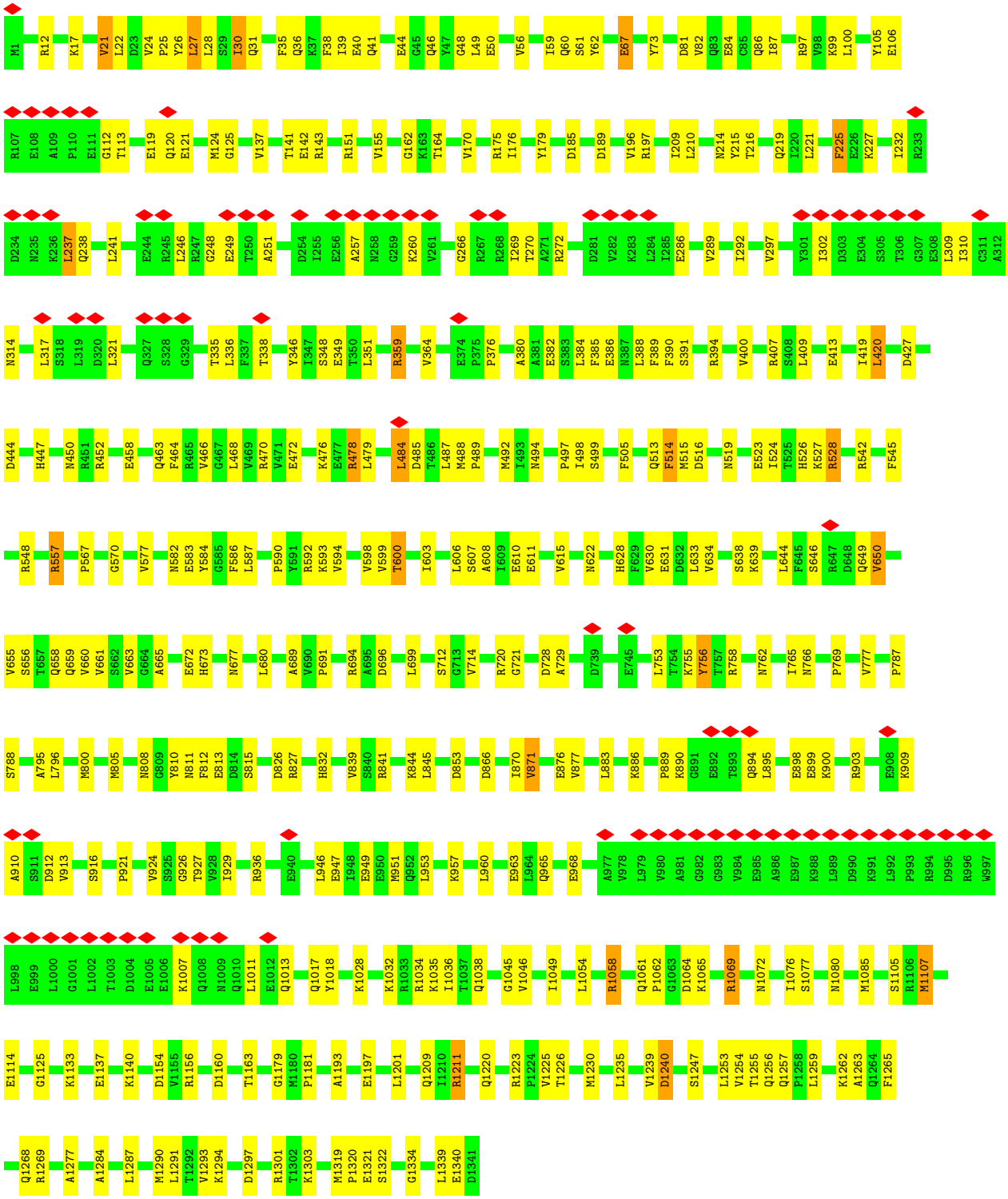
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



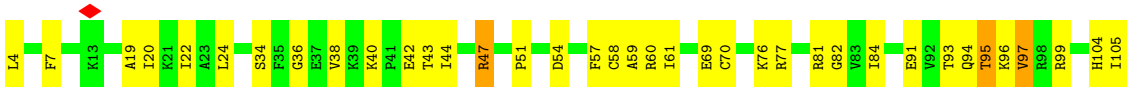
• Molecule 2: DNA-directed RNA polymerase subunit beta

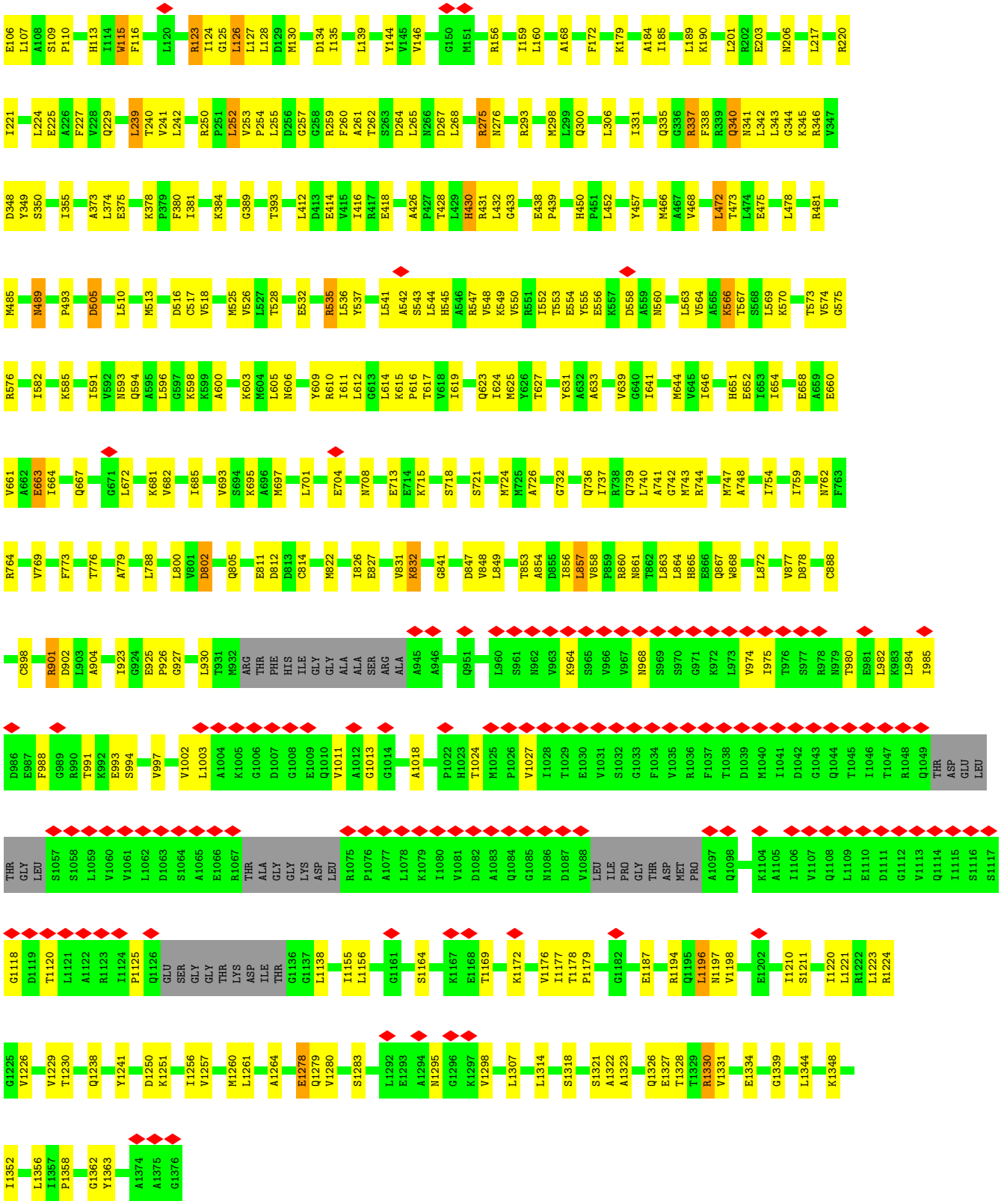
Chain C:



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

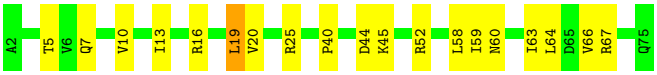
Chain D:



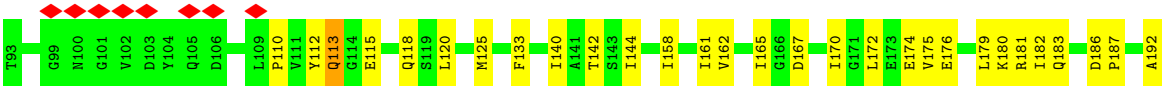


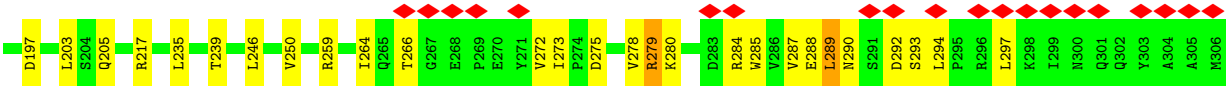
• Molecule 4: DNA-directed RNA polymerase subunit omega

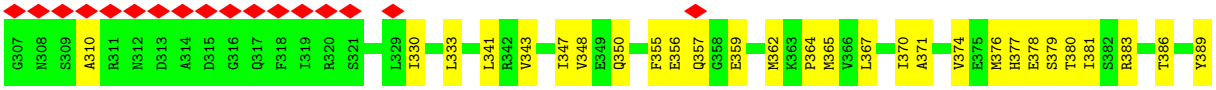
Chain E:

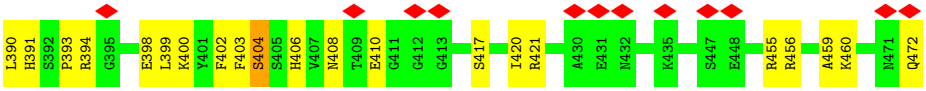


• Molecule 5: RNA polymerase sigma-54 factor

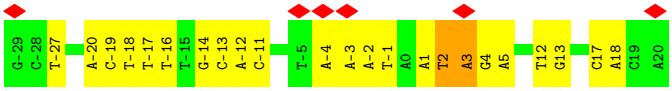








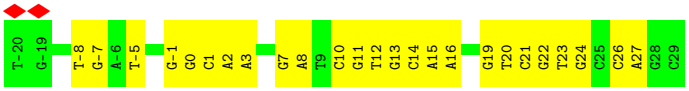
• Molecule 6: DNA (47-MER)



• Molecule 7: RNA (5'-R(P*GP*CP*CP*GP*C)-3')

There are no outlier residues recorded for this chain.

• Molecule 8: DNA (50-MER)



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	570815	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.047	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	220.0, 220.0, 220.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	0.33	0/2396	0.54	1/3252 (0.0%)
1	B	0.37	0/1752	0.54	0/2384
2	C	0.37	0/10235	0.54	2/13877 (0.0%)
3	D	0.37	0/9821	0.53	0/13343
4	E	0.40	0/548	0.60	0/743
5	M	0.32	0/2699	0.50	0/3694
6	N	0.53	0/1074	0.97	3/1652 (0.2%)
7	R	0.28	0/116	0.83	0/176
8	T	0.53	0/1157	0.88	0/1784
All	All	0.38	0/29798	0.58	6/40905 (0.0%)

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	A	0	1
2	C	0	4
3	D	0	3
All	All	0	8

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	N	2	DT	P-O3'-C3'	-9.50	108.30	119.70
2	C	237	LEU	CA-CB-CG	6.69	130.68	115.30
6	N	3	DA	P-O3'-C3'	-6.56	111.82	119.70
2	C	853	ASP	CB-CG-OD1	5.97	123.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	N	1	DA	P-O3'-C3'	-5.36	113.27	119.70
1	A	254	LEU	CA-CB-CG	5.25	127.37	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	235	ARG	Sidechain
2	C	1058	ARG	Sidechain
2	C	1156	ARG	Sidechain
2	C	528	ARG	Sidechain
2	C	557	ARG	Sidechain
3	D	1138	LEU	Peptide
3	D	1330	ARG	Sidechain
3	D	535	ARG	Sidechain

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	2365	0	2387	52	0
1	B	1733	0	1729	64	0
2	C	10080	0	9757	282	0
3	D	9685	0	9418	297	0
4	E	546	0	537	23	0
5	M	2657	0	2371	90	0
6	N	960	0	533	32	0
7	R	106	0	57	0	0
8	T	1030	0	560	20	0
9	D	1	0	0	0	0
10	D	2	0	0	0	0
All	All	29165	0	27349	789	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 14.

