Full wwPDB EM Validation Report ⓘ

May 4, 2025 – 08:05 am BST

PDB ID	:	9GM9 / pdb_00009gm9
EMDB ID	:	EMD-51445
Title	:	MukBEF in a DNA capture state
Authors	:	Burmann, F.; Lowe, J.
Deposited on	:	2024-08-28
Resolution	:	7.80 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:

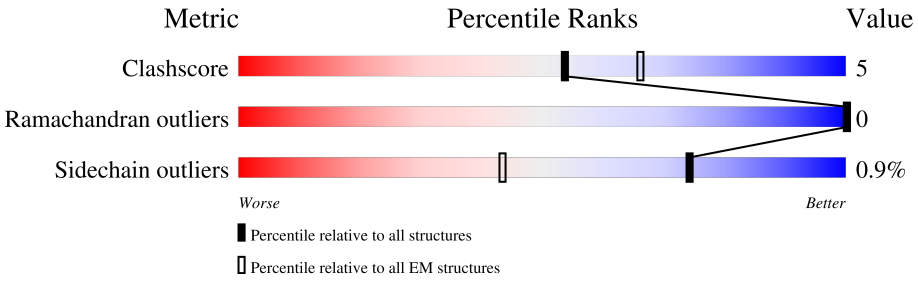
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 7.80 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.



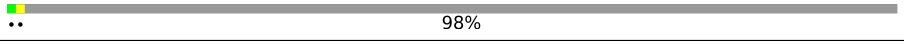
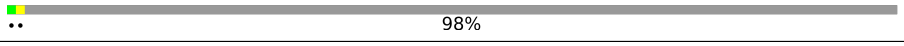
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1482	61% 7% 33%
1	B	1482	54% 13% 33%
2	C	440	87% 12%
2	D	440	65% 7% 28%
3	E	240	68% 19% 12%
3	F	240	63% 18% 18%
3	Q	240	8% 45% 8% 46%
4	G	78	67% 24% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	I	78	
5	K	2124	
6	L	2124	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	4HH	G	36	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 58225 atoms, of which 28572 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 Chromosome partition protein MukB.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	999	Total	C	H	N	O	S	0	0
			16038	4984	8011	1480	1534	29		
1	B	999	Total	C	H	N	O	S	0	0
			16037	4984	8010	1480	1534	29		

- Molecule 2 is a protein called Chromosome partition protein MukF.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	440	Total	C	H	N	O	S	0	0
			6982	2218	3451	614	686	13		
2	D	318	Total	C	H	N	O	S	0	0
			5046	1598	2496	448	493	11		

- Molecule 3 is a protein called Chromosome partition protein MukE.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	212	Total	C	H	N	O	S	0	0
			3441	1090	1719	301	322	9		
3	F	198	Total	C	H	N	O	S	0	0
			3246	1029	1627	284	298	8		
3	Q	129	Total	C	H	N	O	S	0	0
			2101	653	1060	185	196	7		

- Molecule 4 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms							AltConf	Trace
4	G	72	Total	C	H	N	O	P	S	0	0
			1147	360	564	87	133	1	2		
4	I	72	Total	C	H	N	O	P	S	0	0
			1147	360	564	87	133	1	2		

- Molecule 5 is a DNA chain called pFB526.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	K	47	Total	C	H	N	O	P	0	0
			1498	460	525	191	275	47		

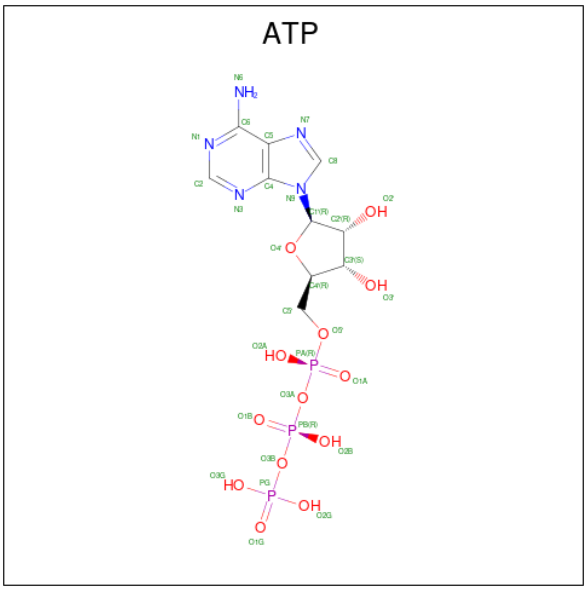
- Molecule 6 is a DNA chain called pFB526.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	L	46	Total	C	H	N	O	P	0	0
			1454	446	521	157	284	46		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Mg	0
			1	1	
7	B	1	Total	Mg	0
			1	1	

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



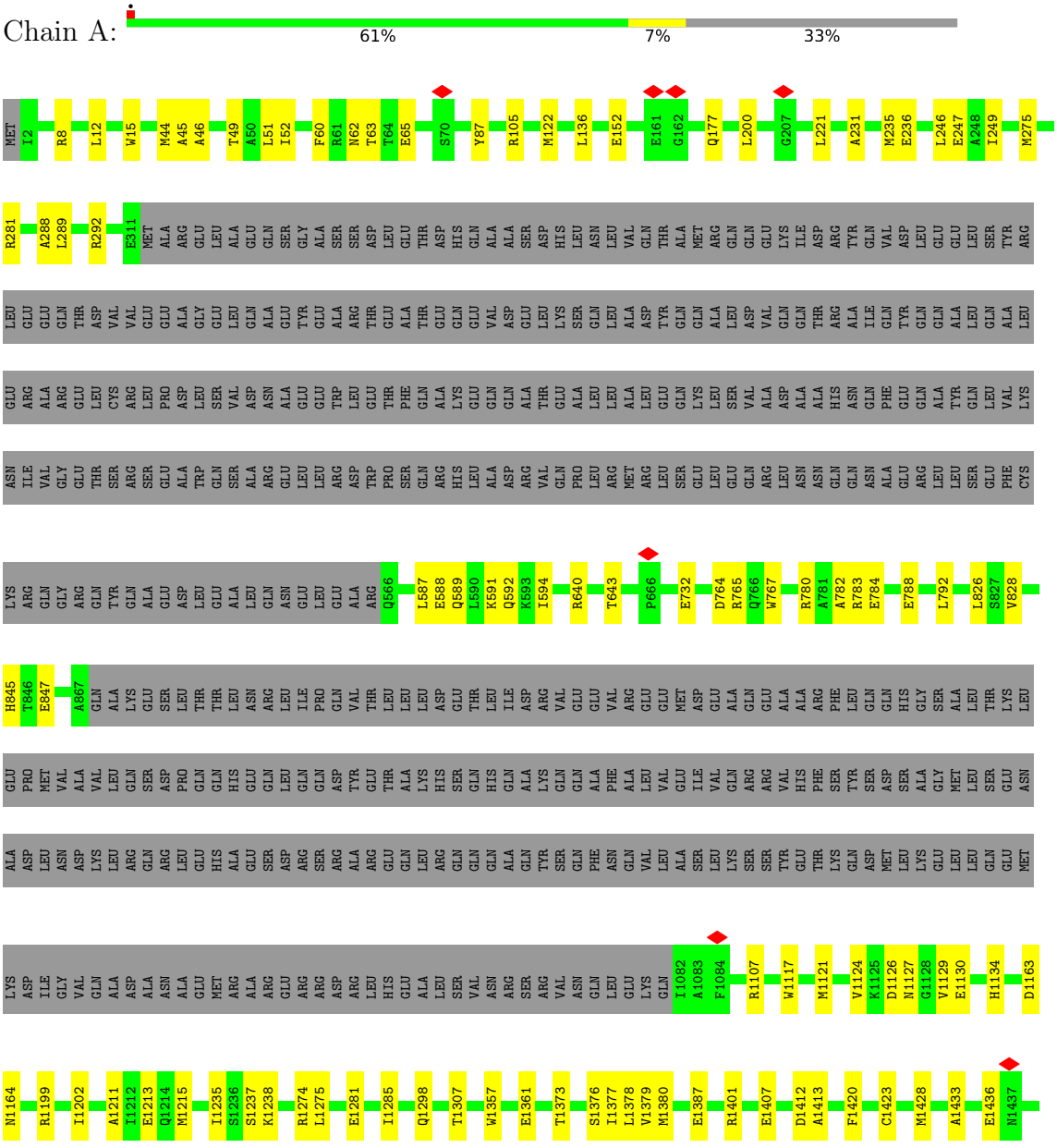
Mol	Chain	Residues	Atoms						AltConf
8	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
8	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

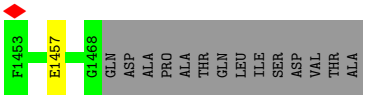
3 Residue-property plots (i)

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: Chromosome partition protein MukB

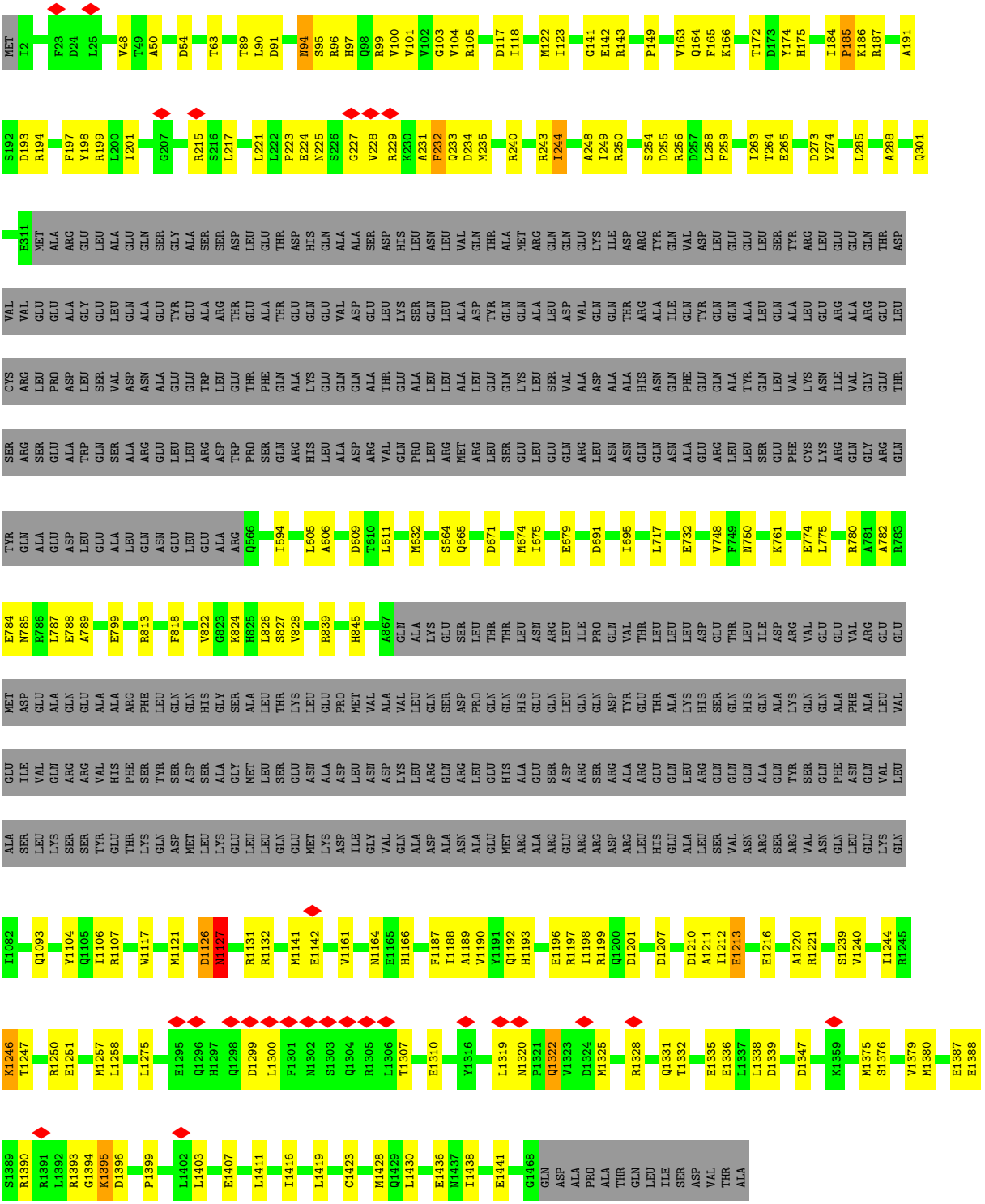
Chain A:





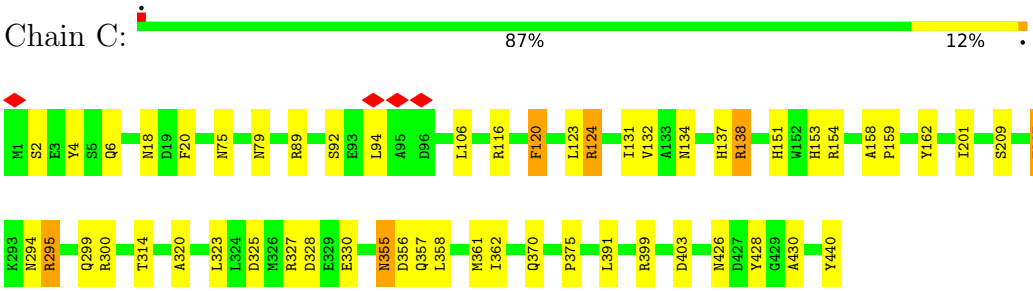
• Molecule 1: Chromosome partition protein MukB

Chain B:



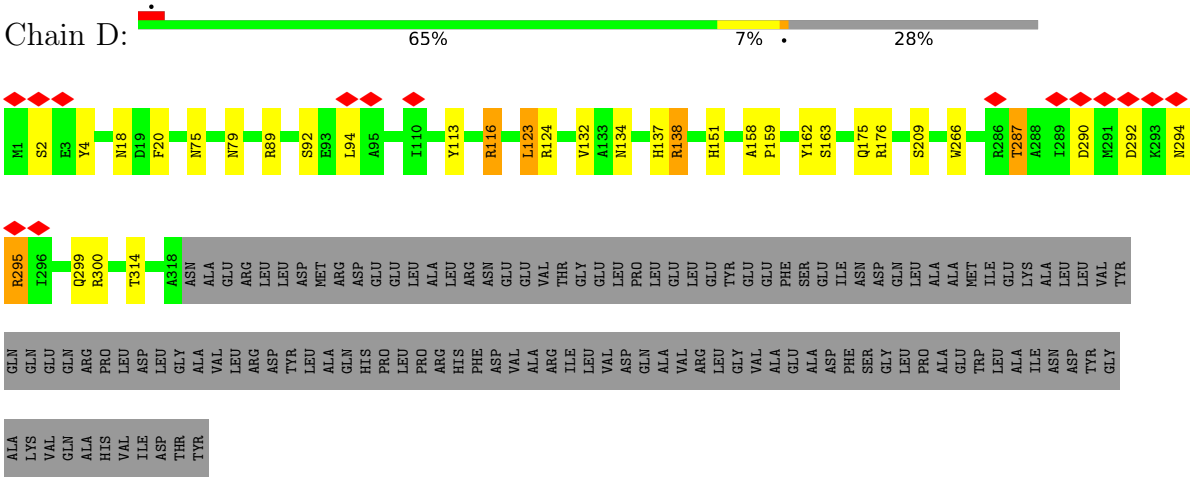
• Molecule 2: Chromosome partition protein MukF

Chain C:



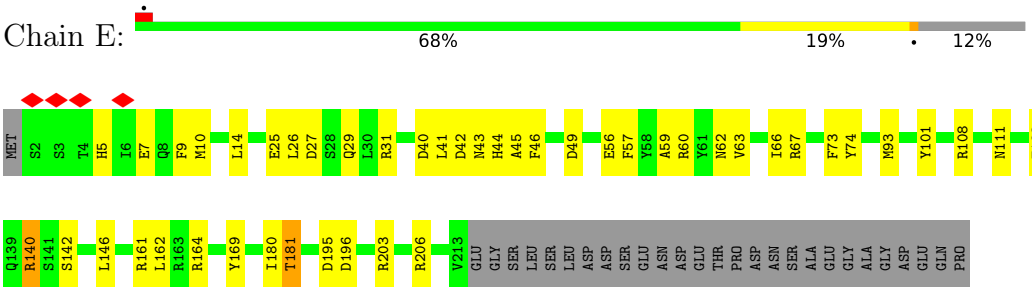
• Molecule 2: Chromosome partition protein MukF

Chain D:



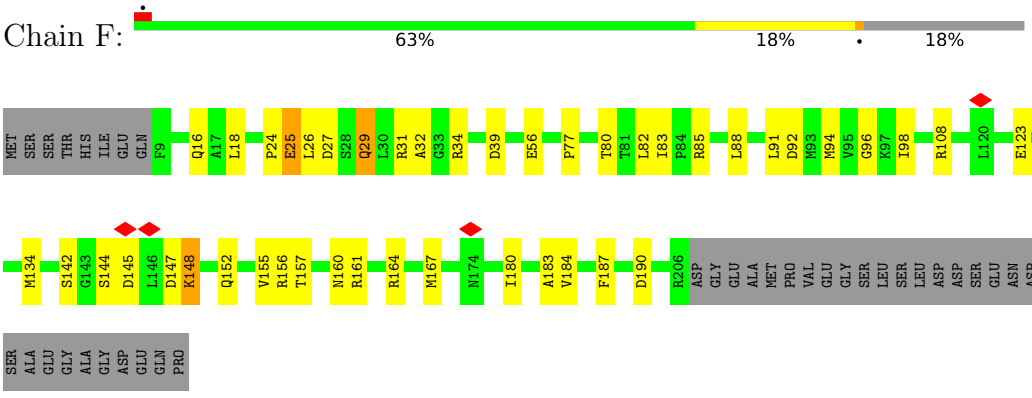
• Molecule 3: Chromosome partition protein MukE

Chain E:



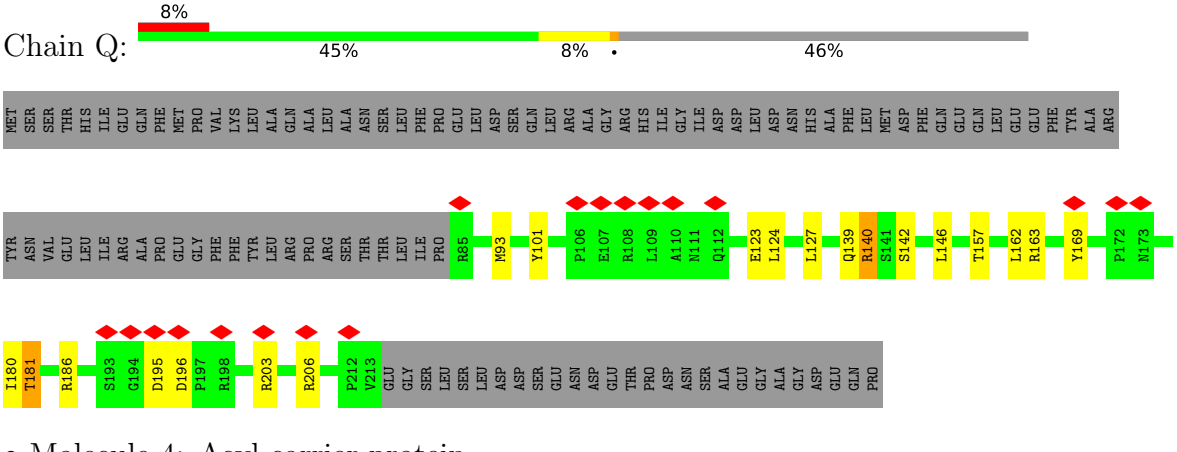
• Molecule 3: Chromosome partition protein MukE

Chain F:



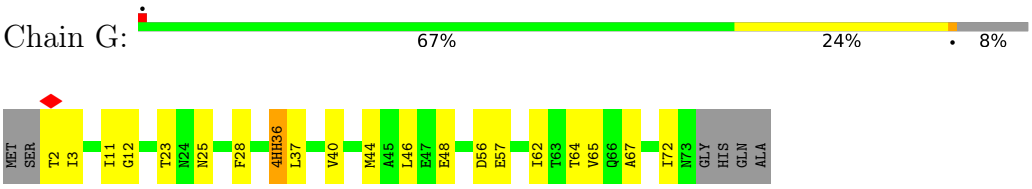
• Molecule 3: Chromosome partition protein MukE

Chain Q:



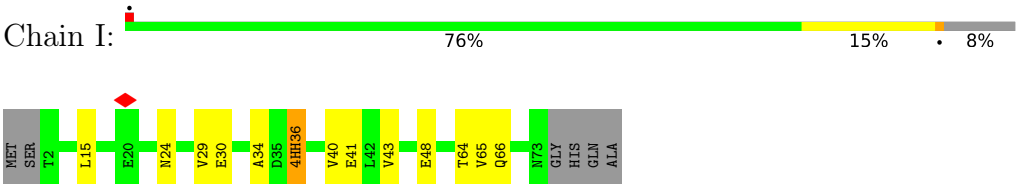
• Molecule 4: Acyl carrier protein

Chain G:



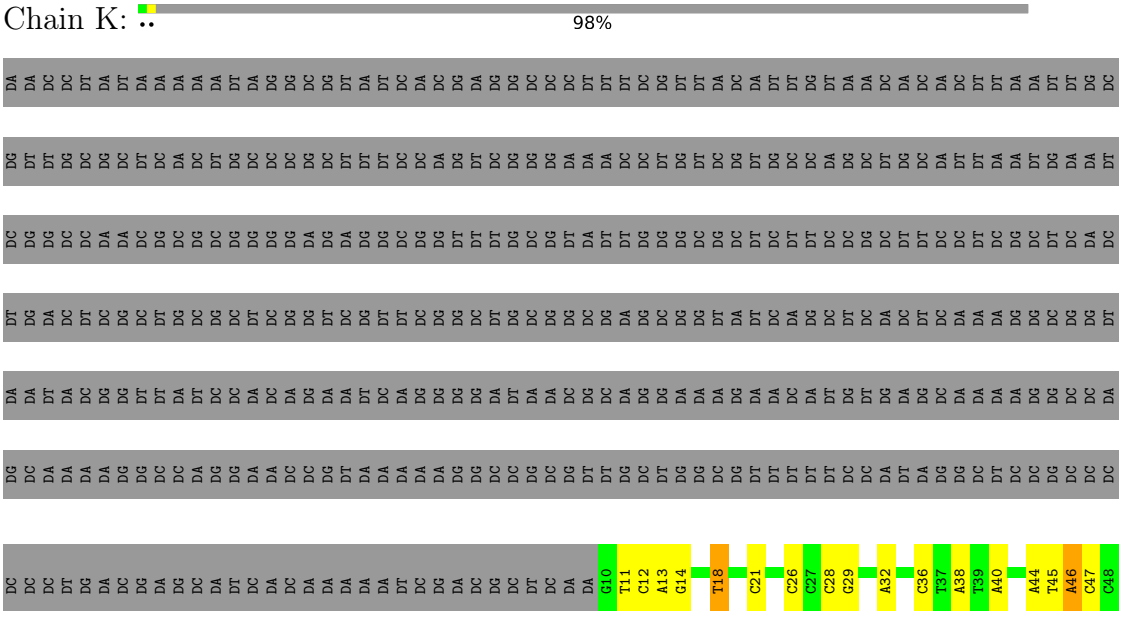
• Molecule 4: Acyl carrier protein

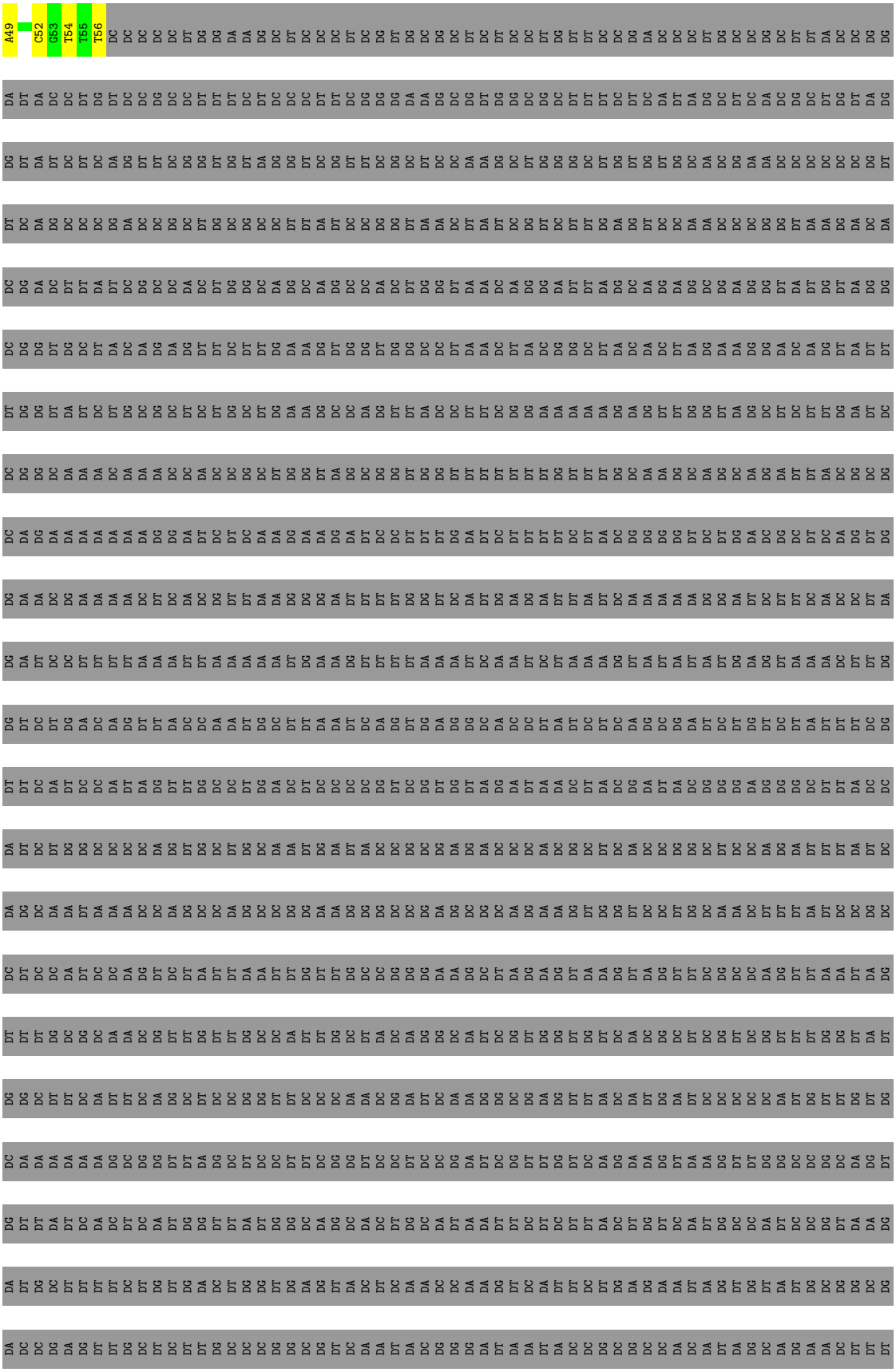
Chain I:

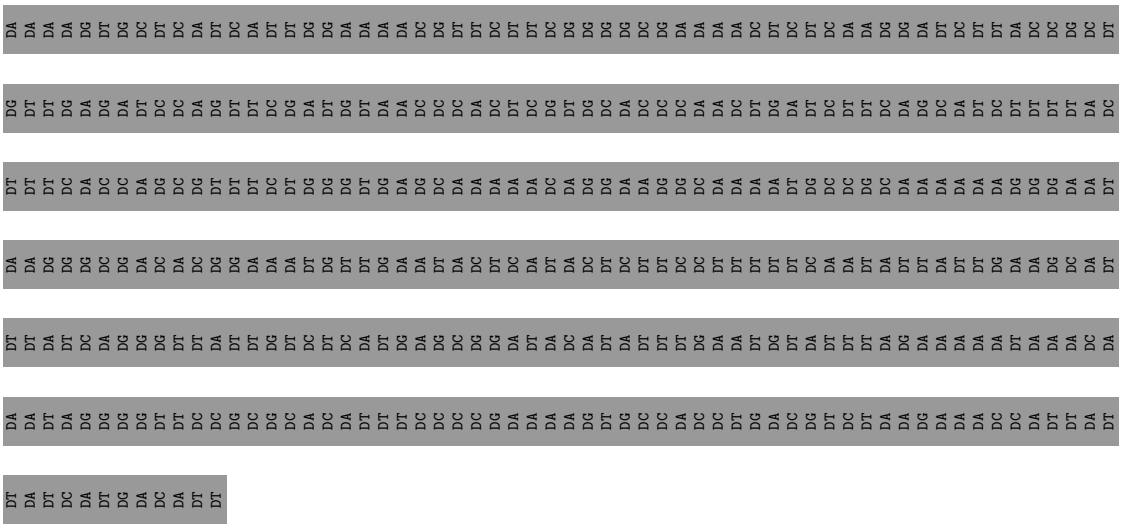


• Molecule 5: pFB526

Chain K:

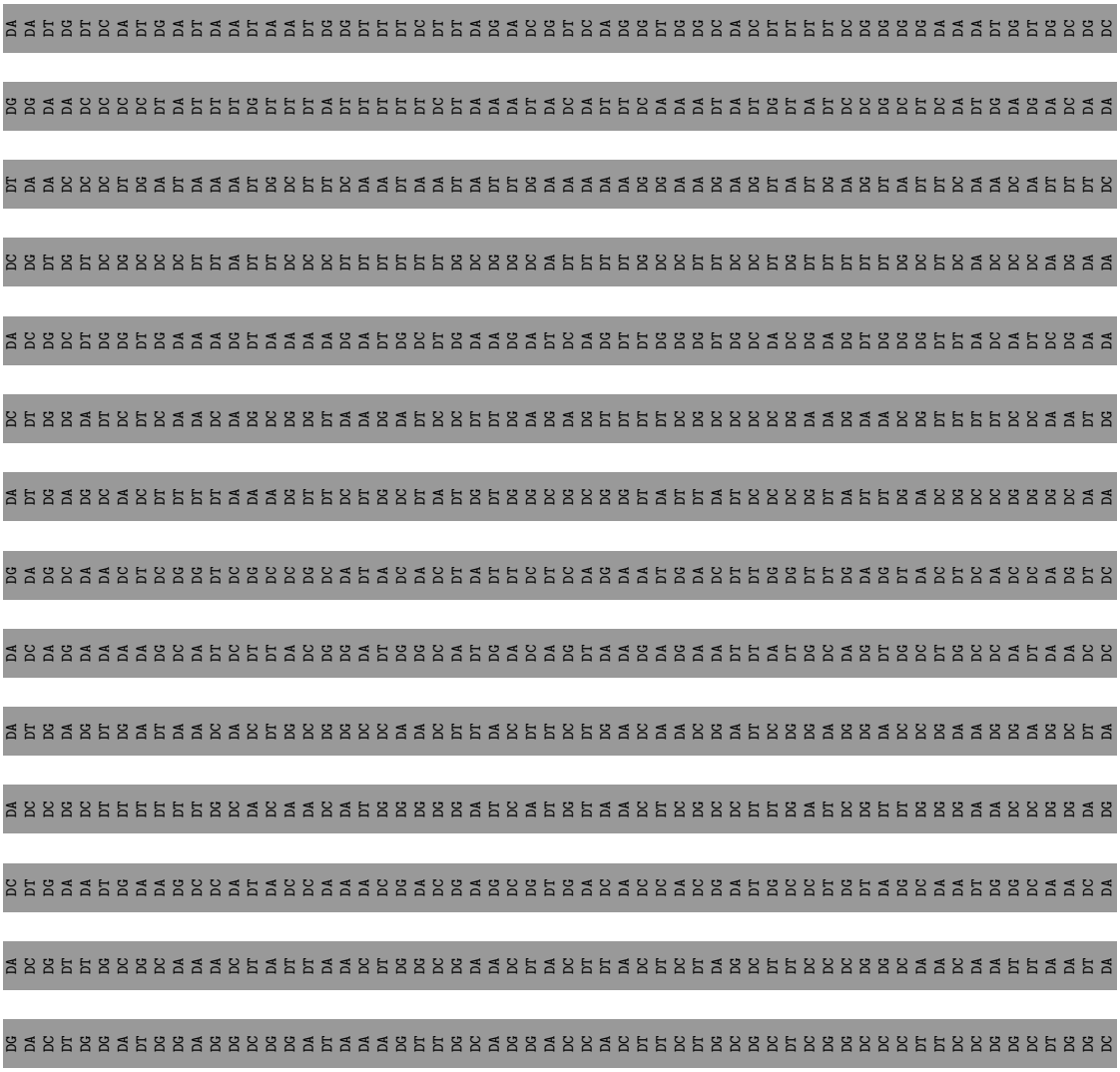


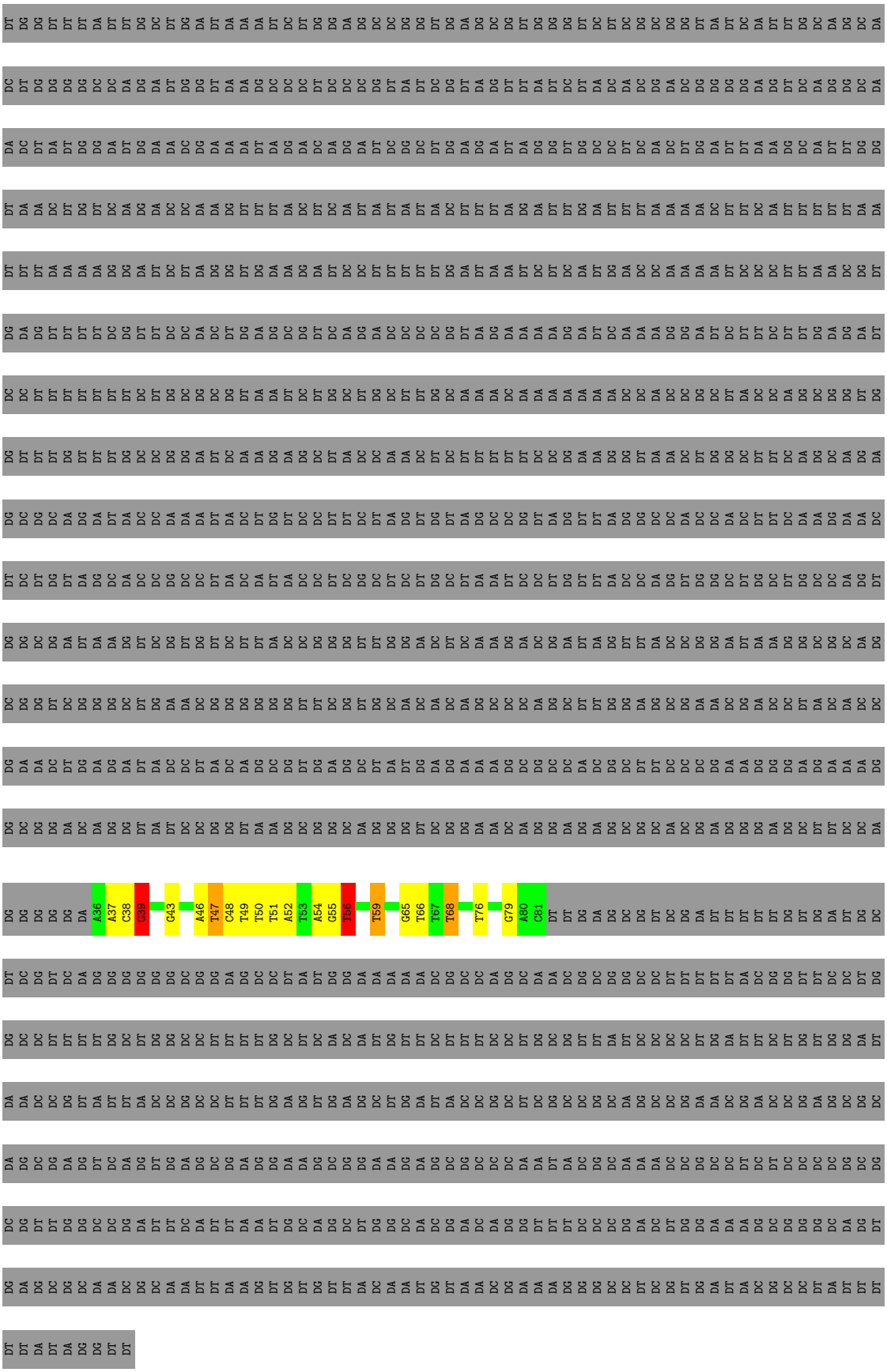

A49
C52
G53
T54
T55
T56



• Molecule 6: pFB526

Chain L: 98%




A36
A37
C38
G39
G43
A46
T47
C48
T49
T50
T51
A52
T53
A54
G55
T56
T59
G65
T66
T67
T68
T76
G79
A80
C81

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7508	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.110	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	460.98074, 460.98074, 460.98074	wwPDB
Map dimensions	184, 184, 184	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.50533, 2.50533, 2.50533	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 4HH, MG, ATP

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	2/8143 (0.0%)	0.67	3/10968 (0.0%)
1	B	1.20	65/8143 (0.8%)	1.29	133/10968 (1.2%)
2	C	0.83	2/3592 (0.1%)	1.30	21/4862 (0.4%)
2	D	0.87	1/2593 (0.0%)	1.44	16/3504 (0.5%)
3	E	1.50	19/1753 (1.1%)	1.71	44/2361 (1.9%)
3	F	1.64	24/1648 (1.5%)	1.68	49/2218 (2.2%)
3	Q	0.99	6/1054 (0.6%)	1.42	7/1413 (0.5%)
4	G	0.13	0/558	0.28	0/754
4	I	0.13	0/558	0.27	0/754
5	K	0.70	0/1095	1.71	8/1689 (0.5%)
6	L	0.71	0/1041	1.71	10/1603 (0.6%)
All	All	0.95	119/30178 (0.4%)	1.25	291/41094 (0.7%)

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
2	C	0	6
2	D	0	5
3	E	0	4
3	Q	0	2
5	K	0	13
6	L	0	12
All	All	0	42

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	295	ARG	C-N	-24.36	1.03	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	295	ARG	C-N	-24.36	1.03	1.33
1	A	589	GLN	C-N	13.54	1.51	1.33
3	E	44	HIS	CE1-NE2	-8.90	1.23	1.32
1	B	175	HIS	CE1-NE2	-8.88	1.23	1.32
1	B	1193	HIS	CE1-NE2	-8.79	1.23	1.32
1	B	1166	HIS	CE1-NE2	-8.79	1.23	1.32
1	B	1193	HIS	CD2-NE2	-8.06	1.28	1.37
1	B	1166	HIS	CD2-NE2	-7.97	1.29	1.37
1	B	175	HIS	CD2-NE2	-7.94	1.29	1.37
3	E	44	HIS	CD2-NE2	-7.93	1.29	1.37
1	B	1131	ARG	CZ-NH2	-7.71	1.23	1.33
3	Q	203	ARG	CZ-NH2	-7.71	1.23	1.33
3	E	206	ARG	CZ-NH2	-7.70	1.23	1.33
3	F	31	ARG	CZ-NH2	-7.68	1.23	1.33
3	Q	206	ARG	CZ-NH2	-7.63	1.23	1.33
3	E	31	ARG	CZ-NH2	-7.60	1.23	1.33
1	B	1093	GLN	C-N	7.59	1.44	1.33
1	B	1221	ARG	CZ-NH2	-7.59	1.23	1.33
3	E	203	ARG	CZ-NH2	-7.57	1.23	1.33
1	B	240	ARG	CZ-NH2	-7.55	1.23	1.33
1	B	1197	ARG	CZ-NH2	-7.55	1.23	1.33
1	B	1132	ARG	CZ-NH2	-7.54	1.23	1.33
1	B	1199	ARG	CZ-NH2	-7.54	1.23	1.33
1	B	250	ARG	CZ-NH2	-7.49	1.23	1.33
3	E	67	ARG	CZ-NH2	-7.46	1.23	1.33
3	F	164	ARG	CZ-NH2	-7.45	1.23	1.33
1	B	199	ARG	CZ-NH2	-7.43	1.23	1.33
1	B	243	ARG	CZ-NH2	-7.40	1.23	1.33
1	B	1328	ARG	CZ-NH2	-7.39	1.23	1.33
3	F	85	ARG	CZ-NH2	-7.39	1.23	1.33
3	E	60	ARG	CZ-NH2	-7.37	1.23	1.33
1	B	229	ARG	CZ-NH2	-7.36	1.23	1.33
3	F	34	ARG	CZ-NH2	-7.36	1.23	1.33
1	B	105	ARG	CZ-NH2	-7.36	1.23	1.33
3	F	161	ARG	CZ-NH2	-7.36	1.23	1.33
1	B	1393	ARG	CZ-NH2	-7.33	1.24	1.33
1	B	1250	ARG	CZ-NH2	-7.32	1.24	1.33
1	B	96	ARG	CZ-NH2	-7.31	1.24	1.33
3	F	156	ARG	CZ-NH2	-7.26	1.24	1.33
1	B	1390	ARG	CZ-NH2	-7.23	1.24	1.33
1	B	301	GLN	C-N	7.14	1.43	1.34
1	B	1394	GLY	N-CA	-6.69	1.37	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1189	ALA	CA-CB	-6.61	1.43	1.53
1	B	248	ALA	CA-CB	-6.54	1.43	1.53
1	A	847	GLU	C-N	6.48	1.42	1.33
3	E	45	ALA	CA-CB	-6.30	1.43	1.53
1	B	231	ALA	CA-CB	-6.27	1.43	1.53
1	B	103	GLY	N-CA	-6.25	1.38	1.45
2	C	320	ALA	CA-CB	-6.21	1.43	1.53
1	B	250	ARG	CZ-NH1	-6.20	1.24	1.32
1	B	191	ALA	CA-CB	-6.18	1.43	1.53
3	E	31	ARG	CZ-NH1	-6.10	1.24	1.32
3	F	164	ARG	CZ-NH1	-6.09	1.24	1.32
1	B	1199	ARG	CZ-NH1	-6.08	1.24	1.32
1	B	240	ARG	CZ-NH1	-6.07	1.24	1.32
3	F	31	ARG	CZ-NH1	-6.07	1.24	1.32
3	E	67	ARG	CZ-NH1	-6.06	1.24	1.32
3	E	203	ARG	CZ-NH1	-6.06	1.24	1.32
3	Q	203	ARG	CZ-NH1	-6.06	1.24	1.32
1	B	50	ALA	CA-CB	-6.05	1.43	1.53
3	E	206	ARG	CZ-NH1	-6.05	1.24	1.32
1	B	105	ARG	CZ-NH1	-6.04	1.24	1.32
3	Q	206	ARG	CZ-NH1	-6.03	1.24	1.32
1	B	243	ARG	CZ-NH1	-6.01	1.24	1.32
3	F	128	ALA	CA-CB	-6.01	1.43	1.53
1	B	1211	ALA	CA-CB	-5.99	1.43	1.53
1	B	1221	ARG	CZ-NH1	-5.98	1.24	1.32
1	B	1132	ARG	CZ-NH1	-5.97	1.24	1.32
3	E	60	ARG	CZ-NH1	-5.97	1.24	1.32
3	F	34	ARG	CZ-NH1	-5.95	1.24	1.32
3	F	96	GLY	N-CA	-5.95	1.38	1.45
1	B	1131	ARG	CZ-NH1	-5.92	1.24	1.32
1	B	96	ARG	CZ-NH1	-5.88	1.24	1.32
1	B	1197	ARG	CZ-NH1	-5.87	1.24	1.32
1	B	1328	ARG	CZ-NH1	-5.87	1.24	1.32
1	B	229	ARG	CZ-NH1	-5.84	1.24	1.32
3	F	156	ARG	CZ-NH1	-5.83	1.24	1.32
1	B	1250	ARG	CZ-NH1	-5.83	1.24	1.32
3	F	131	GLY	N-CA	-5.82	1.38	1.45
1	B	199	ARG	CZ-NH1	-5.81	1.24	1.32
1	B	1393	ARG	CZ-NH1	-5.79	1.24	1.32
3	F	161	ARG	CZ-NH1	-5.79	1.24	1.32
3	E	59	ALA	CA-CB	-5.79	1.43	1.53
3	F	85	ARG	CZ-NH1	-5.78	1.24	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	227	GLY	N-CA	-5.77	1.38	1.45
1	B	1390	ARG	CZ-NH1	-5.76	1.24	1.32
3	F	83	ILE	N-CA	-5.70	1.42	1.46
3	F	32	ALA	CA-CB	-5.65	1.43	1.53
1	B	199	ARG	CD-NE	-5.53	1.38	1.46
1	B	240	ARG	CD-NE	-5.43	1.38	1.46
3	F	85	ARG	CD-NE	-5.42	1.38	1.46
1	B	223	PRO	CA-CB	-5.33	1.46	1.53
1	B	1199	ARG	CD-NE	-5.27	1.38	1.46
3	Q	203	ARG	CD-NE	-5.27	1.38	1.46
3	F	34	ARG	CD-NE	-5.26	1.38	1.46
3	E	203	ARG	CD-NE	-5.26	1.38	1.46
1	B	1132	ARG	CD-NE	-5.25	1.38	1.46
1	B	250	ARG	CD-NE	-5.21	1.39	1.46
3	F	164	ARG	CD-NE	-5.21	1.39	1.46
3	E	60	ARG	CD-NE	-5.18	1.39	1.46
3	F	161	ARG	CD-NE	-5.18	1.39	1.46
1	B	96	ARG	CD-NE	-5.16	1.39	1.46
1	B	1221	ARG	CD-NE	-5.16	1.39	1.46
1	B	105	ARG	CD-NE	-5.16	1.39	1.46
1	B	1390	ARG	CD-NE	-5.13	1.39	1.46
1	B	243	ARG	CD-NE	-5.13	1.39	1.46
3	E	67	ARG	CD-NE	-5.11	1.39	1.46
3	F	142	SER	CA-CB	-5.11	1.45	1.52
3	E	31	ARG	CD-NE	-5.11	1.39	1.46
1	B	1250	ARG	CD-NE	-5.10	1.39	1.46
3	F	31	ARG	CD-NE	-5.09	1.39	1.46
1	B	1393	ARG	CD-NE	-5.09	1.39	1.46
3	Q	206	ARG	CD-NE	-5.09	1.39	1.46
1	B	229	ARG	CD-NE	-5.08	1.39	1.46
3	F	77	PRO	CA-CB	-5.05	1.47	1.53
1	B	1131	ARG	CD-NE	-5.03	1.39	1.46
3	E	206	ARG	CD-NE	-5.03	1.39	1.46
1	B	1197	ARG	CD-NE	-5.01	1.39	1.46