All (789) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:470:ARG:HD2	2:C:497:PRO:HB3	1.37	1.04
3:D:342:LEU:HD13	3:D:1352:ILE:HG12	1.41	1.02
2:C:21:VAL:HG21	2:C:592:ARG:HD2	1.38	0.99
4:E:59:ILE:HD13	4:E:63:ILE:HD11	1.45	0.98
6:N:2:DT:H3'	6:N:3:DA:H5"	1.48	0.95
1:B:108:GLY:H	1:B:133:LEU:HB3	1.32	0.94
1:B:133:LEU:HD13	1:B:133:LEU:H	1.30	0.94
3:D:428:THR:HG23	3:D:433:GLY:HA3	1.51	0.92
1:B:107:ILE:HG23	1:B:133:LEU:HG	1.52	0.91
3:D:596:LEU:HA	3:D:600:ALA:HB3	1.54	0.90
2:C:1062:PRO:HA	2:C:1076:ILE:HB	1.56	0.88
2:C:61:SER:HB3	2:C:479:LEU:HB2	1.55	0.86
4:E:10:VAL:HA	4:E:19:LEU:HD22	1.55	0.86
3:D:1220:ILE:HG23	3:D:1224:ARG:HD2	1.57	0.86
6:N:2:DT:H3'	6:N:3:DA:C5'	2.08	0.83
1:B:16:ILE:HG12	1:B:26:VAL:HG13	1.61	0.82
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.15	0.81
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.15	0.81
1:B:59:VAL:HG22	1:B:144:ILE:HG22	1.63	0.80
4:E:59:ILE:HA	4:E:63:ILE:HD11	1.64	0.80
3:D:556:GLU:HG3	3:D:558:ASP:H	1.47	0.80
5:M:167:ASP:HB3	5:M:170:ILE:HG13	1.64	0.79
3:D:44:ILE:HG22	3:D:51:PRO:HA	1.64	0.78
2:C:400:VAL:HG22	2:C:584:TYR:HD1	1.49	0.78
3:D:848:VAL:HG12	3:D:857:LEU:HD21	1.67	0.77
1:A:38:THR:HG22	1:B:45:ARG:HD3	1.65	0.77
3:D:1226:VAL:O	3:D:1230:THR:HG23	1.84	0.77
3:D:1177:ILE:HG22	3:D:1179:PRO:HD3	1.67	0.76
3:D:1155:ILE:HD13	3:D:1194:ARG:HH12	1.49	0.76
2:C:524:ILE:HD11	2:C:712:SER:HA	1.68	0.76
3:D:800:LEU:HD22	3:D:1256:ILE:HD13	1.68	0.76
3:D:547:ARG:HG2	3:D:573:THR:HG22	1.69	0.75
5:M:279:ARG:HG3	5:M:287:VAL:HG12	1.68	0.75
2:C:49:LEU:HD22	2:C:464:PHE:CD2	2.22	0.75
2:C:582:ASN:HB2	2:C:586:PHE:H	1.52	0.75
5:M:362:MET:CE	5:M:402:PHE:HA	2.18	0.74
1:A:110:VAL:HG22	1:A:131:CYS:HB3	1.68	0.74
2:C:100:LEU:HG	2:C:488:MET:HG2	1.70	0.74
2:C:660:VAL:HG21	3:D:769:VAL:HG13	1.69	0.74
2:C:841:ARG:HD2	5:M:272:VAL:HB	1.69	0.74
3:D:342:LEU:HD12	3:D:343:LEU:HG	1.69	0.74
2:C:1209:GLN:HG2	2:C:1226:THR:HG22	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:984:LEU:HD13	3:D:993:GLU:HB2	1.70	0.73
3:D:693:VAL:HG11	3:D:743:MET:HG3	1.70	0.73
3:D:1156:LEU:HB2	3:D:1223:LEU:HD12	1.71	0.73
2:C:21:VAL:HG21	2:C:592:ARG:CD	2.17	0.73
3:D:984:LEU:O	3:D:991:THR:HA	1.89	0.73
1:B:207:THR:HG22	1:B:209:GLY:H	1.54	0.72
5:M:362:MET:HE1	5:M:402:PHE:HA	1.72	0.72
1:B:104:LYS:HD3	1:B:114:ASP:HB3	1.71	0.71
3:D:426:ALA:HB1	8:T:-1:DG:H1'	1.72	0.71
2:C:841:ARG:HH21	2:C:1046:VAL:HG23	1.55	0.71
2:C:1277:ALA:HB1	3:D:431:ARG:HA	1.72	0.71
3:D:144:TYR:OH	3:D:293:ARG:NH2	2.24	0.71
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.73	0.70
3:D:275:ARG:HD3	3:D:298:MET:HB3	1.71	0.70
1:A:65:LEU:HA	1:A:169:GLY:HA2	1.73	0.70
3:D:848:VAL:HB	3:D:858:VAL:HG22	1.74	0.70
3:D:1238:GLN:NE2	3:D:1250:ASP:OD1	2.24	0.70
3:D:381:ILE:HD11	3:D:412:LEU:HD13	1.73	0.70
1:B:48:LEU:HD11	3:D:535:ARG:HG3	1.73	0.70
1:B:133:LEU:H	1:B:133:LEU:CD1	2.04	0.70
5:M:165:ILE:HG21	5:M:170:ILE:HG21	1.74	0.69
2:C:44:GLU:HB2	2:C:46:GLN:HG2	1.74	0.69
2:C:30:ILE:HG13	2:C:31:GLN:H	1.57	0.69
4:E:63:ILE:HA	4:E:66:VAL:HG22	1.73	0.69
3:D:525:MET:HE2	3:D:548:VAL:HG11	1.75	0.69
3:D:553:THR:HG22	3:D:567:THR:HG23	1.74	0.69
3:D:865:HIS:HE1	3:D:867:GLN:HB2	1.57	0.69
2:C:175:ARG:HH12	6:N:2:DT:H2"	1.57	0.69
2:C:310:ILE:HG13	2:C:321:LEU:HD11	1.74	0.69
3:D:450:HIS:HD2	3:D:452:LEU:H	1.41	0.69
3:D:606:ASN:OD1	3:D:610:ARG:NH1	2.25	0.68
5:M:367:LEU:HB3	5:M:378:GLU:HB3	1.74	0.68
2:C:38:PHE:O	2:C:48:GLY:HA2	1.93	0.68
2:C:577:VAL:HG12	2:C:663:VAL:HG22	1.73	0.68
2:C:484:LEU:HD13	2:C:485:ASP:H	1.59	0.68
1:A:109:PRO:HG3	1:A:132:HIS:NE2	2.09	0.68
2:C:444:ASP:O	2:C:450:ASN:ND2	2.26	0.68
2:C:1284:ALA:HB1	3:D:1356:LEU:HG	1.76	0.67
1:B:108:GLY:H	1:B:133:LEU:CB	2.07	0.67
3:D:552:ILE:HD12	3:D:570:LYS:HB2	1.74	0.67
2:C:463:GLN:O	2:C:466:VAL:HG12	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:221:LEU:HD22	2:C:225:PHE:HE2	1.60	0.66
3:D:542:ALA:HB1	3:D:574:VAL:HG21	1.76	0.66
2:C:1062:PRO:HA	2:C:1076:ILE:CB	2.25	0.66
3:D:438:GLU:OE2	3:D:481:ARG:NH2	2.28	0.66
5:M:378:GLU:O	5:M:381:ILE:HG12	1.96	0.66
1:A:58:GLU:HB3	1:A:172:LEU:HG	1.78	0.66
1:B:86:LYS:HE2	1:B:174:ASP:HB2	1.76	0.66
3:D:430:HIS:CE1	3:D:432:LEU:HB2	2.31	0.66
2:C:225:PHE:CD2	2:C:336:LEU:HD22	2.31	0.65
2:C:394:ARG:NH2	6:N:-2:DA:N7	2.45	0.65
2:C:1254:VAL:HG12	2:C:1255:THR:HG23	1.78	0.65
5:M:158:ILE:HD11	5:M:179:LEU:HD22	1.77	0.65
3:D:342:LEU:CD1	3:D:1352:ILE:HG12	2.21	0.65
3:D:721:SER:HA	3:D:724:MET:HE2	1.78	0.65
3:D:1226:VAL:O	3:D:1229:VAL:HG12	1.97	0.64
1:B:133:LEU:HD13	1:B:133:LEU:N	2.10	0.64
5:M:279:ARG:HH22	5:M:393:PRO:HD2	1.62	0.64
2:C:524:ILE:O	2:C:528:ARG:HG2	1.97	0.64
2:C:765:ILE:HG22	2:C:787:PRO:HG3	1.80	0.64
6:N:2:DT:H2'	6:N:3:DA:H8	1.62	0.64
1:A:58:GLU:HA	1:A:172:LEU:HA	1.79	0.64
3:D:518:VAL:HA	3:D:547:ARG:HH22	1.63	0.64
3:D:923:ILE:HD12	3:D:1256:ILE:HD12	1.80	0.64
2:C:26:TYR:O	2:C:27:LEU:HB2	1.97	0.64
2:C:413:GLU:OE2	2:C:413:GLU:N	2.28	0.64
1:B:74:VAL:HA	1:B:134:THR:HG22	1.80	0.63
5:M:120:LEU:HA	5:M:264:ILE:HD11	1.78	0.63
3:D:901:ARG:O	3:D:1251:LYS:NZ	2.31	0.63
3:D:179:LYS:HB2	3:D:184:ALA:HB2	1.80	0.63
3:D:241:VAL:HG12	3:D:242:LEU:H	1.62	0.63
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.80	0.63
2:C:390:PHE:HA	2:C:419:ILE:HB	1.79	0.63
4:E:7:GLN:HE22	4:E:16:ARG:HH22	1.46	0.63
3:D:128:LEU:HD12	3:D:135:ILE:HD11	1.81	0.63
1:B:143:ARG:HG3	1:B:143:ARG:HH11	1.64	0.63
3:D:105:ILE:HD11	3:D:242:LEU:HD23	1.81	0.63
2:C:910:ALA:O	5:M:259:ARG:NH1	2.31	0.63
2:C:839:VAL:HG22	2:C:1049:ILE:HG23	1.79	0.62
3:D:341:ASN:O	3:D:345:LYS:HG2	1.99	0.62
4:E:59:ILE:HA	4:E:63:ILE:CD1	2.29	0.62
5:M:310:ALA:HB1	6:N:-2:DA:H2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:377:HIS:CE1	8:T:14:DC:H5	2.17	0.62
3:D:36:GLY:HA3	3:D:61:ILE:HG21	1.81	0.62
1:B:179:PRO:O	1:B:207:THR:HG23	1.99	0.62
3:D:615:LYS:N	3:D:616:PRO:HD2	2.14	0.62
5:M:404:SER:HB2	5:M:406:HIS:HD2	1.64	0.62
6:N:4:DG:H2"	6:N:5:DA:H5"	1.82	0.62
8:T:10:DC:H3'	8:T:11:DG:H8	1.63	0.62
2:C:1259:LEU:HD11	5:M:115:GLU:HG3	1.80	0.61
3:D:1323:ALA:O	3:D:1328:THR:HG22	2.00	0.61
6:N:3:DA:H4'	6:N:4:DG:OP1	1.99	0.61
1:B:56:VAL:HG22	1:B:146:VAL:HG12	1.80	0.61
3:D:201:LEU:HD21	3:D:220:ARG:HH11	1.64	0.61
2:C:97:ARG:HB3	2:C:121:GLU:HG3	1.82	0.61
3:D:255:LEU:HD21	3:D:261:ALA:HB2	1.82	0.61
3:D:338:PHE:HD1	3:D:342:LEU:HD11	1.65	0.61
6:N:-13:DC:H2"	6:N:-12:DA:C8	2.36	0.61
2:C:545:PHE:CE1	3:D:788:LEU:HD12	2.36	0.61
3:D:660:GLU:O	3:D:663:GLU:HG3	2.00	0.61
3:D:556:GLU:O	3:D:563:LEU:HA	2.01	0.61
3:D:742:GLY:O	3:D:762:ASN:HB3	2.01	0.60
3:D:77:ARG:NE	3:D:77:ARG:HA	2.16	0.60
3:D:107:LEU:HD21	3:D:242:LEU:HB2	1.83	0.60
8:T:10:DC:H3'	8:T:11:DG:C8	2.36	0.60
5:M:273:ILE:HG22	5:M:275:ASP:H	1.66	0.60
3:D:1164:SER:HB3	3:D:1178:THR:H	1.67	0.60
2:C:1254:VAL:HB	5:M:113:GLN:HG2	1.84	0.60
3:D:355:ILE:HG21	3:D:466:MET:HG3	1.84	0.60
5:M:390:LEU:HD23	5:M:399:LEU:HD23	1.84	0.60
5:M:278:VAL:HG22	5:M:290:ASN:HD22	1.65	0.60
2:C:805:MET:HE2	2:C:1225:VAL:HG21	1.83	0.60
3:D:380:PHE:HZ	3:D:472:LEU:HB3	1.66	0.60
3:D:980:THR:OG1	3:D:997:VAL:O	2.19	0.60
3:D:1011:VAL:HG22	3:D:1013:GLY:H	1.66	0.60
2:C:841:ARG:CZ	2:C:1045:GLY:HA3	2.32	0.59
2:C:606:LEU:HA	2:C:610:GLU:OE1	2.02	0.59
2:C:876:GLU:HG2	2:C:927:THR:HG22	1.84	0.59
2:C:622:ASN:HB2	2:C:630:VAL:HG22	1.83	0.59
3:D:526:VAL:HA	3:D:549:LYS:O	2.03	0.59
3:D:544:LEU:HD23	3:D:574:VAL:HG12	1.84	0.59
1:B:133:LEU:HD23	1:B:135:ASP:HA	1.84	0.59
3:D:708:ASN:HA	3:D:713:GLU:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:105:TYR:HA	2:C:113:THR:HA	1.85	0.59
2:C:221:LEU:HD22	2:C:225:PHE:CE2	2.37	0.59
3:D:110:PRO:HB3	3:D:240:THR:HG22	1.85	0.59
1:B:30:PRO:HG3	1:B:192:VAL:HG21	1.83	0.59
2:C:845:LEU:HD22	2:C:845:LEU:H	1.67	0.59
3:D:4:LEU:O	3:D:81:ARG:NH1	2.35	0.59
3:D:968:ASN:HA	3:D:1118:GLY:HA3	1.85	0.58
5:M:275:ASP:HB3	5:M:391:HIS:HB2	1.85	0.58
1:B:41:ASN:OD1	1:B:44:ARG:NH2	2.36	0.58
3:D:518:VAL:HA	3:D:547:ARG:NH2	2.18	0.58
3:D:802:ASP:OD2	3:D:1348:LYS:NZ	2.26	0.58
3:D:478:LEU:HB3	4:E:20:VAL:HG13	1.86	0.58
1:A:7:GLU:OE1	1:B:150:ARG:NH2	2.36	0.58
3:D:857:LEU:HD12	3:D:858:VAL:HG13	1.85	0.58
6:N:-11:DC:O2	8:T:11:DG:N2	2.36	0.58
1:B:46:ILE:CG2	1:B:223:ILE:HD11	2.34	0.58
1:B:61:ILE:HG12	1:B:142:MET:SD	2.44	0.58
3:D:516:ASP:HB2	3:D:547:ARG:HD3	1.85	0.58
3:D:878:ASP:OD1	3:D:878:ASP:N	2.37	0.58
3:D:338:PHE:HA	3:D:342:LEU:HD11	1.84	0.58
5:M:364:PRO:HA	5:M:404:SER:O	2.03	0.58
3:D:544:LEU:HD22	3:D:575:GLY:HA2	1.85	0.57
2:C:389:PHE:HB3	2:C:420:LEU:HD11	1.85	0.57
2:C:1247:SER:HB3	3:D:375:GLU:O	2.04	0.57
2:C:1253:LEU:HG	5:M:115:GLU:N	2.19	0.57
3:D:38:VAL:HB	3:D:105:ILE:HG22	1.85	0.57
3:D:412:LEU:O	3:D:416:ILE:HG12	2.03	0.57
2:C:189:ASP:OD1	2:C:189:ASP:N	2.35	0.57
2:C:921:PRO:HG2	2:C:924:VAL:HG21	1.87	0.57
2:C:1255:THR:HG21	3:D:341:ASN:ND2	2.19	0.57
5:M:287:VAL:HG11	5:M:348:VAL:HG21	1.85	0.57
2:C:672:GLU:HG2	2:C:673:HIS:CD2	2.40	0.57
3:D:217:LEU:O	3:D:221:ILE:HG12	2.04	0.57
5:M:297:LEU:HD22	5:M:333:LEU:HD22	1.86	0.57
3:D:863:LEU:HD13	3:D:864:LEU:N	2.19	0.57
2:C:106:GLU:N	2:C:112:GLY:O	2.31	0.57
2:C:248:GLY:HA2	2:C:269:ILE:HD12	1.86	0.57
3:D:203:GLU:HA	3:D:206:ASN:HD21	1.68	0.57
3:D:974:VAL:HG22	3:D:1002:VAL:HG22	1.86	0.57
2:C:1062:PRO:HA	2:C:1076:ILE:CG2	2.34	0.57
5:M:343:VAL:O	5:M:347:ILE:HG13	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:815:SER:HB3	2:C:1077:SER:HB3	1.87	0.57
3:D:536:LEU:HD22	3:D:541:LEU:HD12	1.86	0.57
3:D:847:ASP:HB3	3:D:856:ILE:HG21	1.86	0.56
2:C:753:LEU:CD1	2:C:769:PRO:HG3	2.35	0.56
4:E:13:ILE:HD12	4:E:13:ILE:O	2.05	0.56
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.87	0.56
2:C:400:VAL:HG22	2:C:584:TYR:CD1	2.37	0.56
3:D:113:HIS:ND1	3:D:115:TRP:HB2	2.21	0.56
1:A:120:ASP:OD1	1:A:120:ASP:N	2.39	0.56
3:D:594:GLN:HG3	3:D:596:LEU:HD12	1.87	0.56
1:A:158:ARG:HH21	1:A:172:LEU:HD23	1.71	0.56
1:B:207:THR:HG21	1:B:211:ILE:O	2.06	0.56
2:C:143:ARG:NH2	2:C:513:GLN:HA	2.21	0.56
2:C:1277:ALA:CB	3:D:431:ARG:HA	2.35	0.56
8:T:2:DA:H2'	8:T:3:DA:C8	2.40	0.56
5:M:347:ILE:HG23	5:M:365:MET:HE1	1.88	0.56
5:M:417:SER:O	5:M:421:ARG:N	2.30	0.56
6:N:-20:DA:H2"	6:N:-19:DC:H5"	1.87	0.56
3:D:342:LEU:O	3:D:343:LEU:HB2	2.05	0.55
2:C:1262:LYS:HG2	2:C:1263:ALA:H	1.70	0.55
8:T:23:DT:H2'	8:T:24:DG:C8	2.41	0.55
8:T:21:DC:H2"	8:T:22:DG:C8	2.42	0.55
2:C:185:ASP:HB2	2:C:197:ARG:HB3	1.89	0.55
2:C:548:ARG:HB3	2:C:570:GLY:HA3	1.88	0.55
2:C:1223:ARG:HH12	3:D:724:MET:HE1	1.70	0.55
3:D:201:LEU:HB3	3:D:221:ILE:HD11	1.87	0.55
3:D:736:GLN:HA	3:D:739:GLN:HE21	1.71	0.55
5:M:362:MET:HE3	5:M:402:PHE:HA	1.88	0.55
5:M:406:HIS:HB2	5:M:417:SER:H	1.71	0.55
1:A:260:LEU:HB3	1:A:306:VAL:HG11	1.87	0.55
2:C:227:LYS:HA	2:C:336:LEU:HA	1.89	0.55
3:D:576:ARG:HD3	3:D:593:ASN:HA	1.89	0.55
4:E:5:THR:CG2	4:E:7:GLN:HG2	2.37	0.55
4:E:60:ASN:H	4:E:63:ILE:HG12	1.71	0.55
3:D:123:ARG:HA	3:D:126:LEU:HD23	1.87	0.55
4:E:16:ARG:HA	4:E:19:LEU:HD21	1.89	0.55
1:A:111:THR:HG22	1:A:129:VAL:HA	1.87	0.55
2:C:1035:LYS:HA	2:C:1038:GLN:NE2	2.22	0.55
1:B:133:LEU:O	1:B:133:LEU:HD22	2.06	0.54
2:C:394:ARG:HH22	6:N:-2:DA:H62	1.55	0.54
2:C:289:VAL:O	2:C:292:ILE:HG22	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:811:ASN:HA	2:C:815:SER:HB2	1.88	0.54
1:A:61:ILE:HB	1:A:64:VAL:HG22	1.89	0.54
2:C:1293:VAL:O	2:C:1294:LYS:HB3	2.08	0.54
5:M:404:SER:HB2	5:M:406:HIS:CD2	2.42	0.54
1:B:219:ARG:O	1:B:223:ILE:HG23	2.07	0.54
2:C:56:VAL:HG21	2:C:468:LEU:HB3	1.89	0.54
3:D:84:ILE:HD13	3:D:91:GLU:HB2	1.90	0.54
2:C:1137:GLU:OE2	2:C:1137:GLU:N	2.36	0.54
1:A:214:GLU:O	1:A:218:ARG:HG2	2.07	0.54
3:D:128:LEU:HB3	3:D:130:MET:HG2	1.90	0.54
1:A:59:VAL:HB	1:A:171:LEU:HB2	1.89	0.54
2:C:545:PHE:CZ	3:D:788:LEU:HD12	2.43	0.54
2:C:895:LEU:O	2:C:900:LYS:HE3	2.07	0.54
2:C:407:ARG:HH11	2:C:407:ARG:HG3	1.72	0.54
2:C:380:ALA:O	2:C:384:LEU:HG	2.08	0.54
2:C:1137:GLU:H	2:C:1137:GLU:CD	2.11	0.54
2:C:484:LEU:HD13	2:C:485:ASP:N	2.22	0.53
3:D:220:ARG:O	3:D:224:LEU:HG	2.08	0.53
3:D:346:ARG:NH2	8:T:0:DG:OP1	2.41	0.53
3:D:594:GLN:NE2	3:D:600:ALA:HB1	2.23	0.53
1:A:234:LEU:HD13	1:B:26:VAL:HG11	1.91	0.53
2:C:953:LEU:O	2:C:957:LYS:HG3	2.07	0.53
3:D:609:TYR:HD1	3:D:617:THR:HG21	1.72	0.53
2:C:237:LEU:HD23	2:C:237:LEU:O	2.08	0.53
1:A:110:VAL:CG2	1:A:131:CYS:HB3	2.36	0.53
1:B:102:LEU:HG	1:B:142:MET:HB2	1.90	0.53
2:C:232:ILE:HA	2:C:237:LEU:HA	1.90	0.53
3:D:644:MET:O	3:D:764:ARG:NH1	2.41	0.53
5:M:365:MET:O	5:M:403:PHE:HA	2.09	0.53
2:C:216:THR:HG23	2:C:219:GLN:H	1.73	0.53
2:C:756:TYR:HD1	2:C:756:TYR:H	1.56	0.53
2:C:1069:ARG:NH1	2:C:1114:GLU:OE2	2.42	0.53
2:C:548:ARG:NH2	2:C:567:PRO:O	2.41	0.53
3:D:493:PRO:HB3	3:D:904:ALA:HB2	1.91	0.53
5:M:176:GLU:O	5:M:180:LYS:HG3	2.09	0.53
5:M:278:VAL:HG23	5:M:288:GLU:HG3	1.90	0.53
3:D:418:GLU:O	4:E:45:LYS:HD2	2.09	0.53
2:C:384:LEU:O	2:C:388:LEU:HG	2.09	0.53
5:M:367:LEU:CD2	5:M:403:PHE:HE1	2.22	0.53
2:C:141:THR:HG22	2:C:142:GLU:H	1.73	0.52
2:C:936:ARG:NH1	2:C:1046:VAL:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:704:GLU:H	3:D:718:SER:HB3	1.73	0.52
3:D:1187:GLU:OE1	3:D:1187:GLU:N	2.42	0.52
2:C:175:ARG:HH12	6:N:2:DT:C2'	2.22	0.52
2:C:1255:THR:HB	2:C:1322:SER:OG	2.09	0.52
6:N:4:DG:N3	6:N:4:DG:H2'	2.24	0.52
2:C:314:ASN:HD21	2:C:351:LEU:HD13	1.74	0.52
3:D:34:SER:HB2	3:D:104:HIS:HB3	1.91	0.52
2:C:36:GLN:O	2:C:40:GLU:HB3	2.10	0.52
3:D:337:ARG:NE	3:D:341:ASN:OD1	2.43	0.52
3:D:697:MET:SD	3:D:741:ALA:HB3	2.49	0.52
2:C:1294:LYS:HE3	3:D:349:TYR:HB2	1.92	0.52
6:N:17:DC:H2"	6:N:18:DA:C8	2.45	0.52
1:A:20:SER:OG	1:A:21:SER:N	2.42	0.52
2:C:646:SER:H	2:C:649:GLN:NE2	2.08	0.52
3:D:201:LEU:HD21	3:D:220:ARG:NH1	2.24	0.52
3:D:513:MET:HG2	3:D:544:LEU:HD13	1.92	0.52
3:D:556:GLU:HB3	3:D:564:VAL:HG13	1.92	0.52
2:C:1032:LYS:O	2:C:1036:ILE:HG13	2.10	0.52
5:M:125:MET:HE1	5:M:142:THR:HG22	1.90	0.52
1:B:91:ARG:HH21	1:B:124:VAL:HG12	1.75	0.51
2:C:805:MET:CE	2:C:1225:VAL:HG21	2.40	0.51
1:B:133:LEU:HD23	1:B:135:ASP:CA	2.41	0.51
2:C:25:PRO:HG2	2:C:27:LEU:CD1	2.40	0.51
2:C:1255:THR:O	2:C:1257:GLN:HG3	2.10	0.51
2:C:1297:ASP:O	2:C:1301:ARG:HG3	2.10	0.51
3:D:773:PHE:O	3:D:776:THR:OG1	2.28	0.51
3:D:614:LEU:O	3:D:617:THR:HG22	2.11	0.51
3:D:542:ALA:HB1	3:D:574:VAL:CG2	2.38	0.51
2:C:557:ARG:HB3	2:C:587:LEU:HD13	1.91	0.51
3:D:726:ALA:HB2	3:D:737:ILE:HD11	1.93	0.51
2:C:622:ASN:HB2	2:C:630:VAL:CG2	2.40	0.51
3:D:556:GLU:CG	3:D:558:ASP:HB2	2.40	0.51
2:C:251:ALA:HB3	2:C:266:GLY:H	1.75	0.51
2:C:633:LEU:HB3	2:C:644:LEU:HD12	1.93	0.51
3:D:338:PHE:CD1	3:D:342:LEU:HD11	2.46	0.51
3:D:489:ASN:ND2	3:D:489:ASN:O	2.44	0.51
3:D:582:ILE:HD12	3:D:623:GLN:HB3	1.93	0.51
5:M:140:ILE:O	5:M:144:ILE:HG23	2.11	0.51
5:M:400:LYS:HA	5:M:403:PHE:CE2	2.46	0.51
1:A:218:ARG:NH2	1:B:234:LEU:HB3	2.25	0.51
3:D:43:THR:HB	3:D:57:PHE:CD1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:384:LYS:NZ	3:D:414:GLU:HG3	2.26	0.51
5:M:374:VAL:HG23	5:M:376:MET:HB3	1.93	0.51
1:A:166:ARG:NH2	2:C:876:GLU:OE2	2.44	0.51
3:D:255:LEU:HD21	3:D:261:ALA:CB	2.41	0.51
5:M:472:GLN:HA	6:N:-27:DT:H4'	1.93	0.51
6:N:-3:DA:H4'	6:N:-2:DA:OP1	2.11	0.51
3:D:253:VAL:HG22	5:M:112:TYR:CD2	2.45	0.50
1:A:321:TRP:HA	1:A:321:TRP:CE3	2.46	0.50
5:M:285:TRP:CZ3	5:M:355:PHE:HB3	2.47	0.50
2:C:297:VAL:HB	2:C:317:LEU:HD21	1.93	0.50
2:C:658:GLN:O	2:C:661:VAL:HG12	2.12	0.50
3:D:556:GLU:HG3	3:D:558:ASP:HB2	1.92	0.50
3:D:902:ASP:OD1	3:D:902:ASP:N	2.42	0.50
5:M:162:VAL:HG22	5:M:175:VAL:HG21	1.93	0.50
3:D:1327:GLU:HB3	8:T:-5:DT:OP1	2.11	0.50
1:B:50:SER:O	1:B:50:SER:OG	2.27	0.50
2:C:24:VAL:HG13	2:C:25:PRO:HD2	1.93	0.50
2:C:400:VAL:HG11	2:C:452:ARG:HD2	1.94	0.50
8:T:1:DC:C2	8:T:2:DA:C8	3.00	0.50
2:C:606:LEU:HB3	2:C:610:GLU:HB2	1.94	0.50
2:C:810:TYR:O	2:C:1077:SER:OG	2.21	0.50
2:C:844:LYS:HE2	5:M:389:TYR:CE2	2.47	0.50
1:B:215:GLU:OE1	1:B:219:ARG:NE	2.44	0.50
2:C:48:GLY:C	2:C:50:GLU:N	2.65	0.50
2:C:800:MET:HE2	2:C:827:ARG:HH21	1.77	0.50
3:D:337:ARG:NH2	5:M:110:PRO:HG3	2.26	0.50
2:C:519:ASN:ND2	2:C:689:ALA:O	2.44	0.50
2:C:889:PRO:HA	2:C:913:VAL:HG12	1.93	0.50
3:D:38:VAL:HB	3:D:105:ILE:CG2	2.42	0.50
3:D:1169:THR:HG22	3:D:1176:VAL:H	1.76	0.50
2:C:297:VAL:HA	2:C:335:THR:HG22	1.93	0.50
3:D:560:ASN:N	3:D:560:ASN:OD1	2.44	0.50
5:M:365:MET:SD	5:M:370:ILE:HD11	2.51	0.50
2:C:86:GLN:NE2	2:C:142:GLU:OE2	2.45	0.49
3:D:430:HIS:NE2	3:D:432:LEU:HB2	2.27	0.49
5:M:408:ASN:HD21	5:M:410:GLU:HB2	1.77	0.49
1:A:12:ARG:H	1:A:30:PRO:HD2	1.77	0.49
2:C:841:ARG:CD	5:M:272:VAL:HB	2.40	0.49
3:D:264:ASP:OD1	3:D:264:ASP:N	2.45	0.49
3:D:1278:GLU:OE1	3:D:1283:SER:HB2	2.12	0.49
5:M:144:ILE:HD11	5:M:182:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HD13	1:A:36:GLY:HA2	1.93	0.49
3:D:1327:GLU:HG2	3:D:1330:ARG:HH21	1.75	0.49
5:M:186:ASP:HB3	5:M:187:PRO:HD3	1.94	0.49
2:C:608:ALA:O	2:C:611:GLU:HG2	2.13	0.49
2:C:677:ASN:HB3	3:D:779:ALA:HB1	1.93	0.49
2:C:927:THR:O	2:C:929:ILE:HG12	2.13	0.49
3:D:20:ILE:HD12	3:D:1344:LEU:HD21	1.95	0.49
4:E:5:THR:HG22	4:E:7:GLN:HG2	1.95	0.49
2:C:1319:MET:SD	2:C:1320:PRO:HD2	2.52	0.49
2:C:56:VAL:HG13	2:C:472:GLU:OE1	2.13	0.49
2:C:179:TYR:OH	2:C:458:GLU:OE2	2.20	0.49
2:C:894:GLN:O	2:C:894:GLN:HG2	2.12	0.49
3:D:125:GLY:HA2	3:D:135:ILE:CD1	2.42	0.49
3:D:927:GLY:HA2	3:D:930:LEU:HD12	1.93	0.49
5:M:377:HIS:ND1	5:M:379:SER:HB3	2.27	0.49
1:A:39:LEU:O	1:A:43:LEU:HG	2.13	0.49
2:C:832:HIS:CD2	2:C:1058:ARG:HG3	2.48	0.49
3:D:510:LEU:HD11	3:D:624:ILE:HG23	1.95	0.49
5:M:356:GLU:HG2	5:M:357:GLN:HG3	1.94	0.49
1:A:280:ASP:OD1	1:A:281:LEU:N	2.46	0.49
2:C:691:PRO:HB3	2:C:788:SER:HB3	1.95	0.49
2:C:949:GLU:O	2:C:953:LEU:HG	2.13	0.49
3:D:107:LEU:HD12	3:D:239:LEU:O	2.13	0.49
3:D:550:VAL:O	3:D:552:ILE:HG13	2.12	0.49
1:B:25:LYS:HG3	1:B:204:GLU:HG3	1.95	0.49
2:C:1061:GLN:HB2	2:C:1062:PRO:HD2	1.94	0.49
2:C:60:GLN:HB3	2:C:67:GLU:OE2	2.13	0.48
2:C:577:VAL:HG12	2:C:663:VAL:CG2	2.43	0.48