All (291) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	295	ARG	CA-C-N	22.14	147.89	120.88
2	C	295	ARG	C-N-CA	22.14	147.89	120.88
2	D	295	ARG	CA-C-N	22.07	147.81	120.88
2	D	295	ARG	C-N-CA	22.07	147.81	120.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	589	GLN	O-C-N	9.98	132.35	122.07
3	F	82	LEU	CA-C-N	9.41	129.36	122.59
3	F	82	LEU	C-N-CA	9.41	129.36	122.59
1	B	1127	ASN	CA-CB-CG	8.43	121.03	112.60
1	B	259	PHE	CA-CB-CG	7.87	121.67	113.80
1	A	589	GLN	CA-C-N	-7.83	109.65	120.38
1	A	589	GLN	C-N-CA	-7.83	109.65	120.38
2	C	120	PHE	CA-CB-CG	-7.53	106.27	113.80
1	B	232	PHE	CA-CB-CG	7.21	121.01	113.80
5	K	47	DC	O3'-P-O5'	-7.17	93.24	104.00
2	D	294	ASN	N-CA-C	-7.03	103.67	111.82
2	C	294	ASN	N-CA-C	-6.97	103.73	111.82
3	F	160	ASN	CA-CB-CG	6.72	119.32	112.60
2	D	176	ARG	CB-CG-CD	6.72	126.75	111.30
3	E	195	ASP	CA-CB-CG	6.67	119.27	112.60
1	B	301	GLN	O-C-N	-6.65	115.07	122.12
3	E	44	HIS	CA-CB-CG	6.65	120.45	113.80
1	B	197	PHE	CA-CB-CG	6.64	120.44	113.80
3	Q	195	ASP	CA-CB-CG	6.61	119.21	112.60
1	B	225	ASN	CA-CB-CG	6.57	119.17	112.60
3	E	73	PHE	CA-CB-CG	6.53	120.33	113.80
1	B	94	ASN	CA-CB-CG	6.50	119.10	112.60
1	B	1187	PHE	CA-CB-CG	6.46	120.26	113.80
3	E	43	ASN	CA-CB-CG	6.46	119.06	112.60
3	F	187	PHE	CA-CB-CG	6.45	120.25	113.80
3	E	196	ASP	CA-CB-CG	6.45	119.05	112.60
3	Q	196	ASP	CA-CB-CG	6.44	119.04	112.60
1	B	1164	ASN	CA-CB-CG	6.42	119.02	112.60
1	B	1207	ASP	CA-CB-CG	6.41	119.01	112.60
6	L	43	DG	C2'-C3'-O3'	-6.39	101.92	111.50
1	B	175	HIS	CA-CB-CG	6.37	120.17	113.80
1	B	1210	ASP	CA-CB-CG	6.35	118.95	112.60
1	B	187	ARG	NE-CZ-NH2	6.29	124.86	119.20
1	B	1131	ARG	CD-NE-CZ	6.29	133.20	124.40
1	B	54	ASP	CA-CB-CG	6.28	118.88	112.60
1	B	1193	HIS	CA-CB-CG	6.28	120.08	113.80
1	B	255	ASP	CA-CB-CG	6.27	118.87	112.60
1	B	1201	ASP	N-CA-C	6.27	118.63	111.11
2	C	325	ASP	CA-CB-CG	6.22	118.82	112.60
3	E	57	PHE	CA-CB-CG	6.20	120.00	113.80
1	B	97	HIS	CA-C-N	6.20	131.55	123.00
1	B	97	HIS	C-N-CA	6.20	131.55	123.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1221	ARG	CD-NE-CZ	6.19	133.07	124.40
5	K	46	DA	O3'-P-O5'	6.18	113.27	104.00
1	B	243	ARG	CA-CB-CG	6.15	126.40	114.10
1	B	164	GLN	CA-C-N	6.15	131.49	123.00
1	B	164	GLN	C-N-CA	6.15	131.49	123.00
5	K	47	DC	C2'-C3'-O3'	-6.15	102.28	111.50
1	B	1132	ARG	CD-NE-CZ	6.14	133.00	124.40
1	B	234	ASP	CA-CB-CG	6.10	118.70	112.60
1	B	201	ILE	N-CA-CB	6.08	117.67	110.55
1	B	229	ARG	CD-NE-CZ	6.07	132.90	124.40
3	E	62	ASN	CA-CB-CG	6.06	118.66	112.60
1	B	243	ARG	CG-CD-NE	6.05	125.32	112.00
1	B	1328	ARG	CD-NE-CZ	6.04	132.85	124.40
1	B	105	ARG	CD-NE-CZ	6.03	132.84	124.40
1	B	224	GLU	CA-C-N	6.03	131.50	123.00
1	B	224	GLU	C-N-CA	6.03	131.50	123.00
3	E	138	ASN	CA-CB-CG	6.02	118.62	112.60
1	B	198	TYR	N-CA-CB	6.01	118.73	110.01
3	F	145	ASP	CA-CB-CG	6.01	118.61	112.60
3	F	27	ASP	CA-CB-CG	5.98	118.58	112.60
3	E	66	ILE	CA-C-N	5.97	131.79	123.07
3	E	66	ILE	C-N-CA	5.97	131.79	123.07
3	E	138	ASN	CB-CA-C	5.97	120.60	109.86
3	F	156	ARG	CD-NE-CZ	5.96	132.75	124.40
3	E	42	ASP	CA-C-N	5.95	128.18	120.44
3	E	42	ASP	C-N-CA	5.95	128.18	120.44
1	B	118	ILE	CA-C-N	5.94	130.82	122.74
1	B	118	ILE	C-N-CA	5.94	130.82	122.74
1	B	263	ILE	N-CA-CB	5.94	117.09	110.62
3	E	42	ASP	CA-CB-CG	5.93	118.53	112.60
1	B	96	ARG	CD-NE-CZ	5.93	132.70	124.40
1	B	122	MET	CA-C-N	5.92	131.23	122.99
1	B	122	MET	C-N-CA	5.92	131.23	122.99
3	E	60	ARG	CD-NE-CZ	5.92	132.68	124.40
1	B	103	GLY	N-CA-C	5.89	119.20	110.42
2	C	124	ARG	CA-CB-CG	5.89	125.87	114.10
1	B	1244	ILE	N-CA-CB	5.88	117.43	110.55
5	K	32	DA	C5'-C4'-C3'	-5.88	106.08	114.90
1	B	1339	ASP	CA-C-N	5.87	128.14	120.28
1	B	1339	ASP	C-N-CA	5.87	128.14	120.28
3	E	63	VAL	CA-C-N	5.87	130.22	122.30
3	E	63	VAL	C-N-CA	5.87	130.22	122.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	31	ARG	CD-NE-CZ	5.84	132.58	124.40
6	L	47	DT	C5'-C4'-O4'	5.84	118.16	109.40
3	E	31	ARG	CD-NE-CZ	5.82	132.55	124.40
1	B	166	LYS	CA-C-N	5.82	131.19	122.99
1	B	166	LYS	C-N-CA	5.82	131.19	122.99
1	B	1192	GLN	CA-C-N	5.81	128.38	120.54
1	B	1192	GLN	C-N-CA	5.81	128.38	120.54
1	B	235	MET	CA-C-N	5.79	127.97	120.44
1	B	235	MET	C-N-CA	5.79	127.97	120.44
2	C	294	ASN	CA-C-N	5.79	130.79	122.40
2	C	294	ASN	C-N-CA	5.79	130.79	122.40
6	L	56	DT	O3'-P-O5'	-5.79	95.32	104.00
1	B	1395	LYS	CA-CB-CG	5.78	125.66	114.10
3	F	147	ASP	CA-CB-CG	5.77	118.37	112.60
2	D	294	ASN	CA-C-N	5.77	130.76	122.40
2	D	294	ASN	C-N-CA	5.77	130.76	122.40
3	E	25	GLU	CA-C-N	5.76	127.93	120.44
3	E	25	GLU	C-N-CA	5.76	127.93	120.44
1	B	1250	ARG	CD-NE-CZ	5.76	132.46	124.40
1	B	1197	ARG	CA-C-N	5.75	128.21	120.50
1	B	1197	ARG	C-N-CA	5.75	128.21	120.50
1	B	165	PHE	CA-CB-CG	5.74	119.53	113.80
3	F	129	ASP	CA-C-N	5.73	127.96	120.28
3	F	129	ASP	C-N-CA	5.73	127.96	120.28
3	E	74	TYR	CA-C-N	5.73	130.63	122.72
3	E	74	TYR	C-N-CA	5.73	130.63	122.72
3	E	27	ASP	CA-CB-CG	5.71	118.31	112.60
1	B	249	ILE	N-CA-CB	5.69	117.20	110.55
1	B	100	VAL	CA-C-N	5.67	131.04	123.10
1	B	100	VAL	C-N-CA	5.67	131.04	123.10
1	B	103	GLY	CA-C-N	5.67	130.97	122.58
1	B	103	GLY	C-N-CA	5.67	130.97	122.58
1	B	244	ILE	N-CA-CB	5.66	116.56	110.62
2	C	137	HIS	CB-CG-CD2	-5.65	123.86	131.20
3	F	92	ASP	CA-CB-CG	5.64	118.25	112.60
2	C	330	GLU	N-CA-CB	5.64	118.22	109.48
3	E	67	ARG	CG-CD-NE	5.63	124.39	112.00
1	B	256	ARG	CD-NE-CZ	5.63	132.28	124.40
3	F	161	ARG	N-CA-CB	5.63	118.33	109.94
1	B	101	VAL	CA-C-N	5.63	130.16	122.34
1	B	101	VAL	C-N-CA	5.63	130.16	122.34
3	F	26	LEU	CA-C-N	5.62	127.75	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	26	LEU	C-N-CA	5.62	127.75	120.44
1	B	1188	ILE	N-CA-CB	5.62	116.75	110.51
3	E	56	GLU	CA-C-N	5.61	128.05	120.65
3	E	56	GLU	C-N-CA	5.61	128.05	120.65
1	B	163	VAL	CA-C-N	5.61	130.90	123.05
1	B	163	VAL	C-N-CA	5.61	130.90	123.05
1	B	1126	ASP	CA-CB-CG	5.61	118.21	112.60
3	E	46	PHE	N-CA-CB	5.60	118.29	109.94
2	D	137	HIS	CB-CG-CD2	-5.59	123.93	131.20
1	B	1387	GLU	N-CA-CB	5.58	118.33	110.12
3	F	88	LEU	CA-C-N	5.58	130.65	121.39
3	F	88	LEU	C-N-CA	5.58	130.65	121.39
2	D	287	THR	CA-CB-OG1	5.58	117.97	109.60
6	L	39	DG	C4'-C3'-O3'	-5.57	101.65	110.00
2	C	287	THR	CA-CB-OG1	5.56	117.94	109.60
1	B	193	ASP	CA-CB-CG	5.54	118.14	112.60
1	B	104	VAL	CA-C-N	5.54	130.13	122.77
1	B	104	VAL	C-N-CA	5.54	130.13	122.77
2	C	295	ARG	CB-CA-C	5.54	120.26	111.51
1	B	228	VAL	CA-C-N	5.53	127.63	120.44
1	B	228	VAL	C-N-CA	5.53	127.63	120.44
6	L	43	DG	O3'-P-O5'	-5.53	95.71	104.00
2	D	295	ARG	CB-CA-C	5.53	120.24	111.51
3	F	24	PRO	CA-C-N	5.52	127.62	120.44
3	F	24	PRO	C-N-CA	5.52	127.62	120.44
1	B	149	PRO	CA-C-N	5.52	127.61	120.44
1	B	149	PRO	C-N-CA	5.52	127.61	120.44
1	B	1216	GLU	CA-C-N	5.51	127.50	120.56
1	B	1216	GLU	C-N-CA	5.51	127.50	120.56
1	B	1197	ARG	CD-NE-CZ	5.49	132.09	124.40
1	B	99	ARG	CA-C-N	5.48	130.61	122.99
1	B	99	ARG	C-N-CA	5.48	130.61	122.99
1	B	1399	PRO	CA-C-N	5.48	129.02	120.75
1	B	1399	PRO	C-N-CA	5.48	129.02	120.75
3	F	128	ALA	CA-C-N	5.47	129.24	121.42
3	F	128	ALA	C-N-CA	5.47	129.24	121.42
3	E	43	ASN	CA-C-N	5.47	127.55	120.44
3	E	43	ASN	C-N-CA	5.47	127.55	120.44
3	E	44	HIS	CA-C-N	5.46	127.54	120.44
3	E	44	HIS	C-N-CA	5.46	127.54	120.44
1	B	1396	ASP	CA-C-N	5.45	130.21	123.12
1	B	1396	ASP	C-N-CA	5.45	130.21	123.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	117	ASP	CA-C-N	5.45	130.57	122.99
1	B	117	ASP	C-N-CA	5.45	130.57	122.99
1	B	1212	ILE	N-CA-CB	5.45	116.34	110.62
5	K	56	DT	C2'-C3'-O3'	5.45	119.67	111.50
3	E	46	PHE	CA-CB-CG	5.42	119.22	113.80
3	F	155	VAL	N-CA-CB	5.42	116.89	110.55
2	C	116	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	B	1221	ARG	CA-CB-CG	5.39	124.88	114.10
2	C	323	LEU	CA-C-N	5.38	128.41	120.82
2	C	323	LEU	C-N-CA	5.38	128.41	120.82
1	B	227	GLY	CA-C-N	5.38	127.34	120.56
1	B	227	GLY	C-N-CA	5.38	127.34	120.56
3	Q	139	GLN	CB-CG-CD	5.38	121.75	112.60
1	B	48	VAL	N-CA-CB	5.38	117.86	110.54
3	F	129	ASP	CA-CB-CG	5.37	117.97	112.60
3	F	98	ILE	N-CA-CB	5.37	116.83	110.55
1	B	243	ARG	CD-NE-CZ	5.37	131.91	124.40
1	B	233	GLN	CA-C-N	5.36	127.72	120.65
1	B	233	GLN	C-N-CA	5.36	127.72	120.65
1	B	1322	GLN	CA-CB-CG	5.35	124.81	114.10
1	B	194	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	B	186	LYS	CA-CB-CG	5.34	124.78	114.10
1	B	194	ARG	N-CA-CB	-5.33	102.28	110.12
3	F	91	LEU	CA-C-N	5.33	127.37	120.44
3	F	91	LEU	C-N-CA	5.33	127.37	120.44
3	F	123	GLU	CA-C-N	5.33	127.73	120.54
3	F	123	GLU	C-N-CA	5.33	127.73	120.54
1	B	250	ARG	CA-C-N	5.32	127.21	120.72
1	B	250	ARG	C-N-CA	5.32	127.21	120.72
2	C	299	GLN	CA-C-N	5.32	127.72	120.54
2	C	299	GLN	C-N-CA	5.32	127.72	120.54
2	D	116	ARG	NE-CZ-NH2	5.32	123.99	119.20
3	F	148	LYS	CG-CD-CE	5.32	123.53	111.30
3	F	144	SER	CA-C-N	5.31	127.71	120.54
3	F	144	SER	C-N-CA	5.31	127.71	120.54
3	F	161	ARG	CA-C-N	5.30	127.39	120.28
3	F	161	ARG	C-N-CA	5.30	127.39	120.28
1	B	1220	ALA	CA-C-N	5.30	127.70	120.54
1	B	1220	ALA	C-N-CA	5.30	127.70	120.54
2	D	299	GLN	CA-C-N	5.30	127.70	120.54
2	D	299	GLN	C-N-CA	5.30	127.70	120.54
1	B	1328	ARG	CB-CG-CD	5.30	123.48	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	67	ARG	CA-CB-CG	5.29	124.69	114.10
1	B	1188	ILE	CA-C-N	5.29	127.31	120.44
1	B	1188	ILE	C-N-CA	5.29	127.31	120.44
5	K	56	DT	C4'-C3'-O3'	-5.28	102.08	110.00
3	E	62	ASN	CA-C-N	5.28	130.31	122.71
3	E	62	ASN	C-N-CA	5.28	130.31	122.71
2	D	123	LEU	CB-CG-CD2	-5.28	94.87	110.70
2	D	290	ASP	N-CA-C	5.27	118.87	112.23
3	E	67	ARG	CD-NE-CZ	5.27	131.78	124.40
2	C	290	ASP	N-CA-C	5.26	118.86	112.23
3	F	34	ARG	N-CA-CB	5.26	117.78	109.83
1	B	191	ALA	CA-C-N	5.24	127.30	120.28
1	B	191	ALA	C-N-CA	5.24	127.30	120.28
3	F	29	GLN	CA-C-N	5.24	127.25	120.44
3	F	29	GLN	C-N-CA	5.24	127.25	120.44
3	F	147	ASP	CA-C-N	5.23	127.29	120.28
3	F	147	ASP	C-N-CA	5.23	127.29	120.28
5	K	26	DC	C5'-C4'-O4'	5.23	117.25	109.40
3	F	94	MET	CA-C-N	5.23	127.14	120.56
3	F	94	MET	C-N-CA	5.23	127.14	120.56
3	E	26	LEU	CA-C-N	5.22	127.23	120.44
3	E	26	LEU	C-N-CA	5.22	127.23	120.44
1	B	234	ASP	CA-C-N	5.22	127.28	120.28
1	B	234	ASP	C-N-CA	5.22	127.28	120.28
3	E	29	GLN	CA-C-N	5.21	127.22	120.44
3	E	29	GLN	C-N-CA	5.21	127.22	120.44
6	L	48	DC	C5'-C4'-O4'	5.21	117.22	109.40
3	E	206	ARG	N-CA-CB	5.21	117.78	110.12
2	C	151	HIS	CB-CG-CD2	-5.20	124.44	131.20
3	F	80	THR	CA-C-N	5.19	128.47	121.05
3	F	80	THR	C-N-CA	5.19	128.47	121.05
1	B	194	ARG	CA-C-N	5.18	127.18	120.44
1	B	194	ARG	C-N-CA	5.18	127.18	120.44
3	F	156	ARG	CA-C-N	5.18	127.49	120.65
3	F	156	ARG	C-N-CA	5.18	127.49	120.65
3	Q	206	ARG	N-CA-CB	5.18	117.73	110.12
1	B	1164	ASN	N-CA-CB	5.17	117.62	110.17
2	D	151	HIS	CB-CG-CD2	-5.17	124.48	131.20
1	B	1187	PHE	CA-C-N	5.16	127.25	120.60
1	B	1187	PHE	C-N-CA	5.16	127.25	120.60
2	C	6	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	B	1246	LYS	CA-C-N	5.15	127.14	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1246	LYS	C-N-CA	5.15	127.14	120.44
6	L	66	DT	C5'-C4'-O4'	5.12	117.09	109.40
6	L	59	DT	C5'-C4'-O4'	5.12	117.08	109.40
1	B	1190	VAL	N-CA-CB	5.11	116.53	110.55
1	B	240	ARG	N-CA-CB	5.10	117.41	110.01
3	E	27	ASP	N-CA-CB	5.10	117.41	110.01
5	K	18	DT	C5'-C4'-O4'	5.09	117.04	109.40
3	F	148	LYS	CA-C-N	5.08	127.05	120.44
3	F	148	LYS	C-N-CA	5.08	127.05	120.44
1	B	1250	ARG	N-CA-CB	5.08	117.51	109.94
3	F	85	ARG	CA-CB-CG	5.08	124.26	114.10
1	B	1198	ILE	CA-C-N	5.08	128.50	120.89
1	B	1198	ILE	C-N-CA	5.08	128.50	120.89
1	B	185	PRO	CA-C-N	5.07	131.04	122.87
1	B	185	PRO	C-N-CA	5.07	131.04	122.87
6	L	68	DT	C5'-C4'-O4'	5.07	117.01	109.40
3	E	40	ASP	CA-C-N	5.07	127.38	120.54
3	E	40	ASP	C-N-CA	5.07	127.38	120.54
1	B	174	TYR	CA-C-N	5.07	127.07	120.28
1	B	174	TYR	C-N-CA	5.07	127.07	120.28
3	Q	163	ARG	NE-CZ-NH2	5.06	123.76	119.20
3	Q	139	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	B	255	ASP	CA-C-N	5.06	127.02	120.44
1	B	255	ASP	C-N-CA	5.06	127.02	120.44
1	B	1239	SER	CA-C-N	5.06	128.64	120.55
1	B	1239	SER	C-N-CA	5.06	128.64	120.55
2	D	176	ARG	CA-CB-CG	-5.05	104.00	114.10
1	B	123	ILE	CA-C-N	5.05	130.51	122.94
1	B	123	ILE	C-N-CA	5.05	130.51	122.94
1	B	1388	GLU	N-CA-CB	5.04	117.32	110.01
3	F	157	THR	CA-C-N	5.04	127.04	120.28
3	F	157	THR	C-N-CA	5.04	127.04	120.28
3	Q	186	ARG	NE-CZ-NH2	5.04	123.73	119.20
6	L	65	DG	C5'-C4'-O4'	5.01	116.92	109.40
2	C	153	HIS	CB-CG-CD2	-5.00	124.70	131.20