3:D:225:GLU:O	3:D:229:GLN:HG2	2.13	0.48
3:D:664:ILE:HD13	3:D:682:VAL:HG23	1.94	0.48
4:E:60:ASN:OD1	4:E:63:ILE:HG23	2.12	0.48
6:N:-4:DA:H4'	6:N:-3:DA:OP1	2.10	0.48
1:A:170:ARG:O	1:A:171:LEU:HD13	2.12	0.48
3:D:984:LEU:HB2	3:D:993:GLU:H	1.79	0.48
1:A:279:GLY:O	1:A:282:VAL:HG22	2.13	0.48
1:B:16:ILE:HG23	1:B:26:VAL:HG22	1.95	0.48
2:C:41:GLN:HG2	2:C:73:TYR:CZ	2.48	0.48
2:C:494:ASN:O	2:C:497:PRO:HD2	2.13	0.48
1:B:102:LEU:HD11	1:B:142:MET:HG3	1.95	0.48
2:C:137:VAL:HA	2:C:141:THR:O	2.13	0.48
3:D:262:THR:OG1	3:D:267:ASP:OD1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:-17:DT:C2'	6:N:-16:DT:H71	2.44	0.48
2:C:81:ASP:OD2	2:C:84:GLU:HG3	2.14	0.48
2:C:249:GLU:H	2:C:269:ILE:HD13	1.78	0.48
2:C:524:ILE:HD11	2:C:712:SER:CA	2.42	0.48
3:D:433:GLY:O	3:D:457:TYR:HE1	1.96	0.48
3:D:1027:VAL:H	3:D:1120:THR:HG21	1.78	0.48
5:M:390:LEU:HD23	5:M:399:LEU:CD2	2.44	0.48
1:B:77:ASP:OD2	1:B:78:ILE:N	2.46	0.48
2:C:241:LEU:HD23	2:C:241:LEU:H	1.77	0.48
2:C:646:SER:OG	2:C:649:GLN:HG3	2.14	0.48
3:D:203:GLU:HA	3:D:206:ASN:ND2	2.29	0.48
3:D:1196:LEU:HD13	3:D:1210:ILE:O	2.14	0.48
5:M:404:SER:HA	5:M:406:HIS:NE2	2.28	0.48
2:C:516:ASP:O	2:C:523:GLU:HG2	2.13	0.48
2:C:832:HIS:CD2	2:C:1058:ARG:CG	2.97	0.48
3:D:450:HIS:CD2	3:D:452:LEU:H	2.26	0.48
2:C:1247:SER:O	3:D:348:ASP:HB3	2.14	0.48
6:N:12:DT:H2"	6:N:13:DG:C8	2.49	0.48
2:C:41:GLN:HG2	2:C:73:TYR:OH	2.14	0.48
3:D:853:THR:O	3:D:854:ALA:HB3	2.14	0.48
5:M:408:ASN:ND2	5:M:410:GLU:HB2	2.29	0.48
3:D:1155:ILE:HD13	3:D:1194:ARG:NH1	2.22	0.47
3:D:1221:LEU:HD12	3:D:1229:VAL:HG11	1.96	0.47
2:C:542:ARG:HA	6:N:4:DG:H5'	1.96	0.47
3:D:1358:PRO:O	3:D:1363:TYR:HD1	1.96	0.47
4:E:16:ARG:H	4:E:19:LEU:HD21	1.79	0.47
2:C:336:LEU:HD12	2:C:338:THR:H	1.79	0.47
2:C:871:VAL:HG13	2:C:883:LEU:HA	1.96	0.47
3:D:554:GLU:HB2	3:D:566:LYS:HE3	1.96	0.47
2:C:12:ARG:HG2	2:C:1181:PRO:HB2	1.96	0.47
2:C:720:ARG:O	2:C:720:ARG:HG2	2.14	0.47
3:D:1295:ASN:OD1	3:D:1295:ASN:N	2.44	0.47
1:B:58:GLU:HA	1:B:170:ARG:O	2.15	0.47
3:D:338:PHE:HA	3:D:342:LEU:CD1	2.44	0.47
6:N:-18:DT:C6	6:N:-17:DT:H72	2.50	0.47
2:C:385:PHE:CE1	2:C:390:PHE:HZ	2.32	0.47
3:D:1264:ALA:HB2	3:D:1280:VAL:HG22	1.96	0.47
6:N:4:DG:H2"	6:N:5:DA:C8	2.50	0.47
2:C:812:PHE:CD1	2:C:813:GLU:HG2	2.49	0.47
3:D:338:PHE:HA	3:D:342:LEU:CG	2.44	0.47
3:D:537:TYR:CE2	3:D:631:TYR:HE1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:553:THR:HA	3:D:567:THR:HA	1.97	0.47
3:D:681:LYS:O	3:D:685:ILE:HG23	2.14	0.47
3:D:732:GLY:HA2	3:D:736:GLN:OE1	2.15	0.47
4:E:10:VAL:HA	4:E:19:LEU:CD2	2.38	0.47
5:M:278:VAL:HG12	5:M:391:HIS:HB3	1.96	0.47
1:A:279:GLY:HA3	1:A:321:TRP:CH2	2.49	0.47
2:C:225:PHE:HE1	2:C:346:TYR:O	1.97	0.47
2:C:523:GLU:O	2:C:527:LYS:HG3	2.15	0.47
3:D:1024:THR:HG23	3:D:1125:PRO:HG3	1.96	0.47
2:C:100:LEU:H	2:C:100:LEU:HD23	1.79	0.47
2:C:238:GLN:HA	2:C:286:GLU:HA	1.97	0.47
2:C:1105:SER:HA	3:D:736:GLN:OE1	2.14	0.47
5:M:287:VAL:CG1	5:M:348:VAL:HG11	2.45	0.47
2:C:444:ASP:HB3	2:C:447:HIS:HB2	1.96	0.47
2:C:468:LEU:HD23	2:C:498:ILE:HD11	1.95	0.46
3:D:124:ILE:HD11	3:D:185:ILE:HG21	1.97	0.46
8:T:12:DT:H2"	8:T:13:DG:C8	2.49	0.46
1:A:255:ARG:O	1:A:278:ILE:HG12	2.16	0.46
2:C:1340:GLU:HG3	3:D:19:ALA:O	2.14	0.46
5:M:279:ARG:HG2	5:M:280:LYS:N	2.30	0.46
2:C:1339:LEU:HD23	3:D:20:ILE:HG12	1.96	0.46
3:D:40:LYS:HG2	3:D:54:ASP:O	2.16	0.46
3:D:849:LEU:HD12	3:D:856:ILE:HG23	1.96	0.46
1:A:131:CYS:SG	1:A:132:HIS:N	2.89	0.46
2:C:514:PHE:HD1	2:C:514:PHE:H	1.63	0.46
2:C:677:ASN:O	2:C:680:LEU:HB3	2.15	0.46
3:D:335:GLN:HA	3:D:340:GLN:NE2	2.30	0.46
5:M:403:PHE:O	5:M:404:SER:C	2.53	0.46
2:C:728:ASP:OD1	2:C:729:ALA:N	2.47	0.46
2:C:796:LEU:HD23	2:C:796:LEU:H	1.80	0.46
3:D:473:THR:HG22	3:D:475:GLU:H	1.81	0.46
2:C:210:LEU:O	2:C:215:TYR:HB2	2.16	0.46
3:D:549:LYS:HE3	3:D:569:LEU:HD21	1.97	0.46
1:A:17:GLU:HG3	1:A:25:LYS:HB2	1.97	0.46
2:C:926:GLY:HA3	2:C:1054:LEU:HB3	1.97	0.46
2:C:593:LYS:HB3	2:C:600:THR:HG23	1.98	0.46
2:C:1334:GLY:H	3:D:113:HIS:HE2	1.62	0.46
3:D:543:SER:O	3:D:574:VAL:HB	2.15	0.46
1:B:48:LEU:CD1	3:D:535:ARG:HG3	2.42	0.46
2:C:519:ASN:O	2:C:523:GLU:HG3	2.16	0.46
3:D:93:THR:HG22	3:D:94:GLN:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:373:ALA:O	3:D:374:LEU:HB3	2.16	0.46
5:M:371:ALA:HB2	5:M:378:GLU:HG2	1.98	0.46
1:A:70:THR:CG2	2:C:755:LYS:HE2	2.45	0.46
2:C:464:PHE:CE2	2:C:468:LEU:HD11	2.51	0.46
2:C:1140:LYS:HE2	2:C:1140:LYS:HB3	1.58	0.46
3:D:254:PRO:C	3:D:255:LEU:HD22	2.37	0.46
3:D:416:ILE:HG23	3:D:439:PRO:HG2	1.96	0.46
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.98	0.46
3:D:1356:LEU:HD23	3:D:1362:GLY:HA2	1.97	0.46
1:B:212:ASP:OD1	1:B:213:PRO:HD2	2.16	0.45
2:C:125:GLY:HA2	2:C:499:SER:HB3	1.98	0.45
3:D:1260:MET:HG2	3:D:1307:LEU:O	2.15	0.45
2:C:965:GLN:O	2:C:968:GLU:HG3	2.16	0.45
5:M:235:LEU:O	5:M:239:THR:HG23	2.15	0.45
1:B:73:GLY:O	1:B:134:THR:HB	2.16	0.45
3:D:1003:LEU:HA	3:D:1018:ALA:HA	1.98	0.45
5:M:294:LEU:HD11	5:M:330:ILE:HG23	1.98	0.45
5:M:456:ARG:HD2	5:M:459:ALA:HB3	1.98	0.45
2:C:151:ARG:HD2	6:N:3:DA:H62	1.82	0.45
3:D:82:GLY:HA2	3:D:91:GLU:OE1	2.17	0.45
3:D:146:VAL:HB	3:D:160:LEU:HD21	1.98	0.45
4:E:40:PRO:O	4:E:52:ARG:NH2	2.47	0.45
1:A:64:VAL:HG11	1:A:78:ILE:HD12	1.97	0.45
2:C:841:ARG:HG3	2:C:1045:GLY:O	2.16	0.45
5:M:383:ARG:NH2	6:N:-14:DG:O6	2.49	0.45
1:A:104:LYS:HZ2	1:A:110:VAL:HG12	1.81	0.45
2:C:67:GLU:OE2	2:C:67:GLU:HA	2.17	0.45
2:C:196:VAL:HG21	2:C:209:ILE:HG21	1.99	0.45
2:C:886:LYS:HB3	2:C:916:SER:O	2.17	0.45
3:D:94:GLN:O	3:D:95:THR:HB	2.17	0.45
3:D:257:GLY:HA2	5:M:272:VAL:O	2.15	0.45
3:D:555:TYR:HB3	3:D:563:LEU:HB3	1.98	0.45
5:M:417:SER:HA	5:M:420:ILE:HB	1.99	0.45
1:B:60:GLU:HB3	1:B:143:ARG:CZ	2.47	0.45
2:C:1034:ARG:O	2:C:1038:GLN:HG3	2.17	0.45
3:D:537:TYR:HA	3:D:542:ALA:O	2.17	0.45
3:D:964:LYS:H	3:D:975:ILE:HG23	1.81	0.45
5:M:370:ILE:O	5:M:374:VAL:HG22	2.16	0.45
2:C:214:ASN:OD1	2:C:359:ARG:HG3	2.16	0.45
2:C:661:VAL:HG22	2:C:665:ALA:HB3	1.98	0.45
3:D:105:ILE:HG12	3:D:242:LEU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:872:LEU:HB2	3:D:877:VAL:HG11	1.98	0.45
5:M:292:ASP:OD1	5:M:293:SER:N	2.50	0.45
2:C:1193:ALA:O	2:C:1197:GLU:HG2	2.16	0.45
2:C:1303:LYS:HB2	2:C:1303:LYS:HE3	1.84	0.45
3:D:418:GLU:H	4:E:45:LYS:HE2	1.82	0.45
6:N:-2:DA:H1'	6:N:-1:DT:C2	2.51	0.45
2:C:899:GLU:O	2:C:903:ARG:HG3	2.17	0.45
2:C:1065:LYS:HD3	2:C:1235:LEU:HD12	1.99	0.45
3:D:663:GLU:O	3:D:667:GLN:HG3	2.17	0.45
1:B:46:ILE:HD11	1:B:224:LEU:HD13	1.98	0.44
3:D:744:ARG:HB3	3:D:759:ILE:HB	1.98	0.44
3:D:930:LEU:HD11	3:D:1241:TYR:CE1	2.52	0.44
3:D:1220:ILE:CG2	3:D:1224:ARG:HD2	2.37	0.44
1:B:46:ILE:HG23	1:B:223:ILE:HD11	1.99	0.44
2:C:175:ARG:NH1	6:N:2:DT:H2"	2.30	0.44
2:C:877:VAL:HG22	2:C:926:GLY:O	2.17	0.44
3:D:505:ASP:OD1	3:D:505:ASP:N	2.49	0.44
3:D:1196:LEU:HD12	3:D:1198:VAL:O	2.17	0.44
2:C:1133:LYS:HD3	2:C:1133:LYS:HA	1.82	0.44
2:C:1226:THR:HG21	3:D:639:VAL:O	2.16	0.44
3:D:7:PHE:HD1	3:D:7:PHE:H	1.65	0.44
3:D:96:LYS:O	3:D:99:ARG:HG3	2.16	0.44
3:D:116:PHE:O	3:D:124:ILE:HG22	2.17	0.44
3:D:416:ILE:CG2	3:D:439:PRO:HG2	2.47	0.44
3:D:841:GLY:HA2	3:D:863:LEU:HD11	1.99	0.44
5:M:183:GLN:HE21	5:M:192:ALA:HA	1.82	0.44
5:M:403:PHE:H	5:M:403:PHE:HD2	1.65	0.44
1:A:104:LYS:NZ	1:A:110:VAL:HG12	2.32	0.44
1:B:81:ILE:HD12	1:B:131:CYS:HB3	1.99	0.44
2:C:488:MET:HB2	2:C:489:PRO:CD	2.47	0.44
3:D:342:LEU:C	3:D:344:GLY:H	2.20	0.44
3:D:654:ILE:O	3:D:658:GLU:HG3	2.18	0.44
5:M:367:LEU:HD21	5:M:403:PHE:HE1	1.81	0.44
2:C:542:ARG:HA	6:N:4:DG:C5'	2.48	0.44
2:C:753:LEU:HD12	2:C:769:PRO:HG3	1.99	0.44
2:C:1160:ASP:OD2	2:C:1163:THR:HG23	2.18	0.44
2:C:1256:GLN:HG3	2:C:1321:GLU:HG3	2.00	0.44
3:D:516:ASP:HA	3:D:545:HIS:O	2.17	0.44
8:T:7:DG:H2"	8:T:8:DA:C8	2.52	0.44
1:A:231:PHE:CZ	1:B:28:LEU:HD22	2.51	0.44
1:B:104:LYS:HG3	1:B:110:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:48:GLY:C	2:C:50:GLU:H	2.21	0.44
2:C:634:VAL:HG21	2:C:650:VAL:HG11	2.00	0.44
2:C:1269:ARG:HD3	8:T:-1:DG:H5'	2.00	0.44
3:D:106:GLU:O	3:D:276:ASN:ND2	2.51	0.44
3:D:127:LEU:HD23	3:D:189:LEU:HD11	1.99	0.44
3:D:536:LEU:HB3	3:D:541:LEU:HB2	1.99	0.44
3:D:591:ILE:O	3:D:594:GLN:NE2	2.51	0.44
5:M:278:VAL:HG23	5:M:288:GLU:CG	2.48	0.44
1:A:96:ASP:O	1:A:147:GLN:HA	2.18	0.44
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.98	0.44
2:C:141:THR:HG21	2:C:514:PHE:CE2	2.52	0.44
3:D:254:PRO:HA	3:D:260:PHE:CD1	2.53	0.44
3:D:255:LEU:HB2	3:D:259:ARG:O	2.17	0.44
1:A:70:THR:HG21	2:C:755:LYS:HE2	2.00	0.44
2:C:119:GLU:HG2	2:C:120:GLN:H	1.82	0.44
5:M:203:LEU:HD13	5:M:217:ARG:HA	1.99	0.44
1:A:159:ILE:HD13	1:A:159:ILE:HA	1.85	0.44
2:C:221:LEU:HD11	2:C:313:ALA:HB1	1.99	0.44
5:M:289:LEU:HD12	5:M:341:LEU:HB2	2.00	0.44
5:M:456:ARG:HD2	5:M:456:ARG:HA	1.80	0.44
1:A:230:ALA:O	1:A:234:LEU:HD23	2.17	0.43
2:C:808:ASN:H	3:D:633:ALA:HB2	1.82	0.43
3:D:105:ILE:CG1	3:D:242:LEU:HB3	2.48	0.43
5:M:144:ILE:HG22	5:M:161:ILE:HD13	2.00	0.43
8:T:-8:DT:H2"	8:T:-7:DG:H8	1.83	0.43
2:C:871:VAL:HG21	2:C:883:LEU:HD22	1.99	0.43
2:C:22:LEU:HD23	2:C:603:ILE:HD13	2.00	0.43
2:C:714:VAL:HG13	2:C:787:PRO:HD2	2.00	0.43
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.50	0.43
4:E:60:ASN:O	4:E:64:LEU:HG	2.17	0.43
1:A:253:LEU:HD23	1:A:279:GLY:HA3	1.99	0.43
2:C:349:GLU:OE2	2:C:349:GLU:N	2.50	0.43
3:D:555:TYR:CE2	3:D:585:LYS:HD3	2.53	0.43
4:E:44:ASP:OD1	4:E:52:ARG:NH1	2.52	0.43
5:M:285:TRP:CH2	5:M:355:PHE:HB3	2.53	0.43
2:C:391:SER:OG	2:C:394:ARG:HB2	2.19	0.43
2:C:631:GLU:HG3	2:C:633:LEU:O	2.19	0.43
3:D:849:LEU:CD1	3:D:856:ILE:HG12	2.47	0.43
3:D:1221:LEU:HD23	3:D:1221:LEU:O	2.18	0.43
5:M:279:ARG:HG2	5:M:279:ARG:HH11	1.83	0.43
5:M:455:ARG:HD3	5:M:455:ARG:C	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:2:DT:H2'	6:N:3:DA:C8	2.49	0.43
8:T:13:DG:C5	8:T:14:DC:C4	3.07	0.43
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.99	0.43
2:C:699:LEU:HD23	2:C:699:LEU:HA	1.86	0.43
2:C:1211:ARG:HD3	2:C:1220:GLN:CD	2.38	0.43
1:A:228:LEU:HD11	1:B:224:LEU:HG	2.00	0.43
1:B:47:LEU:HD23	1:B:51:MET:SD	2.58	0.43
1:B:130:ILE:HD12	1:B:130:ILE:N	2.33	0.43
3:D:472:LEU:H	3:D:472:LEU:HG	1.57	0.43
2:C:22:LEU:HG	2:C:655:VAL:HG11	2.00	0.43
2:C:598:VAL:HB	2:C:628:HIS:CE1	2.54	0.43
2:C:758:ARG:NH1	2:C:762:ASN:OD1	2.45	0.43
2:C:1256:GLN:CG	3:D:99:ARG:HH12	2.31	0.43
3:D:201:LEU:HB3	3:D:221:ILE:CD1	2.49	0.43
2:C:756:TYR:CD1	2:C:756:TYR:N	2.87	0.43
2:C:1080:ASN:HB3	2:C:1085:MET:SD	2.59	0.43
2:C:1287:LEU:O	2:C:1291:LEU:HG	2.19	0.43
3:D:393:THR:HG22	5:M:181:ARG:HH22	1.83	0.43
3:D:888:CYS:HA	3:D:898:CYS:SG	2.58	0.43
5:M:161:ILE:O	5:M:165:ILE:HG12	2.19	0.43
2:C:606:LEU:HD22	2:C:610:GLU:HB3	2.01	0.43
2:C:1062:PRO:C	2:C:1064:ASP:H	2.22	0.43
2:C:1107:MET:HG3	3:D:740:LEU:HD21	2.00	0.43
3:D:331:ILE:O	3:D:1328:THR:HG21	2.18	0.43
4:E:66:VAL:HG23	4:E:67:ARG:N	2.34	0.43
1:A:258:ASP:OD1	1:A:258:ASP:N	2.51	0.42
2:C:35:PHE:O	2:C:39:ILE:HG12	2.18	0.42
2:C:346:TYR:O	2:C:348:SER:N	2.42	0.42
2:C:364:VAL:HG23	2:C:376:PRO:HG2	2.00	0.42
3:D:826:ILE:HG22	3:D:831:VAL:HB	2.01	0.42
3:D:1155:ILE:HG12	3:D:1211:SER:HB3	2.01	0.42
3:D:1314:LEU:HD21	3:D:1326:GLN:CB	2.48	0.42
2:C:25:PRO:O	2:C:27:LEU:HD22	2.19	0.42
2:C:721:GLY:HA3	2:C:777:VAL:HG12	2.01	0.42
2:C:755:LYS:HA	2:C:766:ASN:OD1	2.19	0.42
3:D:268:LEU:HD13	3:D:306:LEU:HA	2.01	0.42
3:D:603:LYS:HE3	3:D:603:LYS:HB3	1.84	0.42
3:D:651:HIS:CE1	3:D:652:GLU:HG3	2.54	0.42
5:M:174:GLU:OE1	5:M:174:GLU:N	2.49	0.42
1:A:280:ASP:HB3	1:A:321:TRP:HE1	1.84	0.42
2:C:515:MET:HA	2:C:526:HIS:ND1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:605:LEU:HD23	3:D:605:LEU:HA	1.88	0.42
3:D:982:LEU:HD23	3:D:982:LEU:HA	1.91	0.42
3:D:1172:LYS:H	6:N:17:DC:P	2.42	0.42
1:A:125:LYS:HE3	1:A:127:GLN:HE21	1.83	0.42
2:C:484:LEU:C	2:C:484:LEU:HD22	2.40	0.42
3:D:123:ARG:O	3:D:127:LEU:HB2	2.20	0.42
3:D:250:ARG:HB3	3:D:265:LEU:HD23	2.02	0.42
3:D:252:LEU:H	3:D:252:LEU:HG	1.58	0.42
3:D:615:LYS:O	3:D:619:ILE:HG13	2.19	0.42
3:D:982:LEU:O	3:D:994:SER:HA	2.19	0.42
1:B:17:GLU:OE1	1:B:25:LYS:HD3	2.19	0.42
1:B:46:ILE:HG21	1:B:223:ILE:HD11	2.00	0.42
1:B:107:ILE:CG2	1:B:133:LEU:HG	2.36	0.42
5:M:403:PHE:N	5:M:403:PHE:CD2	2.88	0.42
8:T:26:DC:H2"	8:T:27:DA:C8	2.53	0.42
2:C:302:ILE:HD12	2:C:309:LEU:HB3	2.02	0.42
2:C:1061:GLN:HE22	2:C:1240:ASP:CG	2.23	0.42
3:D:860:ARG:O	3:D:861:ASN:C	2.57	0.42
3:D:1322:ALA:O	3:D:1331:VAL:HG21	2.19	0.42
6:N:-14:DG:H2"	6:N:-13:DC:C6	2.55	0.42
2:C:99:LYS:HG2	2:C:121:GLU:HB3	2.01	0.42
2:C:909:LYS:HE2	2:C:909:LYS:HB3	1.83	0.42
3:D:93:THR:HG21	3:D:97:VAL:HG11	2.01	0.42
3:D:124:ILE:O	3:D:128:LEU:HG	2.19	0.42
3:D:623:GLN:O	3:D:627:THR:HG22	2.20	0.42
5:M:371:ALA:CB	5:M:378:GLU:HG2	2.50	0.42
8:T:19:DG:H2'	8:T:20:DT:H71	2.02	0.42
2:C:25:PRO:HG2	2:C:27:LEU:HD13	2.00	0.42
2:C:100:LEU:CG	2:C:488:MET:HG2	2.45	0.42
2:C:270:THR:C	2:C:272:ARG:N	2.72	0.42
2:C:947:GLU:O	2:C:951:MET:HG3	2.19	0.42
3:D:126:LEU:HG	3:D:127:LEU:N	2.33	0.42
3:D:168:ALA:O	3:D:172:PHE:N	2.50	0.42
3:D:582:ILE:HD13	3:D:582:ILE:HA	1.91	0.42
3:D:1318:SER:OG	3:D:1321:SER:OG	2.27	0.42
8:T:15:DA:H2"	8:T:16:DA:C8	2.55	0.42
1:A:248:GLU:N	3:D:389:GLY:HA3	2.34	0.42
1:A:307:LEU:HD23	1:A:307:LEU:HA	1.83	0.42
3:D:58:CYS:SG	3:D:59:ALA:N	2.92	0.42
3:D:544:LEU:HD22	3:D:575:GLY:CA	2.50	0.42
8:T:14:DC:H2"	8:T:15:DA:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:82:VAL:HG13	2:C:137:VAL:HG21	2.01	0.41
2:C:143:ARG:HA	2:C:513:GLN:O	2.19	0.41
3:D:450:HIS:CD2	3:D:452:LEU:HB2	2.55	0.41
3:D:1197:ASN:HB3	3:D:1210:ILE:O	2.20	0.41
3:D:1230:THR:HG22	3:D:1257:VAL:HG11	2.01	0.41
3:D:1295:ASN:HD22	3:D:1298:VAL:HG21	1.85	0.41
1:A:218:ARG:HH22	1:B:234:LEU:HB3	1.85	0.41
1:B:107:ILE:H	1:B:107:ILE:HD12	1.85	0.41
2:C:162:GLY:HA2	2:C:170:VAL:HA	2.02	0.41
2:C:478:ARG:HH21	2:C:492:MET:H	1.67	0.41
3:D:646:ILE:HD12	3:D:762:ASN:ND2	2.35	0.41
1:B:133:LEU:HD23	1:B:135:ASP:N	2.36	0.41
2:C:59:ILE:HD11	2:C:476:LYS:HD2	2.02	0.41
2:C:638:SER:OG	2:C:639:LYS:N	2.53	0.41
3:D:217:LEU:HD13	3:D:217:LEU:HA	1.94	0.41
4:E:5:THR:HG22	4:E:7:GLN:H	1.85	0.41
5:M:187:PRO:HG3	5:M:264:ILE:HG21	2.01	0.41
2:C:60:GLN:HB3	2:C:67:GLU:CD	2.41	0.41
2:C:215:TYR:HA	2:C:219:GLN:OE1	2.20	0.41
2:C:582:ASN:HD22	2:C:586:PHE:HB2	1.86	0.41
2:C:1013:GLN:O	2:C:1017:GLN:HG2	2.21	0.41
2:C:1294:LYS:HE3	3:D:349:TYR:CD1	2.55	0.41
3:D:598:LYS:O	3:D:598:LYS:HG3	2.21	0.41
3:D:860:ARG:HG2	3:D:860:ARG:HH11	1.86	0.41
2:C:22:LEU:CG	2:C:655:VAL:HG11	2.51	0.41
2:C:409:LEU:HD13	2:C:427:ASP:HB3	2.02	0.41
2:C:946:LEU:HD12	2:C:946:LEU:H	1.84	0.41
2:C:1293:VAL:HG23	2:C:1301:ARG:HA	2.02	0.41
3:D:22:ILE:O	3:D:1339:GLY:HA2	2.20	0.41
1:B:83:LEU:HD22	3:D:526:VAL:CG1	2.51	0.41
2:C:84:GLU:HA	2:C:87:ILE:HG22	2.02	0.41
2:C:382:GLU:O	2:C:386:GLU:HG2	2.20	0.41
2:C:590:PRO:O	2:C:659:GLN:NE2	2.44	0.41
2:C:960:LEU:HD11	2:C:1028:LYS:NZ	2.35	0.41
3:D:47:ARG:CD	5:M:386:THR:HG21	2.51	0.41
3:D:337:ARG:O	3:D:342:LEU:HG	2.21	0.41
3:D:748:ALA:HB3	3:D:754:ILE:HA	2.03	0.41
5:M:246:LEU:O	5:M:250:VAL:HG13	2.20	0.41
2:C:35:PHE:CE2	2:C:39:ILE:HD13	2.54	0.41
3:D:40:LYS:HB3	3:D:42:GLU:CD	2.41	0.41
3:D:556:GLU:HB3	3:D:564:VAL:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:611:ILE:HG22	3:D:612:LEU:HD23	2.02	0.41
3:D:847:ASP:HB3	3:D:856:ILE:CG2	2.49	0.41
2:C:1256:GLN:HG2	3:D:99:ARG:HH12	1.86	0.41
2:C:1268:GLN:HG2	3:D:350:SER:HB3	2.02	0.41
3:D:69:GLU:HA	3:D:76:LYS:HA	2.02	0.41
1:A:228:LEU:O	1:A:232:VAL:HG23	2.21	0.41
2:C:257:ALA:N	2:C:260:LYS:O	2.39	0.41
2:C:615:VAL:HG12	2:C:650:VAL:HA	2.03	0.41
2:C:898:GLU:CD	2:C:898:GLU:H	2.24	0.41
2:C:1125:GLY:HA3	2:C:1179:GLY:HA2	2.01	0.41
2:C:1294:LYS:O	2:C:1294:LYS:HG2	2.21	0.41
3:D:139:LEU:HA	3:D:139:LEU:HD23	1.87	0.41
3:D:350:SER:HA	3:D:468:VAL:O	2.20	0.41
4:E:16:ARG:O	4:E:16:ARG:HG3	2.20	0.41
6:N:-17:DT:H2"	6:N:-16:DT:H71	2.02	0.41
1:A:234:LEU:HD12	1:B:217:ILE:HG21	2.03	0.41
3:D:189:LEU:HD12	3:D:189:LEU:HA	1.91	0.41
3:D:661:VAL:O	3:D:664:ILE:HG22	2.21	0.41
3:D:1226:VAL:HG22	3:D:1261:LEU:HD13	2.03	0.41
1:A:64:VAL:HG11	1:A:78:ILE:CD1	2.51	0.40
1:B:228:LEU:O	1:B:232:VAL:HG23	2.21	0.40
2:C:155:VAL:HG23	2:C:176:ILE:HG12	2.03	0.40
2:C:607:SER:OG	2:C:610:GLU:HG3	2.21	0.40
2:C:696:ASP:O	2:C:795:ALA:HB1	2.22	0.40
2:C:755:LYS:HA	2:C:755:LYS:HE3	2.03	0.40
3:D:433:GLY:O	3:D:457:TYR:CE1	2.74	0.40
3:D:641:ILE:HD12	3:D:641:ILE:HA	1.92	0.40
3:D:827:GLU:CB	3:D:832:LYS:HE2	2.52	0.40
3:D:865:HIS:CE1	3:D:868:TRP:CD1	3.10	0.40
3:D:1155:ILE:HG12	3:D:1194:ARG:HH22	1.86	0.40
5:M:192:ALA:HB1	5:M:197:ASP:HB3	2.03	0.40
1:A:135:ASP:OD1	1:A:135:ASP:N	2.54	0.40
1:B:56:VAL:HG22	1:B:146:VAL:CG1	2.50	0.40
2:C:832:HIS:CD2	2:C:1058:ARG:HG2	2.56	0.40
2:C:841:ARG:NH1	2:C:1045:GLY:HA3	2.36	0.40
3:D:24:LEU:HD21	3:D:116:PHE:CZ	2.56	0.40
1:B:108:GLY:N	1:B:133:LEU:HB3	2.16	0.40
2:C:658:GLN:O	2:C:660:VAL:N	2.54	0.40
2:C:1007:LYS:HA	2:C:1011:LEU:HD12	2.04	0.40
3:D:159:ILE:HD12	3:D:159:ILE:HA	1.92	0.40
3:D:374:LEU:HD12	3:D:381:ILE:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:985:ILE:HG23	3:D:988:PHE:O	2.21	0.40
5:M:377:HIS:O	5:M:381:ILE:HG23	2.21	0.40
1:B:102:LEU:CD1	1:B:142:MET:HB2	2.51	0.40
2:C:656:SER:O	2:C:659:GLN:HB2	2.22	0.40
2:C:866:ASP:N	2:C:870:ILE:O	2.52	0.40
3:D:1330:ARG:O	3:D:1334:GLU:HG2	2.21	0.40
2:C:960:LEU:HD11	2:C:1028:LYS:HZ2	1.86	0.40
3:D:528:THR:HG22	3:D:532:GLU:OE1	2.22	0.40
5:M:183:GLN:NE2	5:M:192:ALA:HA	2.37	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	304/321 (95%)	282 (93%)	21 (7%)	1 (0%)	41 72
1	B	232/321 (72%)	215 (93%)	16 (7%)	1 (0%)	34 66
2	C	1339/1341 (100%)	1265 (94%)	73 (6%)	1 (0%)	51 81
3	D	1318/1373 (96%)	1232 (94%)	84 (6%)	2 (0%)	47 78
4	E	72/74 (97%)	68 (94%)	4 (6%)	0	100 100
5	M	378/380 (100%)	350 (93%)	24 (6%)	4 (1%)	14 41
All	All	3643/3810 (96%)	3412 (94%)	222 (6%)	9 (0%)	50 78