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	120	PHE	Sidechain
2	C	138	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	C	300	ARG	Sidechain
2	C	327	ARG	Sidechain
2	C	4	TYR	Sidechain
2	C	89	ARG	Sidechain
2	D	116	ARG	Sidechain
2	D	138	ARG	Sidechain
2	D	300	ARG	Sidechain
2	D	4	TYR	Sidechain
2	D	89	ARG	Sidechain
3	E	101	TYR	Sidechain
3	E	140	ARG	Sidechain
3	E	161	ARG	Sidechain
3	E	164	ARG	Sidechain
5	K	11	DT	Sidechain
5	K	12	DC	Sidechain
5	K	14	DG	Sidechain
5	K	18	DT	Sidechain
5	K	28	DC	Sidechain
5	K	29	DG	Sidechain
5	K	36	DC	Sidechain
5	K	44	DA	Sidechain
5	K	45	DT	Sidechain
5	K	46	DA	Sidechain
5	K	49	DA	Sidechain
5	K	52	DC	Sidechain
5	K	54	DT	Sidechain
6	L	37	DA	Sidechain
6	L	38	DC	Sidechain
6	L	39	DG	Sidechain
6	L	46	DA	Sidechain
6	L	47	DT	Sidechain
6	L	49	DT	Sidechain
6	L	50	DT	Sidechain
6	L	51	DT	Sidechain
6	L	56	DT	Sidechain
6	L	59	DT	Sidechain
6	L	68	DT	Sidechain
6	L	76	DT	Sidechain
3	Q	101	TYR	Sidechain
3	Q	140	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	8027	8011	8007	76	0
1	B	8027	8010	8007	92	0
2	C	3531	3451	3450	69	0
2	D	2550	2496	2495	57	0
3	E	1722	1719	1718	15	0
3	F	1619	1627	1626	14	0
3	Q	1041	1060	1059	8	0
4	G	583	564	563	26	0
4	I	583	564	563	10	0
5	K	973	525	526	4	0
6	L	933	521	520	5	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	31	12	12	0	0
8	B	31	12	12	0	0
All	All	29653	28572	28558	293	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 (293) 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:158:ALA:HB1	2:D:123:LEU:HG	1.19	1.18
2:C:162:TYR:HB3	2:D:124:ARG:HG3	1.23	1.17
2:C:158:ALA:CB	2:D:123:LEU:HG	1.82	1.08
2:C:131:ILE:HD11	2:D:163:SER:OG	1.56	1.05
4:G:36:4HH:CL3	4:G:40:VAL:HG21	1.87	1.04
1:B:1127:ASN:O	1:B:1127:ASN:ND2	1.91	1.03
2:C:138:ARG:NH1	2:D:134:ASN:ND2	2.10	1.00
2:C:162:TYR:HB3	2:D:124:ARG:CG	1.93	0.97
2:C:134:ASN:HD21	2:D:138:ARG:HH12	1.11	0.95
1:B:1107:ARG:NE	4:I:48:GLU:OE1	2.04	0.90
2:C:131:ILE:CD1	2:D:163:SER:OG	2.18	0.90
2:C:138:ARG:NH1	2:D:134:ASN:HD21	1.70	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:138:ARG:HH12	2:D:134:ASN:ND2	1.70	0.88
1:A:292:ARG:HD3	4:G:36:4HH:SU	2.14	0.88
2:C:158:ALA:CB	2:D:123:LEU:CG	2.51	0.87
2:C:162:TYR:CB	2:D:124:ARG:HG3	2.04	0.87
2:C:162:TYR:CG	2:D:124:ARG:HB2	2.12	0.84
1:B:665:GLN:NE2	1:B:671:ASP:OD2	2.11	0.82
1:B:1127:ASN:HD22	1:B:1127:ASN:C	1.88	0.82
2:C:123:LEU:HG	2:D:158:ALA:HB1	1.61	0.81
2:C:134:ASN:HD21	2:D:138:ARG:NH1	1.80	0.80
2:C:158:ALA:HB2	2:D:123:LEU:CD2	2.13	0.79
2:C:123:LEU:HD21	2:D:158:ALA:HB2	1.67	0.77
4:G:36:4HH:HT3	4:G:56:ASP:OD1	1.85	0.77
1:A:1412:ASP:OD1	1:A:1413:ALA:N	2.20	0.73
2:C:124:ARG:HA	2:D:162:TYR:CB	2.20	0.72
2:C:131:ILE:HD11	2:D:163:SER:CB	2.18	0.72
1:B:172:THR:HG21	5:K:21:DC:H5”	1.71	0.71
4:G:36:4HH:CL3	4:G:40:VAL:CG2	2.68	0.70
2:C:124:ARG:HA	2:D:162:TYR:HB3	1.73	0.70
1:A:288:ALA:HB1	4:G:44:MET:HE1	1.73	0.70
4:G:36:4HH:HB2	4:G:36:4HH:HJ2	1.74	0.69
1:B:273:ASP:OD1	1:B:274:TYR:N	2.26	0.68
1:A:1298:GLN:N	1:A:1298:GLN:OE1	2.26	0.67
1:A:1436:GLU:O	1:A:1436:GLU:OE1	2.12	0.67
4:G:23:THR:OG1	4:G:25:ASN:OD1	2.04	0.67
1:A:784:GLU:OE1	1:A:784:GLU:N	2.28	0.67
4:G:36:4HH:HJ2	4:G:36:4HH:CB	2.25	0.67
1:A:826:LEU:HD21	1:B:827:SER:HA	1.75	0.67
2:C:158:ALA:HB2	2:D:123:LEU:HD21	1.77	0.65
2:C:123:LEU:HG	2:D:158:ALA:CB	2.26	0.65
4:G:46:LEU:HD21	4:G:72:ILE:HD11	1.78	0.64
3:F:167:MET:HE2	3:F:167:MET:HA	1.79	0.63
1:B:1332:THR:O	1:B:1336:GLU:N	2.30	0.63
4:G:36:4HH:ON	4:G:40:VAL:CG2	2.48	0.62
2:C:162:TYR:HB3	2:D:124:ARG:CB	2.29	0.62
2:D:314:THR:HA	3:Q:93:MET:HE2	1.81	0.62
1:A:231:ALA:HB2	1:B:665:GLN:CB	2.30	0.62
1:B:1141:MET:HE3	1:B:1141:MET:HA	1.80	0.62
1:B:1322:GLN:O	1:B:1322:GLN:CD	2.43	0.61
2:C:158:ALA:HB2	2:D:123:LEU:CG	2.31	0.61
2:C:314:THR:HA	3:E:93:MET:HE2	1.81	0.61
1:B:254:SER:O	1:B:258:LEU:HD22	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:124:ARG:HB2	2:D:162:TYR:CD1	2.35	0.61
2:C:138:ARG:NH1	2:D:134:ASN:HD22	2.00	0.60
2:C:123:LEU:CG	2:D:158:ALA:CB	2.79	0.60
2:C:162:TYR:CG	2:D:124:ARG:CB	2.85	0.60
1:A:289:LEU:HD22	4:G:36:4HH:HS3	1.83	0.59
2:C:123:LEU:CG	2:D:158:ALA:HB1	2.30	0.59
1:A:1457:GLU:OE1	1:A:1457:GLU:N	2.28	0.59
1:B:788:GLU:OE1	1:B:789:ALA:N	2.35	0.59
4:I:24:ASN:O	4:I:66:GLN:N	2.35	0.59
2:C:158:ALA:HB3	2:C:159:PRO:HD3	1.84	0.58
1:B:1142:GLU:OE1	1:B:1142:GLU:N	2.36	0.58
3:E:10:MET:SD	3:F:18:LEU:HD11	2.43	0.58
1:B:674:MET:HE3	1:B:674:MET:HA	1.85	0.57
1:B:1107:ARG:HE	4:I:48:GLU:CD	2.12	0.56
2:C:124:ARG:HA	2:D:162:TYR:CG	2.41	0.56
1:A:231:ALA:HB2	1:B:665:GLN:HB2	1.89	0.54
1:B:273:ASP:OD1	1:B:273:ASP:C	2.49	0.54
1:A:236:GLU:OE2	1:A:1307:THR:HG21	2.08	0.54
1:B:822:VAL:HA	1:B:826:LEU:HD23	1.88	0.54
4:G:36:4HH:HJ3	4:G:37:LEU:N	2.22	0.54
1:A:828:VAL:HG12	1:A:828:VAL:O	2.08	0.54
1:B:1423:CYS:SG	1:B:1430:LEU:HD11	2.48	0.54
3:E:7:GLU:OE1	3:E:7:GLU:N	2.38	0.54
3:F:148:LYS:HD3	3:F:148:LYS:N	2.23	0.54
2:C:328:ASP:OD1	2:C:328:ASP:O	2.25	0.53
1:A:289:LEU:HD22	4:G:36:4HH:CS	2.39	0.53
1:B:1299:ASP:OD1	1:B:1300:LEU:N	2.42	0.53
2:C:123:LEU:HD11	2:D:158:ALA:CB	2.39	0.53
1:B:1258:LEU:HD21	1:B:1380:MET:HG2	1.90	0.53
1:B:1395:LYS:O	1:B:1395:LYS:HD3	2.09	0.53
2:D:79:ASN:CG	3:E:142:SER:HB3	2.34	0.53
3:Q:124:LEU:C	3:Q:124:LEU:HD23	2.34	0.53
1:A:1126:ASP:O	1:A:1127:ASN:OD1	2.27	0.53
2:C:123:LEU:CD2	2:D:158:ALA:HB2	2.36	0.53
2:C:79:ASN:CG	3:Q:142:SER:HB3	2.34	0.52
3:E:124:LEU:C	3:E:124:LEU:HD23	2.34	0.52
1:A:1281:GLU:O	1:A:1285:ILE:HD12	2.08	0.52
1:A:1420:PHE:HA	1:A:1423:CYS:SG	2.48	0.52
1:A:122:MET:HE1	1:A:177:GLN:HB3	1.90	0.52
1:B:799:GLU:C	1:B:799:GLU:OE1	2.52	0.52
1:B:665:GLN:C	1:B:665:GLN:OE1	2.53	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:828:VAL:HG12	1:B:828:VAL:O	2.10	0.52
1:A:65:GLU:O	1:A:65:GLU:HG3	2.08	0.52
1:A:44:MET:HE3	1:A:1433:ALA:HB2	1.92	0.52
2:D:158:ALA:HB3	2:D:159:PRO:HD3	1.91	0.52
3:E:10:MET:HE3	3:E:14:LEU:HD22	1.92	0.51
1:A:764:ASP:N	1:A:764:ASP:OD1	2.40	0.51
4:G:62:ILE:HG22	4:G:62:ILE:O	2.11	0.51
1:B:732:GLU:H	1:B:732:GLU:CD	2.18	0.51
1:B:63:THR:HG21	1:B:1407:GLU:HG3	1.92	0.51
1:B:1441:GLU:OE1	1:B:1441:GLU:N	2.37	0.51
1:B:1246:LYS:HD2	1:B:1246:LYS:O	2.11	0.51
1:B:1319:LEU:HD12	1:B:1320:ASN:N	2.26	0.51
6:L:39:DG:H3'	3:Q:157:THR:HG23	1.93	0.51
2:C:131:ILE:CD1	2:D:163:SER:CB	2.83	0.51
2:C:370:GLN:OE1	2:C:370:GLN:O	2.29	0.50
1:B:1257:MET:SD	1:B:1257:MET:C	2.95	0.50
1:B:91:ASP:C	1:B:91:ASP:OD1	2.54	0.50
1:B:1161:VAL:HG12	1:B:1161:VAL:O	2.09	0.50
1:B:217:LEU:HG	1:B:221:LEU:HD12	1.91	0.50
2:C:124:ARG:HB2	2:D:162:TYR:CG	2.46	0.50
2:C:356:ASP:C	2:C:356:ASP:OD1	2.55	0.50
3:F:16:GLN:C	3:F:16:GLN:OE1	2.55	0.50
1:A:1163:ASP:OD1	1:A:1164:ASN:N	2.45	0.50
1:B:1196:GLU:N	1:B:1196:GLU:OE1	2.45	0.49
4:I:36:4HH:O	4:I:40:VAL:HG23	2.12	0.49
2:C:162:TYR:CD1	2:D:124:ARG:HD2	2.47	0.49
2:C:358:LEU:HG	2:C:362:ILE:HD11	1.94	0.49
1:A:200:LEU:HD12	1:A:1378:LEU:HD22	1.94	0.49
4:G:36:4HH:CB	4:G:36:4HH:CJ	2.90	0.49
1:A:1361:GLU:OE1	1:A:1361:GLU:HA	2.12	0.49
1:A:235:MET:HA	1:A:235:MET:HE2	1.95	0.49
2:D:75:ASN:HD21	3:E:146:LEU:HB2	1.78	0.49
1:A:1211:ALA:O	1:A:1215:MET:HG2	2.13	0.49
1:B:1107:ARG:CZ	4:I:48:GLU:OE1	2.60	0.49
1:B:1376:SER:O	1:B:1379:VAL:HG22	2.13	0.49
1:A:1376:SER:O	1:A:1379:VAL:HG22	2.12	0.48
2:C:134:ASN:ND2	2:D:138:ARG:NH1	2.57	0.48
2:C:124:ARG:CB	2:D:162:TYR:CG	2.96	0.48
4:G:36:4HH:ON	4:G:40:VAL:HG23	2.14	0.48
2:C:123:LEU:CG	2:D:158:ALA:HB2	2.44	0.48
2:C:292:ASP:CG	2:C:295:ARG:HA	2.39	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:391:LEU:HD13	2:C:428:TYR:CE2	2.49	0.48
3:F:56:GLU:OE1	3:F:56:GLU:HA	2.13	0.48
1:B:244:ILE:HD13	3:E:41:LEU:HD21	1.94	0.48
2:C:106:LEU:HB2	2:D:113:TYR:CD1	2.49	0.48
1:B:94:ASN:OD1	1:B:95:SER:N	2.47	0.48
4:G:11:ILE:HG23	4:G:12:GLY:N	2.29	0.48
1:A:732:GLU:OE1	1:A:732:GLU:N	2.46	0.47
1:B:1322:GLN:O	1:B:1322:GLN:OE1	2.32	0.47
2:C:75:ASN:HD21	3:Q:146:LEU:HB2	1.78	0.47
4:G:2:THR:OG1	4:G:3:ILE:N	2.45	0.47
2:C:162:TYR:CB	2:D:124:ARG:CB	2.93	0.47
2:D:292:ASP:CG	2:D:295:ARG:HA	2.39	0.47
4:G:57:GLU:OE1	4:G:57:GLU:N	2.45	0.47
1:B:184:ILE:HG23	1:B:185:PRO:HD2	1.97	0.47
3:F:180:ILE:HG23	3:F:184:VAL:HG21	1.96	0.47
1:A:1237:SER:OG	1:A:1238:LYS:N	2.45	0.47
1:B:1161:VAL:O	1:B:1161:VAL:CG1	2.62	0.47
2:C:391:LEU:HD13	2:C:428:TYR:CD2	2.50	0.47
1:B:664:SER:OG	1:B:665:GLN:HG3	2.15	0.47
1:B:774:GLU:N	1:B:774:GLU:OE1	2.48	0.47
1:A:62:ASN:OD1	1:A:63:THR:N	2.48	0.46
3:Q:140:ARG:HD2	3:Q:140:ARG:O	2.15	0.46
1:A:588:GLU:O	1:A:592:GLN:HG3	2.15	0.46
1:B:1117:TRP:O	1:B:1121:MET:HG2	2.14	0.46
2:C:375:PRO:HA	2:C:440:TYR:OH	2.15	0.46
3:E:5:HIS:CD2	3:E:7:GLU:OE1	2.69	0.46
1:A:1285:ILE:HD12	1:A:1285:ILE:H	1.81	0.46
4:G:28:PHE:CE1	4:G:65:VAL:HG22	2.51	0.46
1:B:285:LEU:HD13	4:I:41:GLU:OE2	2.15	0.46
1:B:782:ALA:O	1:B:785:ASN:N	2.47	0.46
3:F:39:ASP:OD1	3:F:39:ASP:N	2.49	0.46
1:A:12:LEU:HD21	1:A:46:ALA:HB2	1.97	0.46
1:A:765:ARG:HH11	1:B:748:VAL:HG23	1.81	0.46
1:B:824:LYS:HG2	1:B:824:LYS:O	2.15	0.46
1:A:8:ARG:HH21	1:A:8:ARG:HG3	1.80	0.46
1:B:1275:LEU:HD12	1:B:1347:ASP:O	2.15	0.46
1:B:1320:ASN:ND2	3:E:49:ASP:OD2	2.49	0.46
3:F:25:GLU:CD	3:F:25:GLU:H	2.23	0.46
1:B:782:ALA:O	1:B:785:ASN:CB	2.64	0.46
2:C:426:ASN:OD1	2:C:430:ALA:HB3	2.16	0.46
2:C:106:LEU:HD13	2:D:113:TYR:CG	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:134:ASN:ND2	2:D:138:ARG:HH12	1.95	0.45
1:B:1375:MET:HG2	1:B:1419:LEU:HD11	1.99	0.45
1:A:275:MET:HE1	1:A:1134:HIS:ND1	2.31	0.45
1:A:1213:GLU:OE1	1:B:813:ARG:NE	2.49	0.45
1:B:784:GLU:HA	1:B:787:LEU:HG	1.98	0.45
1:B:679:GLU:OE1	1:B:679:GLU:HA	2.16	0.45
3:F:134:MET:N	3:F:134:MET:HE2	2.32	0.45
1:B:611:LEU:C	1:B:611:LEU:HD23	2.42	0.45
5:K:38:DA:C2	6:L:54:DA:C2	3.05	0.45
1:A:247:GLU:HA	1:A:247:GLU:OE1	2.17	0.45
1:A:1127:ASN:OD1	1:A:1127:ASN:C	2.60	0.45
1:A:640:ARG:O	1:A:643:THR:HG22	2.17	0.44
1:A:1275:LEU:HD23	1:A:1380:MET:HE2	1.98	0.44
2:C:138:ARG:HH11	2:D:134:ASN:HD21	1.56	0.44
3:F:190:ASP:C	3:F:190:ASP:OD1	2.60	0.44
1:A:1121:MET:HA	1:A:1124:VAL:HG12	1.99	0.44
4:G:36:4HH:OM	4:G:37:LEU:HA	2.17	0.44
5:K:40:DA:C2	6:L:52:DA:C2	3.05	0.44
1:B:232:PHE:CZ	1:B:1240:VAL:HG11	2.53	0.44
1:B:750:ASN:HB3	1:B:761:LYS:HB3	2.00	0.44
4:G:36:4HH:ON	4:G:40:VAL:HG21	2.06	0.44
4:I:64:THR:HG22	4:I:65:VAL:N	2.33	0.44
1:B:632:MET:HE1	1:B:818:PHE:HB3	2.00	0.43
1:B:782:ALA:O	1:B:785:ASN:HB3	2.18	0.43
1:B:839:ARG:HG2	1:B:839:ARG:HH21	1.82	0.43
2:C:158:ALA:CB	2:D:123:LEU:CD2	2.85	0.43
2:C:355:ASN:OD1	2:C:355:ASN:N	2.49	0.43
3:Q:180:ILE:HG22	3:Q:181:THR:N	2.33	0.43
1:B:1104:TYR:CE1	1:B:1107:ARG:NH1	2.86	0.43
3:E:180:ILE:HG22	3:E:181:THR:N	2.33	0.43
1:A:275:MET:HE1	1:A:1134:HIS:CE1	2.52	0.43
1:B:215:ARG:HG2	1:B:1325:MET:HE2	2.01	0.43
1:A:1401:ARG:HB3	1:A:1428:MET:HE2	1.99	0.43
2:C:358:LEU:HA	2:C:361:MET:SD	2.59	0.43
1:B:1436:GLU:O	1:B:1438:ILE:HG23	2.19	0.43
1:A:51:LEU:O	1:A:52:ILE:HD13	2.18	0.43
1:A:152:GLU:OE1	1:A:152:GLU:N	2.51	0.43
1:A:782:ALA:C	1:A:783:ARG:HD3	2.43	0.43
1:A:1274:ARG:HG3	1:A:1357:TRP:CZ3	2.53	0.43
1:B:691:ASP:OD1	1:B:780:ARG:HB3	2.17	0.43
2:C:18:ASN:HB3	2:C:20:PHE:CZ	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1387:GLU:C	1:A:1387:GLU:OE1	2.61	0.43
3:Q:127:LEU:HD23	3:Q:127:LEU:C	2.44	0.43
2:C:124:ARG:CA	2:D:162:TYR:CG	3.01	0.43
2:C:154:ARG:HA	2:D:123:LEU:HD21	2.00	0.43
2:C:399:ARG:O	2:C:403:ASP:OD2	2.36	0.43
1:A:1129:VAL:O	1:A:1130:GLU:C	2.61	0.43
1:B:89:THR:C	1:B:90:LEU:HD12	2.43	0.43
1:A:1285:ILE:HD11	3:F:108:ARG:NH1	2.34	0.42
1:A:292:ARG:HD3	4:G:36:4HH:CT	2.49	0.42
1:B:605:LEU:O	1:B:609:ASP:OD2	2.37	0.42
3:F:25:GLU:O	3:F:29:GLN:HG3	2.19	0.42
1:A:1235:ILE:HG21	1:B:675:ILE:HD13	2.01	0.42
1:B:606:ALA:HA	1:B:609:ASP:OD2	2.20	0.42
1:B:1213:GLU:H	1:B:1213:GLU:CD	2.26	0.42
2:D:175:GLN:HB3	2:D:266:TRP:CE2	2.55	0.42
1:B:1325:MET:SD	1:B:1325:MET:N	2.90	0.42
1:A:105:ARG:HD2	1:A:105:ARG:C	2.44	0.42
1:A:782:ALA:O	1:A:783:ARG:HD3	2.19	0.42
1:A:1199:ARG:O	1:A:1199:ARG:HG2	2.19	0.42
2:D:18:ASN:HB3	2:D:20:PHE:CZ	2.55	0.42
1:A:782:ALA:O	1:A:783:ARG:C	2.63	0.42
1:A:1387:GLU:C	1:A:1387:GLU:CD	2.87	0.42
1:B:695:ILE:N	1:B:695:ILE:HD12	2.35	0.42
1:B:1246:LYS:HD2	1:B:1246:LYS:C	2.45	0.42
1:B:1247:THR:O	1:B:1251:GLU:OE1	2.37	0.42
1:B:594:ILE:HD12	1:B:845:HIS:CE1	2.55	0.42
3:E:127:LEU:C	3:E:127:LEU:HD23	2.44	0.42
1:A:12:LEU:HD22	1:A:15:TRP:CG	2.55	0.41
1:A:46:ALA:O	1:A:49:THR:HG22	2.21	0.41
1:A:767:TRP:CE3	1:B:717:LEU:HD13	2.55	0.41
1:B:1142:GLU:CD	1:B:1142:GLU:H	2.28	0.41
1:B:1395:LYS:HD3	1:B:1395:LYS:C	2.45	0.41
1:B:288:ALA:HB2	1:B:1106:ILE:HG22	2.03	0.41
1:B:775:LEU:N	1:B:775:LEU:HD22	2.34	0.41
2:C:131:ILE:HD11	2:D:163:SER:HB2	1.99	0.41
1:A:1202:ILE:O	1:A:1202:ILE:HG22	2.20	0.41
1:B:1126:ASP:O	1:B:1127:ASN:HB3	2.21	0.41
1:A:1380:MET:HE3	1:A:1380:MET:HB3	1.96	0.41
1:A:12:LEU:HD21	1:A:46:ALA:CB	2.50	0.41
1:A:1373:THR:O	1:A:1377:ILE:HG12	2.19	0.41
6:L:55:DG:H2"	6:L:56:DT:C6	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ALA:HB1	1:A:60:PHE:CE2	2.55	0.41
1:A:587:LEU:HD11	1:A:591:LYS:HE2	2.03	0.41
1:B:141:GLY:O	1:B:143:ARG:NH1	2.54	0.41
1:B:264:THR:HG23	1:B:265:GLU:N	2.36	0.41
3:F:167:MET:HE1	3:F:183:ALA:HB1	2.01	0.41
4:I:40:VAL:O	4:I:43:VAL:HG12	2.20	0.41
1:B:1411:LEU:HB2	1:B:1416:ILE:HD11	2.03	0.41
2:C:162:TYR:CD2	2:D:124:ARG:HB2	2.54	0.41
1:A:246:LEU:O	1:A:249:ILE:CG2	2.69	0.41
2:C:131:ILE:CD1	2:D:163:SER:HB2	2.51	0.41
2:C:357:GLN:O	2:C:361:MET:SD	2.78	0.41
5:K:13:DA:C2	6:L:79:DG:C2	3.08	0.41
1:A:281:ARG:C	1:A:281:ARG:HD2	2.46	0.41
1:A:1407:GLU:HA	1:A:1407:GLU:OE1	2.21	0.41
1:B:1335:GLU:HA	1:B:1338:LEU:HG	2.03	0.41
2:C:201:ILE:HD13	2:C:289:ILE:HD11	2.02	0.41
1:A:594:ILE:HD12	1:A:845:HIS:CE1	2.56	0.40
1:B:1331:GLN:OE1	1:B:1331:GLN:N	2.54	0.40
4:G:36:4HH:O	4:G:40:VAL:HG23	2.21	0.40
1:B:1338:LEU:N	1:B:1338:LEU:HD23	2.36	0.40
1:B:1403:LEU:HD13	1:B:1428:MET:HE3	2.03	0.40
2:C:124:ARG:CB	2:D:162:TYR:CD1	3.04	0.40
4:G:64:THR:HG23	4:G:67:ALA:H	1.85	0.40
1:A:788:GLU:O	1:A:792:LEU:HD13	2.21	0.40
1:B:1307:THR:OG1	1:B:1310:GLU:HG3	2.22	0.40
3:E:9:PHE:CE1	3:F:16:GLN:HG2	2.57	0.40
3:E:108:ARG:NH1	3:E:111:ASN:HD21	2.19	0.40
4:I:29:VAL:HG13	4:I:30:GLU:N	2.36	0.40
1:A:87:TYR:CD2	1:A:136:LEU:HD23	2.56	0.40
1:A:1107:ARG:NE	4:G:48:GLU:OE1	2.53	0.40
3:E:140:ARG:HD2	3:E:140:ARG:O	2.22	0.40
4:I:15:LEU:HD22	4:I:34:ALA:HB2	2.03	0.40
1:A:780:ARG:O	1:A:783:ARG:N	2.46	0.40
1:A:1117:TRP:CE3	1:A:1121:MET:HE1	2.56	0.40
1:B:142:GLU:HA	1:B:143:ARG:CZ	2.51	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	993/1482 (67%)	962 (97%)	31 (3%)	0	100	100
1	B	993/1482 (67%)	953 (96%)	40 (4%)	0	100	100
2	C	438/440 (100%)	426 (97%)	12 (3%)	0	100	100
2	D	316/440 (72%)	309 (98%)	7 (2%)	0	100	100
3	E	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
3	F	196/240 (82%)	191 (97%)	5 (3%)	0	100	100
3	Q	127/240 (53%)	123 (97%)	4 (3%)	0	100	100
4	G	69/78 (88%)	68 (99%)	1 (1%)	0	100	100
4	I	69/78 (88%)	66 (96%)	3 (4%)	0	100	100
All	All	3411/4720 (72%)	3304 (97%)	107 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	861/1281 (67%)	860 (100%)	1 (0%)	92	95
1	B	861/1281 (67%)	859 (100%)	2 (0%)	92	94
2	C	376/376 (100%)	369 (98%)	7 (2%)	52	69
2	D	274/376 (73%)	268 (98%)	6 (2%)	47	65
3	E	189/212 (89%)	184 (97%)	5 (3%)	41	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	F	177/212 (84%)	175 (99%)	2 (1%)	70 80
3	Q	116/212 (55%)	112 (97%)	4 (3%)	32 51
4	G	62/66 (94%)	62 (100%)	0	100 100
4	I	62/66 (94%)	62 (100%)	0	100 100
All	All	2978/4082 (73%)	2951 (99%)	27 (1%)	74 83

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	LEU
1	B	1127	ASN
1	B	1213	GLU
2	C	2	SER
2	C	92	SER
2	C	94	LEU
2	C	132	VAL
2	C	209	SER
2	C	287	THR
2	C	355	ASN
2	D	2	SER
2	D	92	SER
2	D	94	LEU
2	D	132	VAL
2	D	209	SER
2	D	287	THR
3	E	123	GLU
3	E	138	ASN
3	E	162	LEU
3	E	169	TYR
3	E	181	THR
3	F	25	GLU
3	F	152	GLN
3	Q	123	GLU
3	Q	162	LEU
3	Q	169	TYR
3	Q	181	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	GLN
1	A	865	GLN
1	A	1105	GLN
1	A	1109	GLN
1	A	1242	ASN
1	A	1293	GLN
1	B	62	ASN
1	B	78	HIS
1	B	98	GLN
1	B	175	HIS
1	B	306	GLN
1	B	566	GLN
1	B	766	GLN
1	B	864	GLN
1	B	1091	ASN
1	B	1193	HIS
1	B	1342	ASN
1	B	1437	ASN
2	C	75	ASN
2	C	134	ASN
2	C	155	ASN
2	C	198	GLN
2	C	435	HIS
2	D	75	ASN
2	D	134	ASN
2	D	198	GLN
2	D	269	GLN
3	E	8	GLN
3	E	111	ASN
3	E	152	GLN
3	Q	111	ASN
3	Q	201	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	4HH	I	36	4	21,26,27	0.46	0	27,35,37	1.72	3 (11%)
4	4HH	G	36	4	21,26,27	0.45	0	27,35,37	3.13	4 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	4HH	I	36	4	-	6/32/35/37	-
4	4HH	G	36	4	-	5/32/35/37	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	36	4HH	O1P-P-OG	11.65	161.86	107.75
4	G	36	4HH	OG-P-O2P	-8.86	74.46	109.07
4	G	36	4HH	P-OG-CB	6.12	157.57	121.68
4	I	36	4HH	P-OG-CB	-5.40	90.01	121.68
4	I	36	4HH	O1P-P-OG	4.64	129.31	107.75
4	I	36	4HH	OG-CB-CA	4.36	112.39	108.14
4	G	36	4HH	OG-CB-CA	2.84	110.91	108.14