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ASP
5	M	398	GLU
1	B	137	ASN

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Mol	Chain	Res	Type
2	C	30	ILE
5	M	404	SER
5	M	113	GLN
3	D	109	SER
5	M	266	THR
3	D	97	VAL

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	259/280 (92%)	248 (96%)	11 (4%)	30	63
1	B	184/280 (66%)	175 (95%)	9 (5%)	25	57
2	C	1038/1156 (90%)	1002 (96%)	36 (4%)	36	70
3	D	943/1145 (82%)	899 (95%)	44 (5%)	26	59
4	E	53/64 (83%)	50 (94%)	3 (6%)	20	50
5	M	231/333 (69%)	219 (95%)	12 (5%)	23	55
All	All	2708/3258 (83%)	2593 (96%)	115 (4%)	33	63

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	17	GLU
1	A	64	VAL
1	A	91	ARG
1	A	110	VAL
1	A	114	ASP
1	A	120	ASP
1	A	233	ASP
1	A	255	ARG
1	A	258	ASP
1	A	321	TRP
1	B	4	SER

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Mol	Chain	Res	Type
1	B	12	ARG
1	B	75	GLN
1	B	117	HIS
1	B	120	ASP
1	B	133	LEU
1	B	136	GLU
1	B	191	ARG
1	B	205	MET
2	C	17	LYS
2	C	21	VAL
2	C	27	LEU
2	C	62	TYR
2	C	67	GLU
2	C	124	MET
2	C	164	THR
2	C	225	PHE
2	C	246	LEU
2	C	359	ARG
2	C	420	LEU
2	C	478	ARG
2	C	484	LEU
2	C	487	LEU
2	C	514	PHE
2	C	583	GLU
2	C	600	THR
2	C	650	VAL
2	C	694	ARG
2	C	756	TYR
2	C	826	ASP
2	C	871	VAL
2	C	890	LYS
2	C	912	ASP
2	C	963	GLU
2	C	1018	TYR
2	C	1069	ARG
2	C	1107	MET
2	C	1154	ASP
2	C	1201	LEU
2	C	1211	ARG
2	C	1230	MET
2	C	1239	VAL
2	C	1240	ASP

Continued on next page...

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Mol	Chain	Res	Type
2	C	1265	PHE
2	C	1290	MET
3	D	47	ARG
3	D	60	ARG
3	D	70	CYS
3	D	95	THR
3	D	115	TRP
3	D	123	ARG
3	D	126	LEU
3	D	134	ASP
3	D	156	ARG
3	D	190	LYS
3	D	227	PHE
3	D	239	LEU
3	D	252	LEU
3	D	275	ARG
3	D	300	GLN
3	D	337	ARG
3	D	340	GLN
3	D	378	LYS
3	D	430	HIS
3	D	472	LEU
3	D	485	MET
3	D	489	ASN
3	D	505	ASP
3	D	517	CYS
3	D	566	LYS
3	D	625	MET
3	D	663	GLU
3	D	672	LEU
3	D	695	LYS
3	D	701	LEU
3	D	715	LYS
3	D	747	MET
3	D	802	ASP
3	D	805	GLN
3	D	811	GLU
3	D	812	ASP
3	D	814	CYS
3	D	822	MET
3	D	832	LYS
3	D	857	LEU

Continued on next page...

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Mol	Chain	Res	Type
3	D	901	ARG
3	D	1196	LEU
3	D	1278	GLU
3	D	1279	GLN
4	E	19	LEU
4	E	25	ARG
4	E	58	LEU
5	M	118	GLN
5	M	133	PHE
5	M	172	LEU
5	M	205	GLN
5	M	279	ARG
5	M	284	ARG
5	M	289	LEU
5	M	350	GLN
5	M	359	GLU
5	M	380	THR
5	M	394	ARG
5	M	460	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
2	C	517	GLN
2	C	518	ASN
2	C	582	ASN
2	C	673	HIS
2	C	1061	GLN
3	D	94	GLN
3	D	206	ASN
3	D	229	GLN
3	D	450	HIS
3	D	739	GLN
3	D	1249	ASN
3	D	1350	ASN
4	E	7	GLN
5	M	406	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	R	3/5 (60%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	N	1
7	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	-9:DC	O3’	-5:DT	P	14.72
1	R	2:G	O3’	3:C	P	3.08

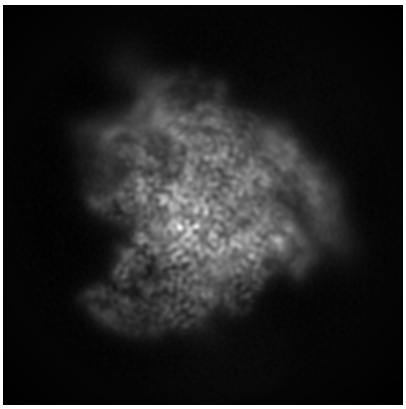
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19079. These allow visual inspection of the internal detail of the map and identification of artifacts.

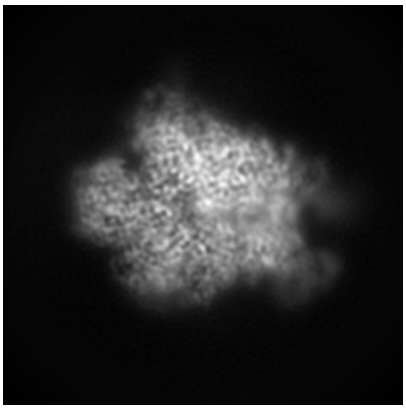
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

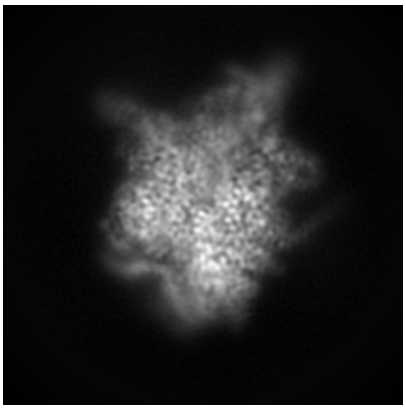
6.1.1 Primary map



X

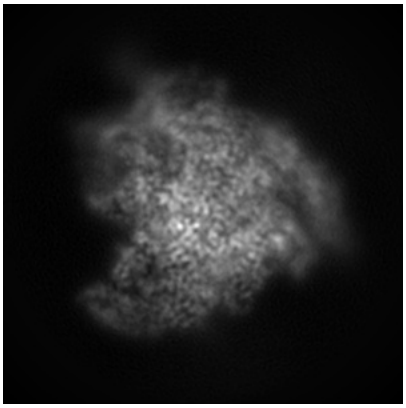


Y

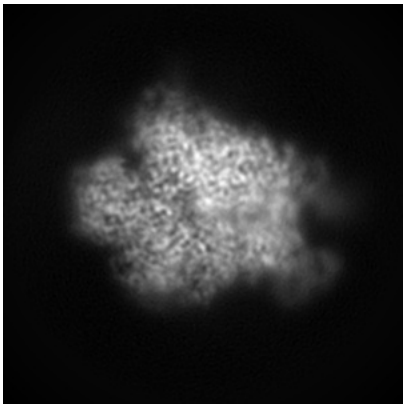


Z

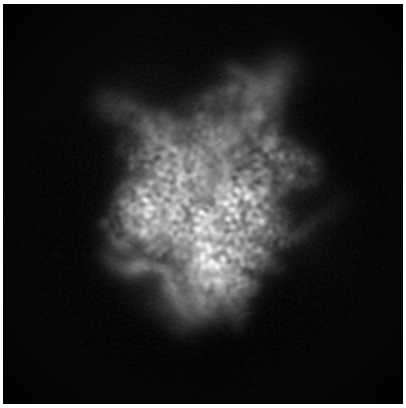
6.1.2 Raw map



X



Y

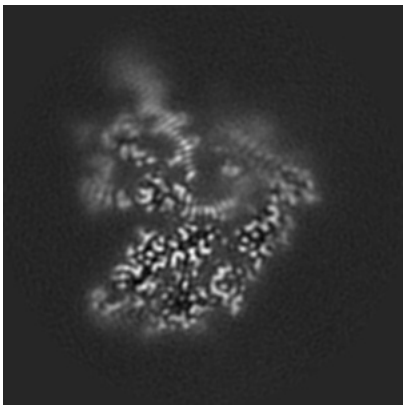


Z

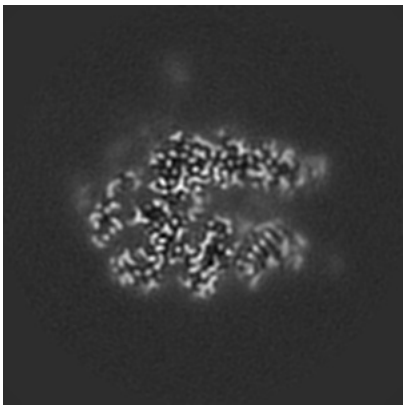
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

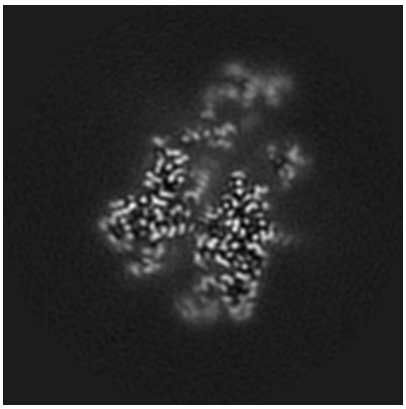
6.2.1 Primary map



X Index: 100

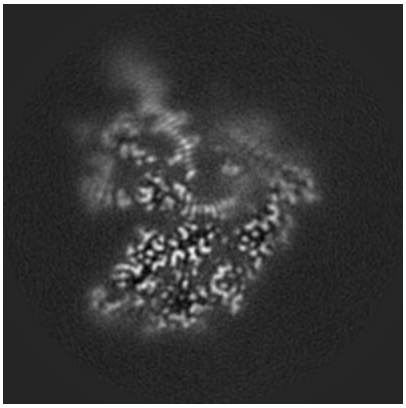


Y Index: 100

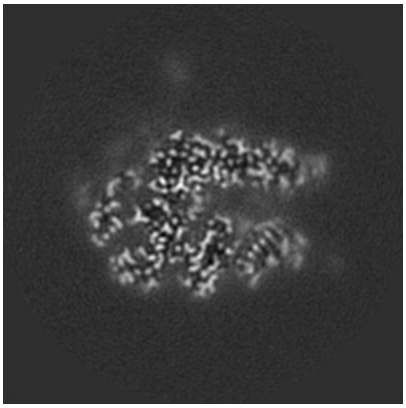


Z Index: 100

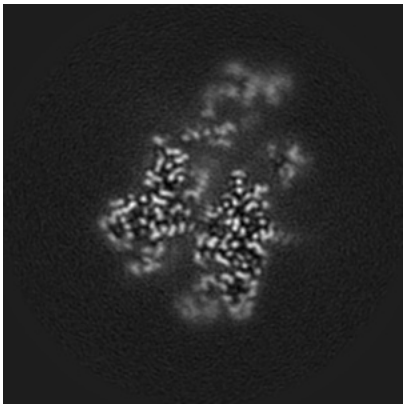
6.2.2 Raw map



X Index: 100



Y Index: 100

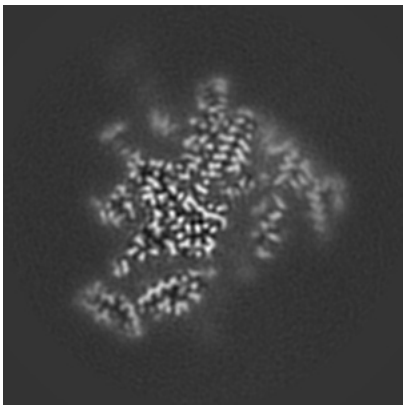


Z Index: 100

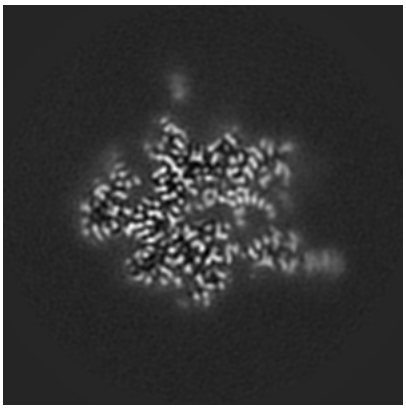
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