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	36	4HH	N-CA-CB-OG
4	I	36	4HH	CB-OG-P-O1P
4	G	36	4HH	CJ-O3P-P-OG
4	G	36	4HH	CB-OG-P-O3P
4	I	36	4HH	CO-CP-CQ-NR
4	I	36	4HH	CO-CP-CQ-OR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	I	36	4HH	CB-OG-P-O3P
4	G	36	4HH	ON-CL3-CM-OM
4	I	36	4HH	ON-CL3-CM-OM
4	G	36	4HH	CT-CS-NR-CQ
4	G	36	4HH	CB-OG-P-O2P

There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	36	4HH	1	0
4	G	36	4HH	16	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	ATP	B	1502	7	26,33,33	0.63	0	31,52,52	1.12	4 (12%)
8	ATP	A	1502	7	26,33,33	0.61	0	31,52,52	1.13	3 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ATP	B	1502	7	-	2/18/38/38	0/3/3/3
8	ATP	A	1502	7	-	1/18/38/38	0/3/3/3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1502	ATP	C5-C6-N6	2.37	123.96	120.35
8	A	1502	ATP	C5-C6-N6	2.35	123.93	120.35
8	A	1502	ATP	O2'-C2'-C3'	-2.32	104.31	111.82
8	B	1502	ATP	O2'-C2'-C3'	-2.18	104.76	111.82
8	B	1502	ATP	O3'-C3'-C2'	-2.14	104.90	111.82
8	A	1502	ATP	O3'-C3'-C2'	-2.07	105.13	111.82
8	B	1502	ATP	O2'-C2'-C1'	-2.00	103.46	110.85

There are no chirality outliers.

All (3) torsion outliers are listed below:

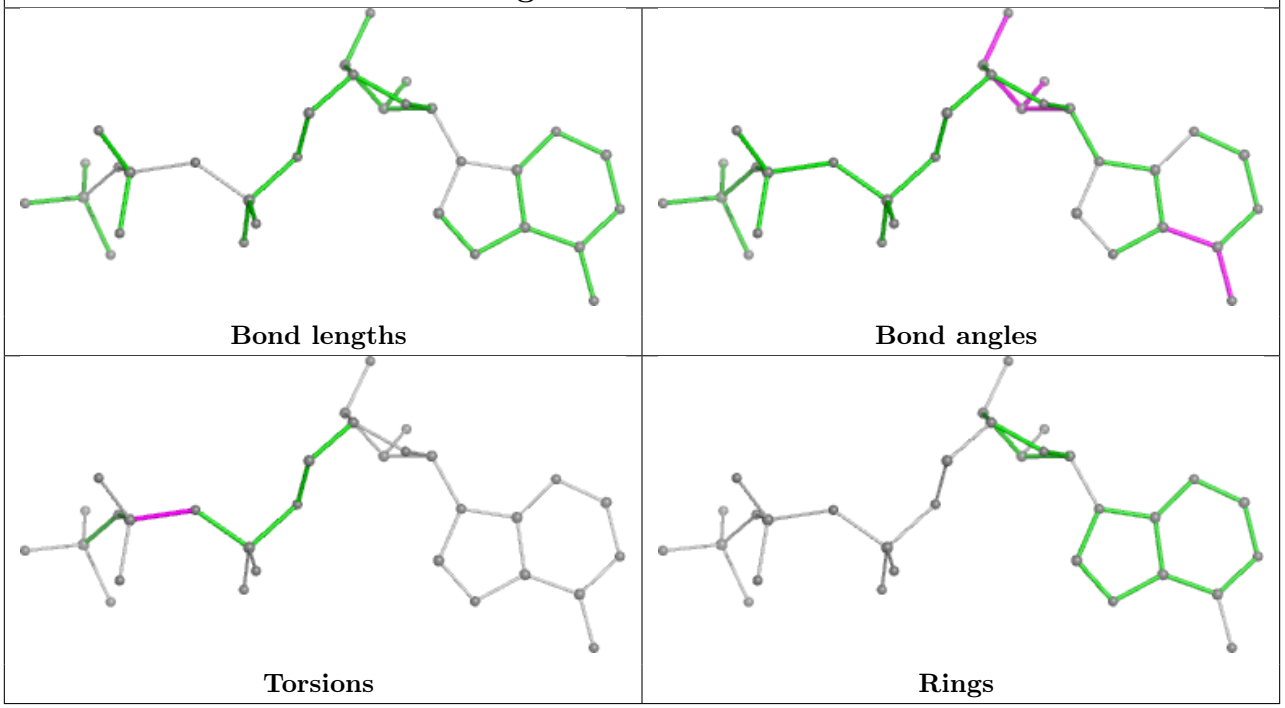
Mol	Chain	Res	Type	Atoms
8	A	1502	ATP	PA-O3A-PB-O2B
8	B	1502	ATP	PA-O3A-PB-O1B
8	B	1502	ATP	PA-O3A-PB-O2B

There are no ring outliers.