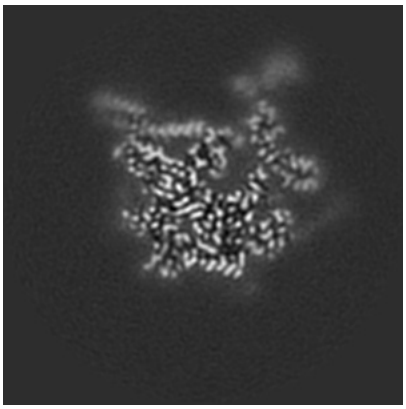
6.3.1 Primary map



X Index: 113

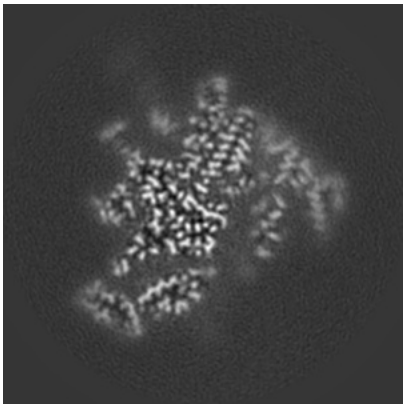


Y Index: 93

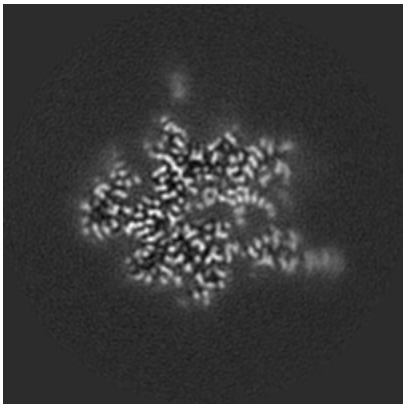


Z Index: 82

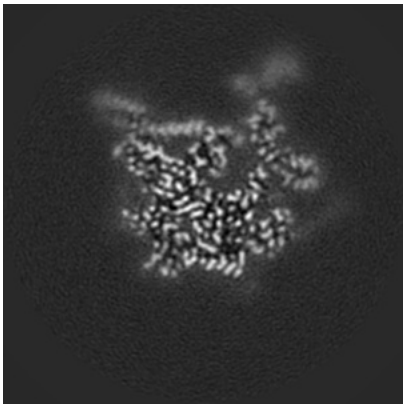
6.3.2 Raw map



X Index: 113



Y Index: 93

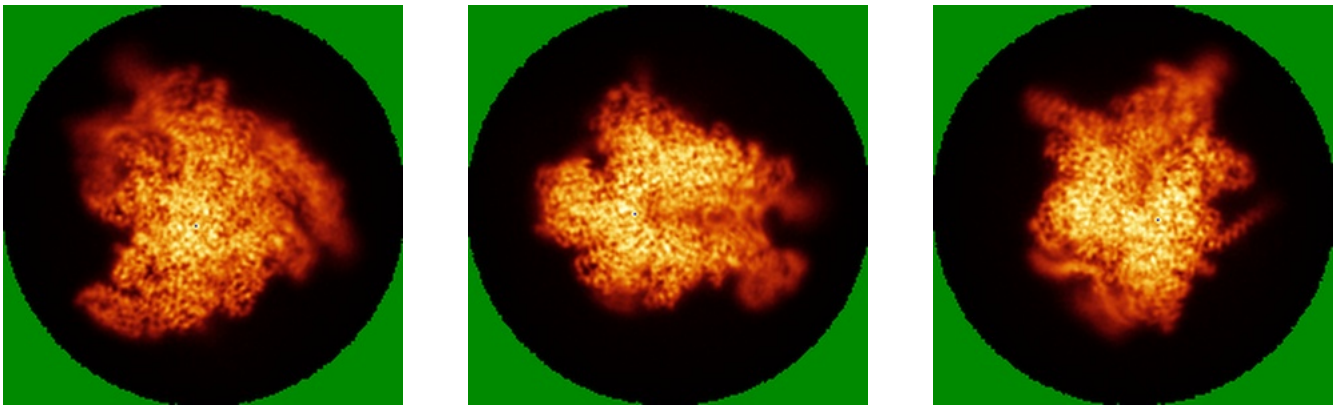


Z Index: 82

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

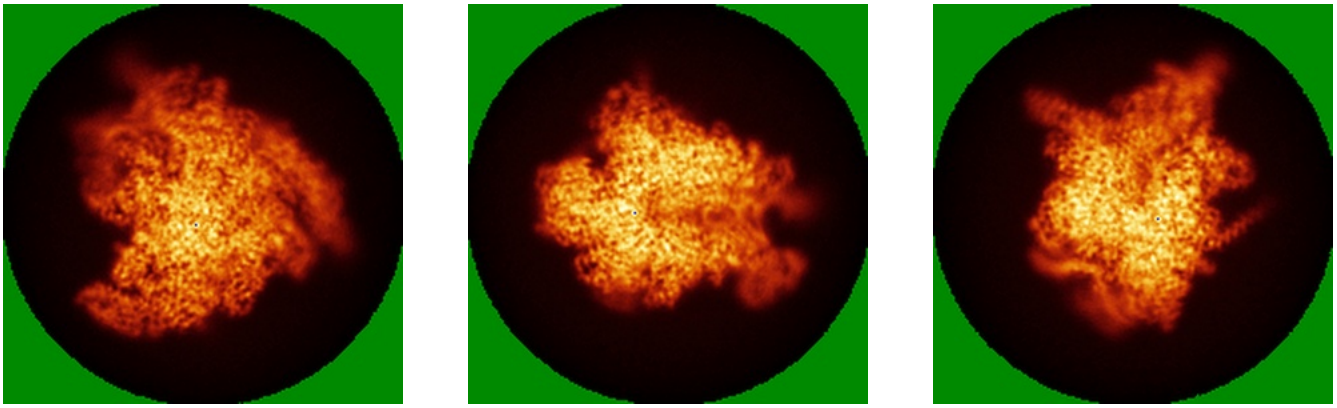
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

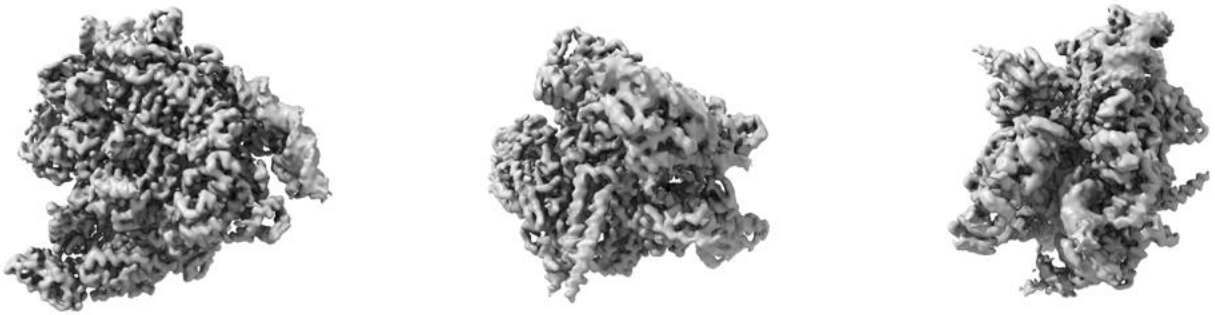


X Y Z

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)

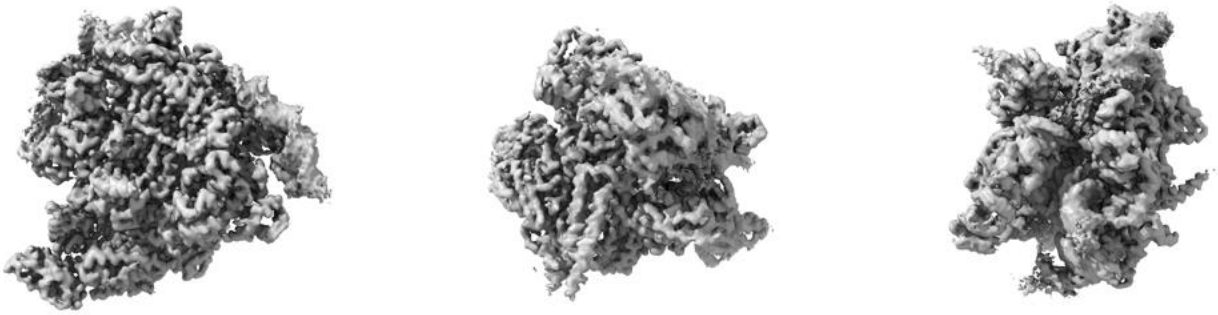
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

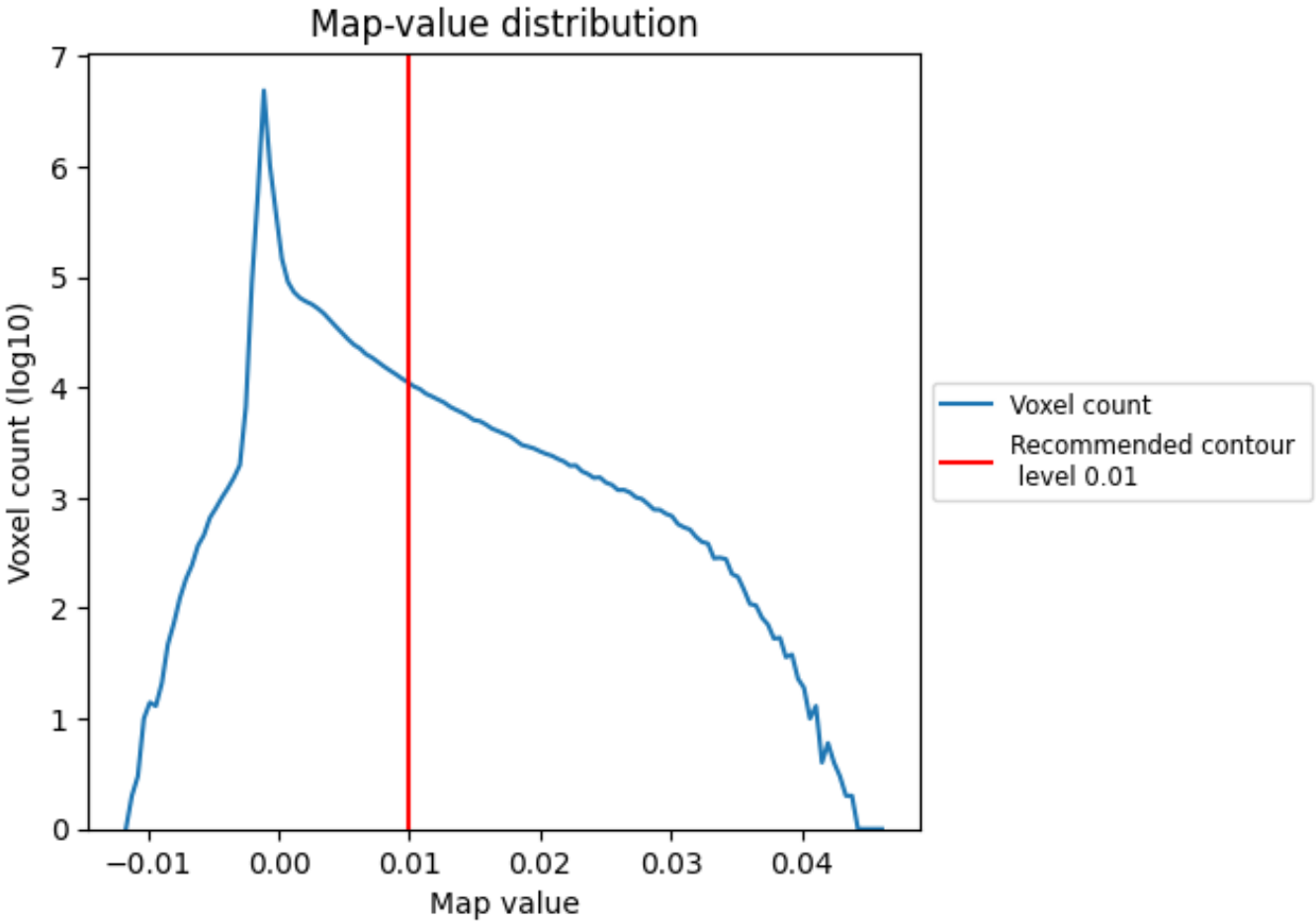
6.6 Mask visualisation (i)

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

7 Map analysis

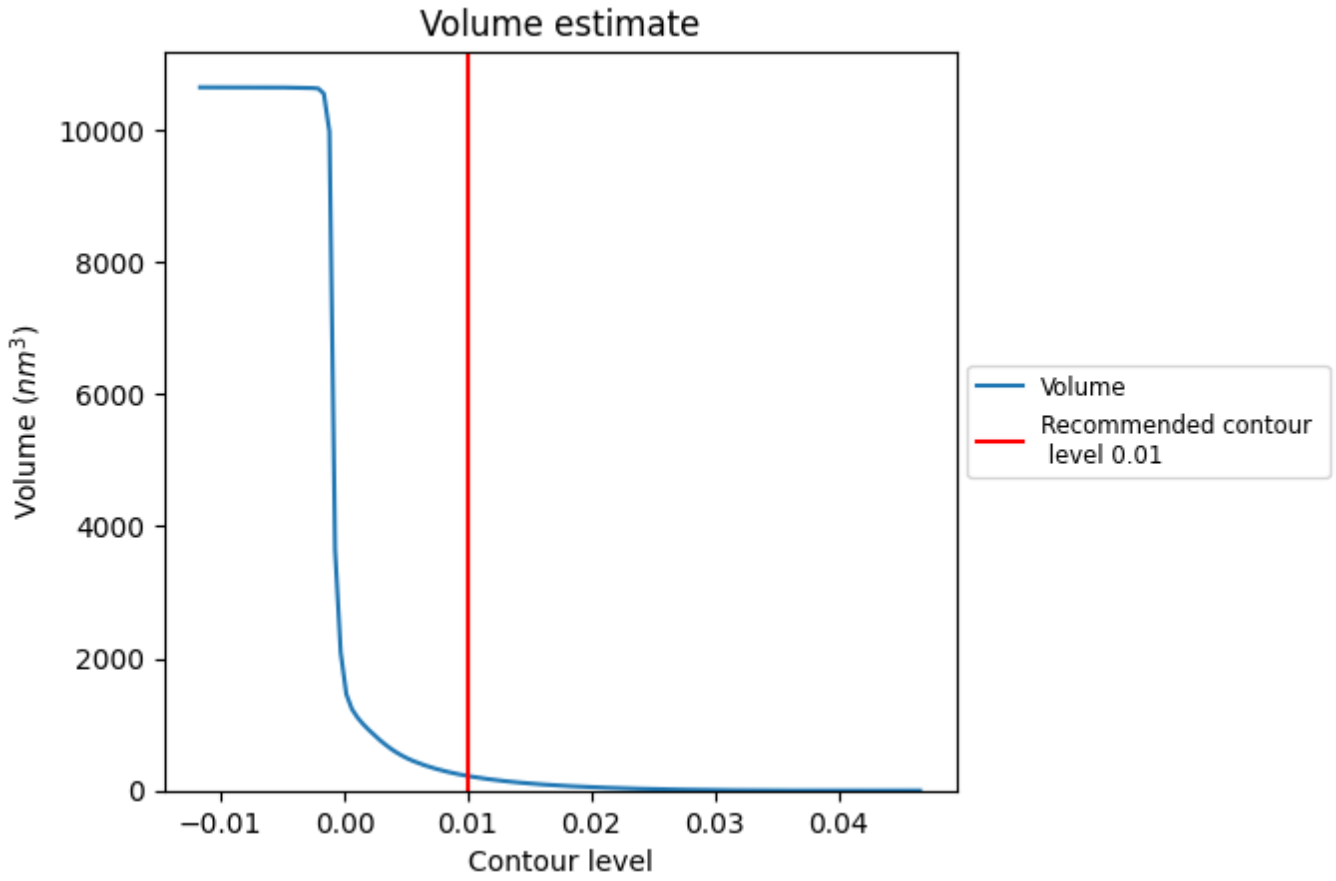
This section contains the results of statistical analysis of the map.

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.

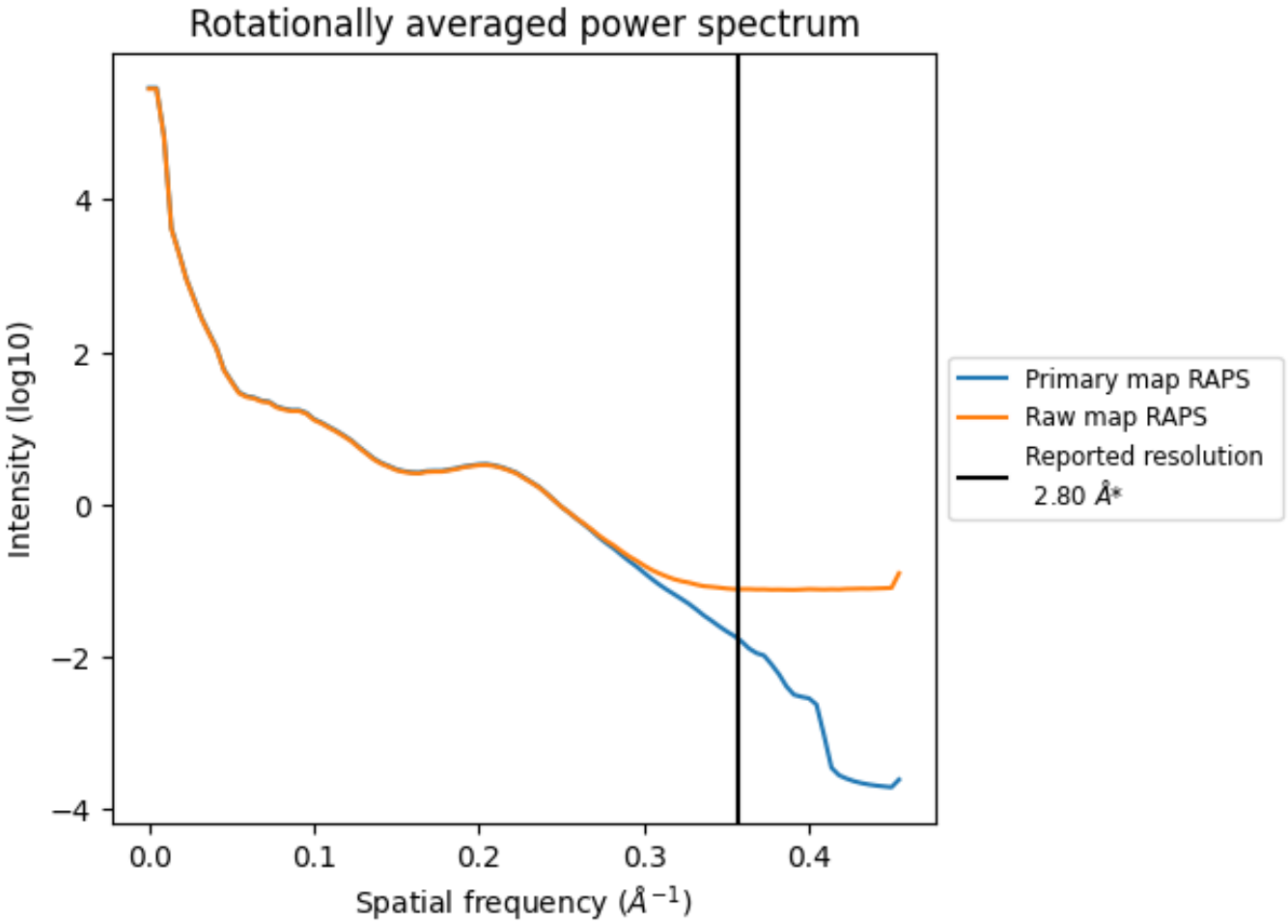
7.2 Volume estimate



The volume at the recommended contour level is 221 nm^3; this corresponds to an approximate mass of 200 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)

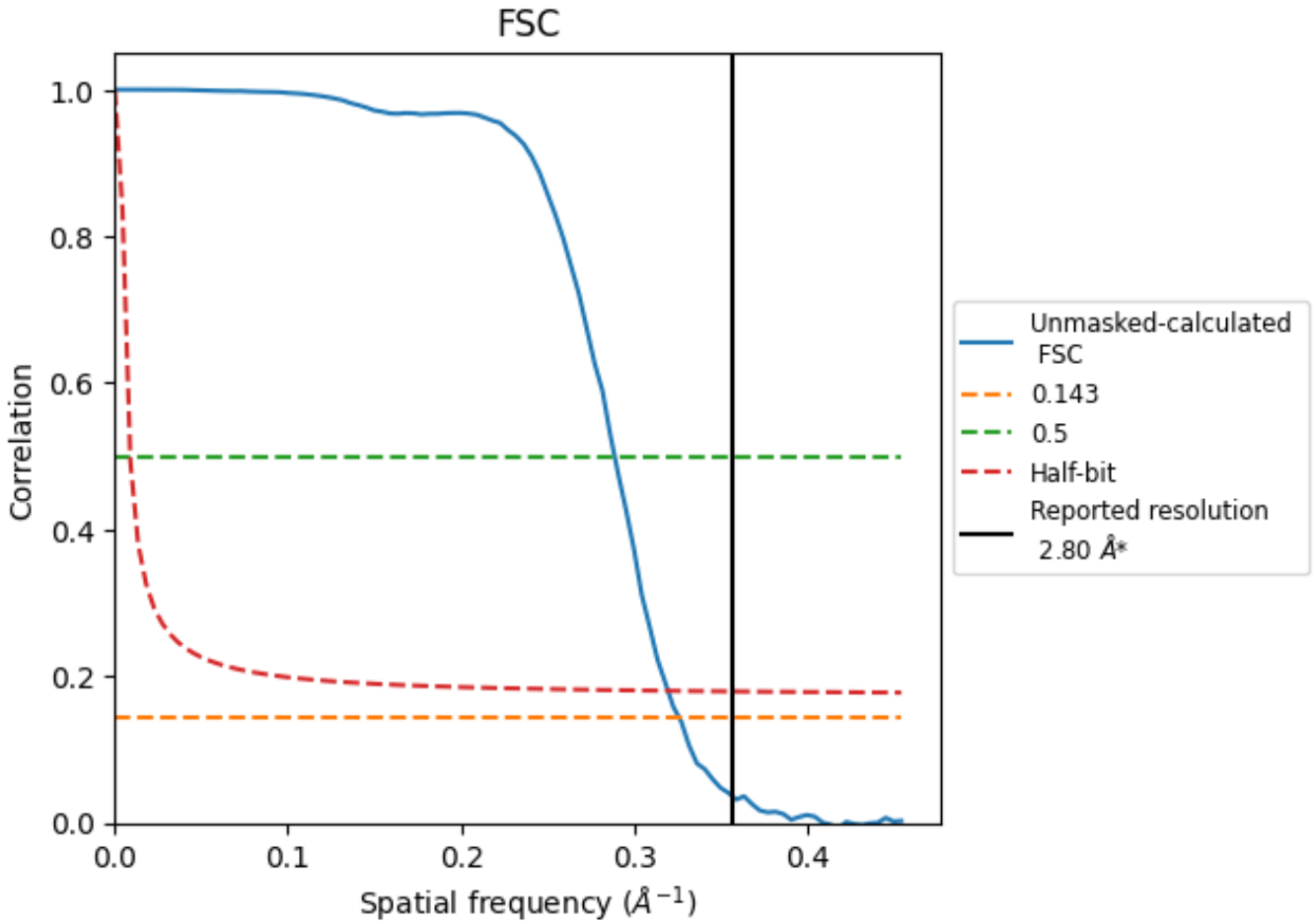


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

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 0.357 Å^{-1}

8.2 Resolution estimates (i)

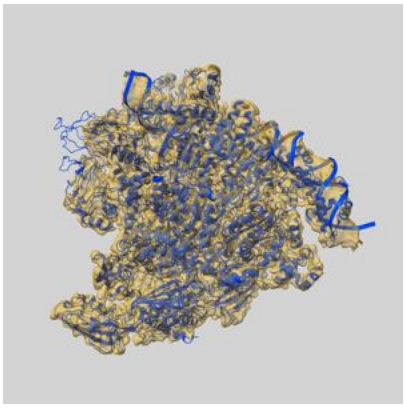
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.07	3.46	3.13

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

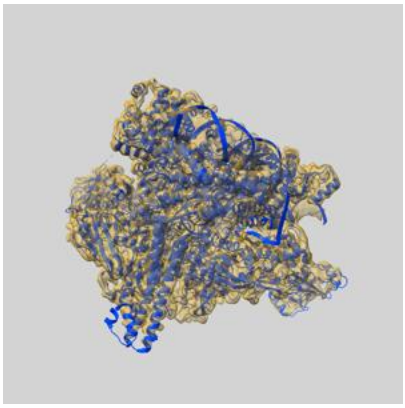
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19079 and PDB model 8RE4. Per-residue inclusion information can be found in section 3 on page 6.

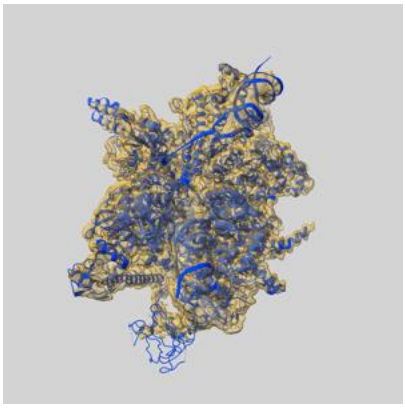
9.1 Map-model overlay



X



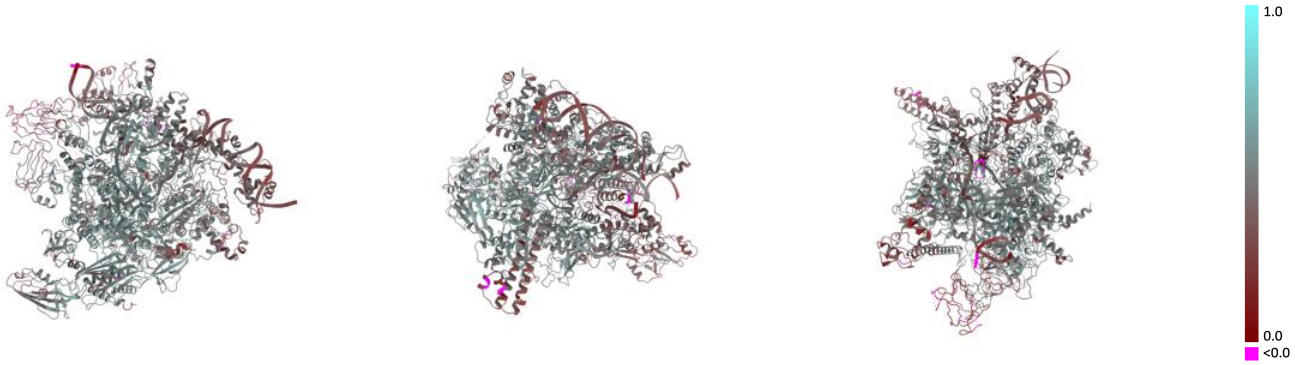
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

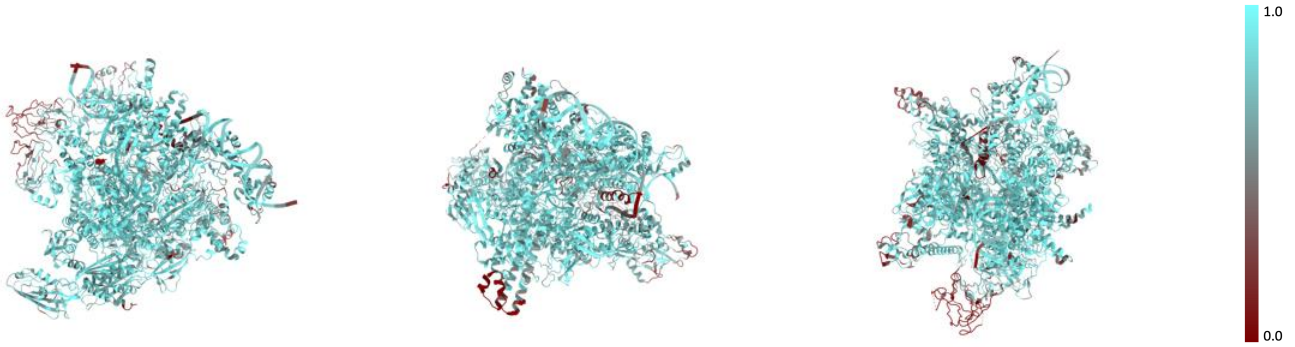
9.2 Q-score mapped to coordinate model (i)



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.

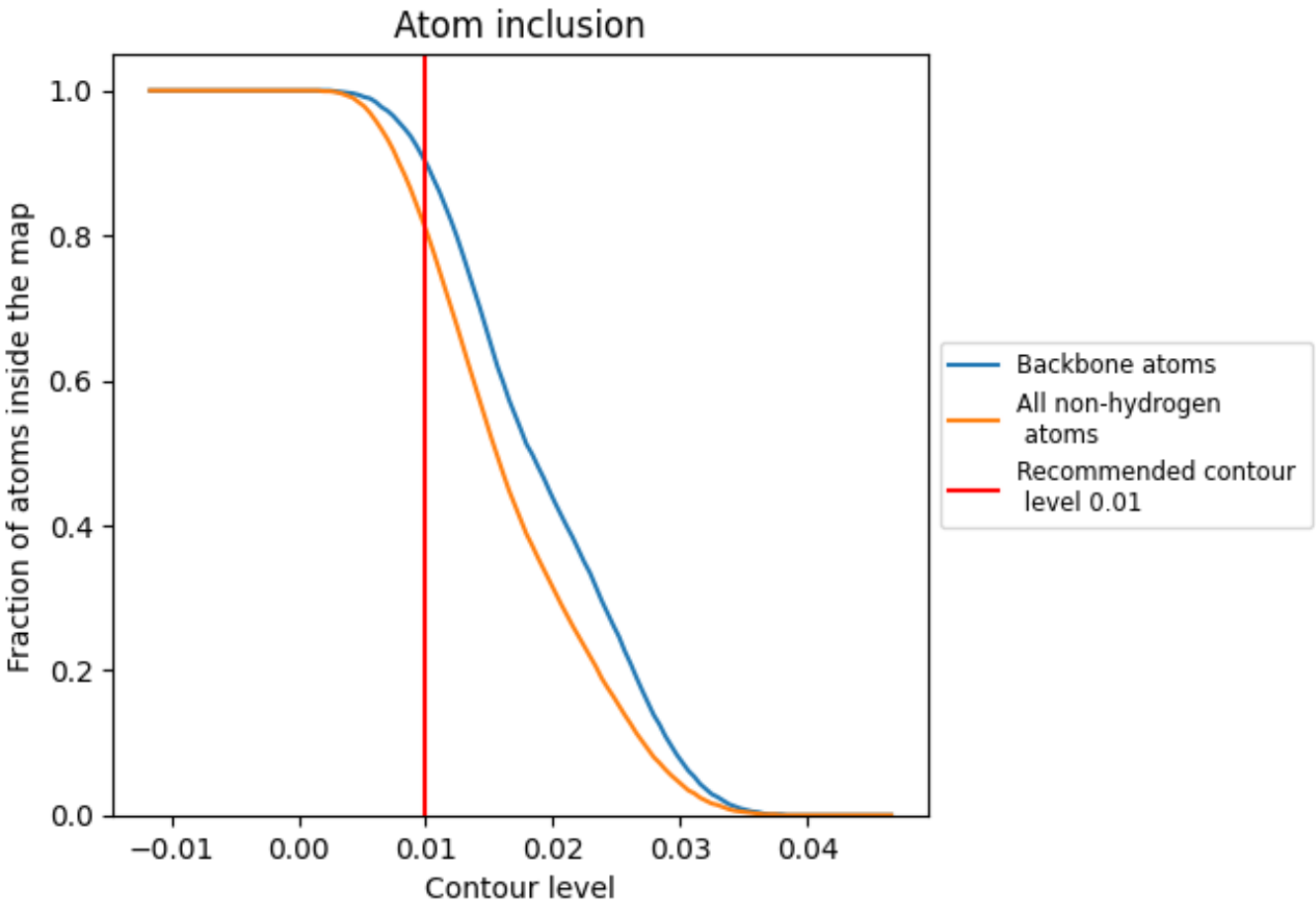
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 81% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8090	0.4700
A	0.7990	0.5020
B	0.7670	0.4720
C	0.8270	0.4840
D	0.8200	0.4820
E	0.8740	0.5160
M	0.7290	0.4080
N	0.7500	0.3410
R	0.9530	0.5110
T	0.8330	0.3850