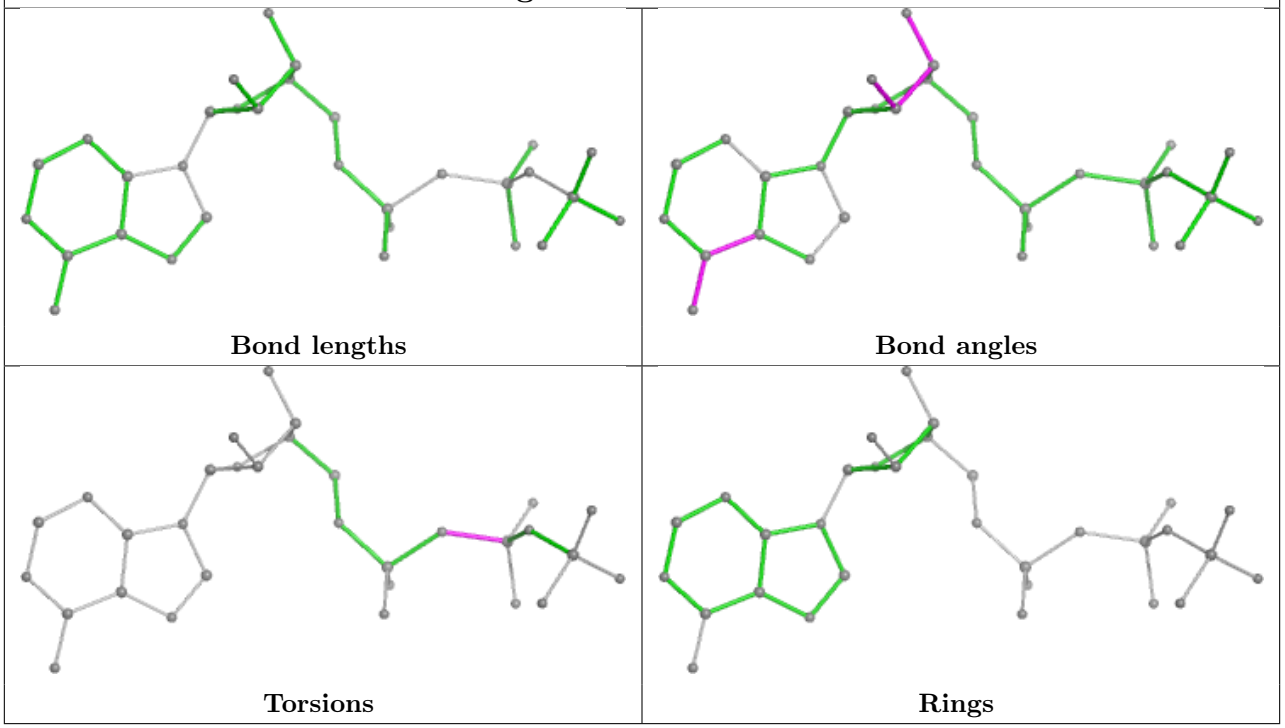
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP B 1502



Ligand ATP A 1502



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
2	C	1
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	295:ARG	C	296:ILE	N	1.03
1	D	295:ARG	C	296:ILE	N	1.03

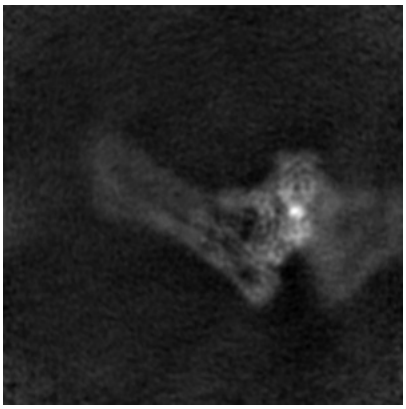
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51445. These allow visual inspection of the internal detail of the map and identification of artifacts.

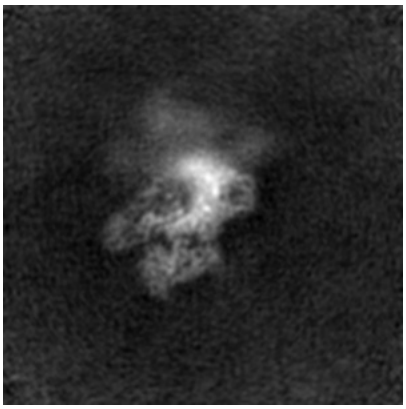
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

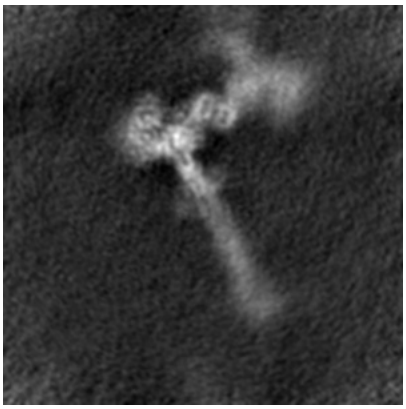
6.1.1 Primary map



X

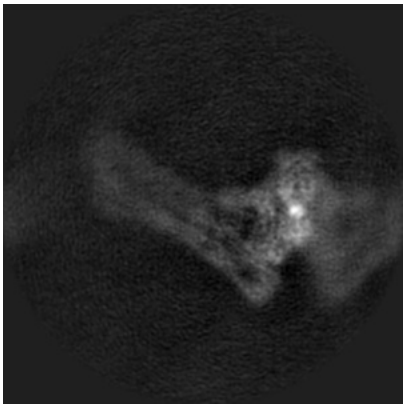


Y

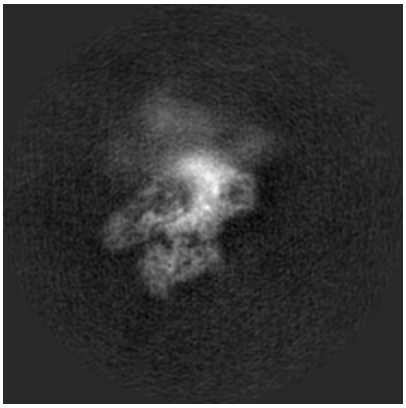


Z

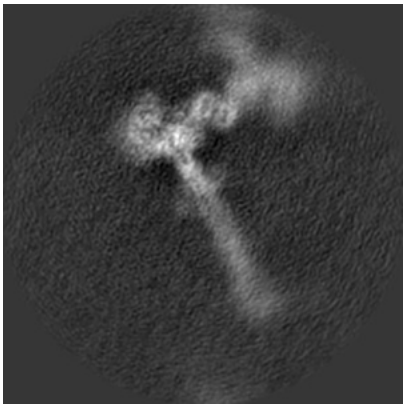
6.1.2 Raw map



X



Y

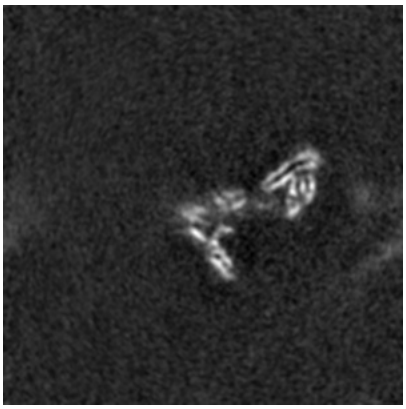


Z

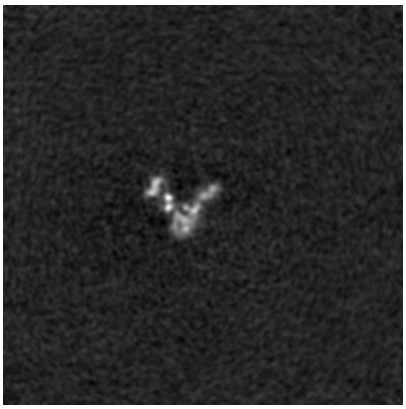
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

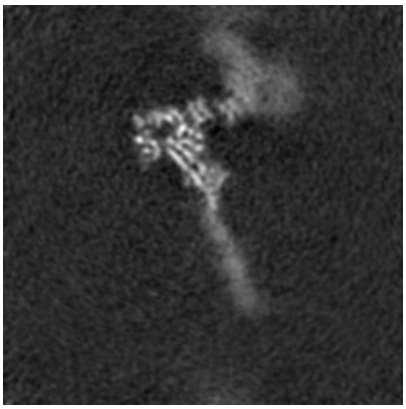
6.2.1 Primary map



X Index: 92

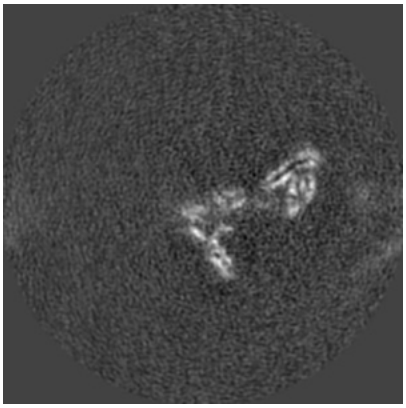


Y Index: 92

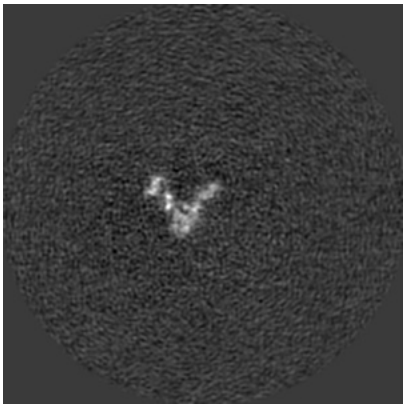


Z Index: 92

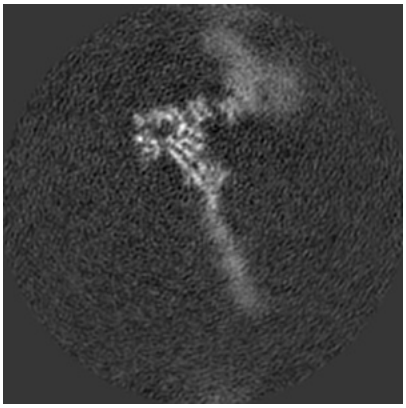
6.2.2 Raw map



X Index: 92



Y Index: 92

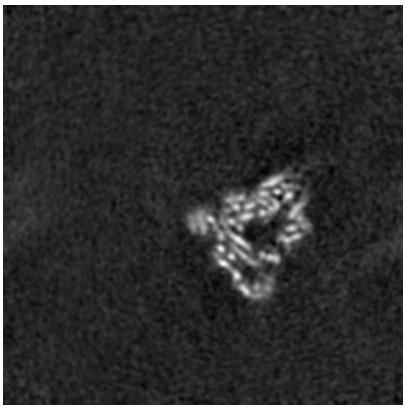


Z Index: 92

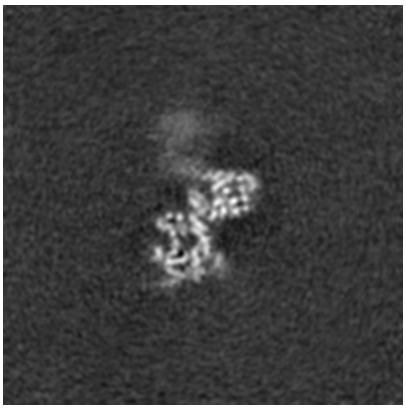
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

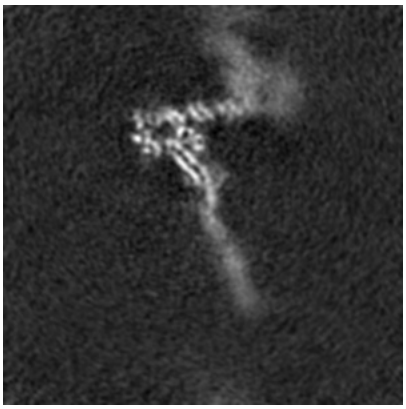
6.3.1 Primary map



X Index: 86

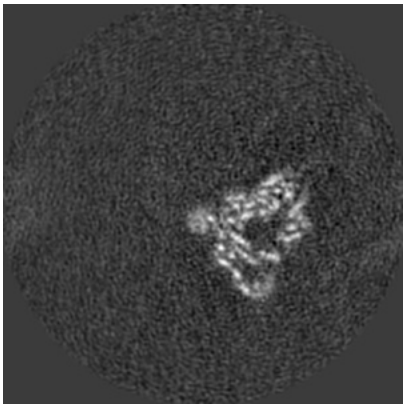


Y Index: 132

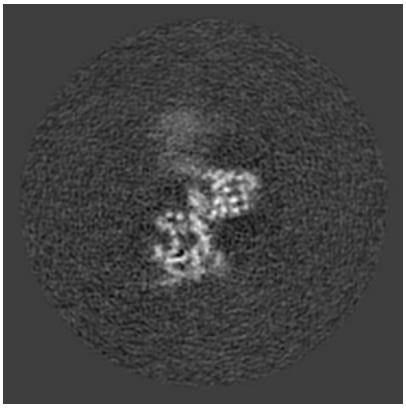


Z Index: 91

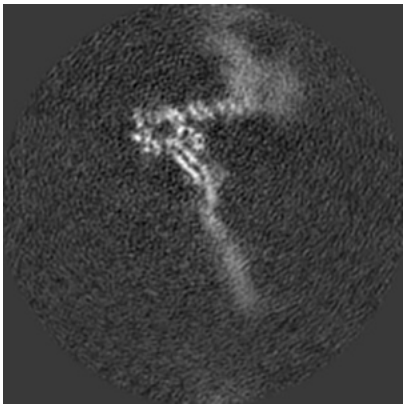
6.3.2 Raw map



X Index: 86



Y Index: 132

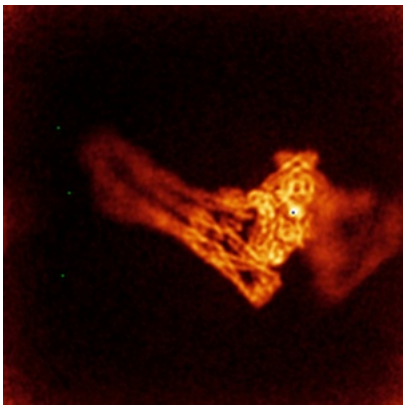


Z Index: 91

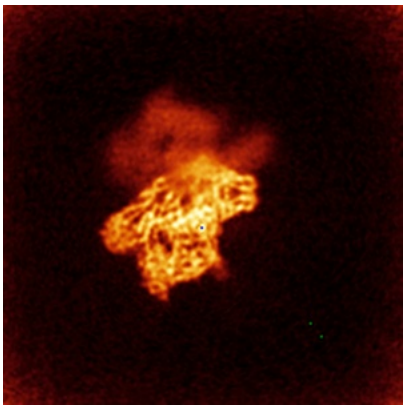
The images above show the largest variance slices of the map in three orthogonal directions.

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

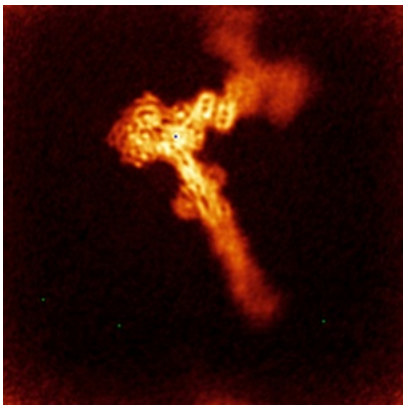
6.4.1 Primary map



X

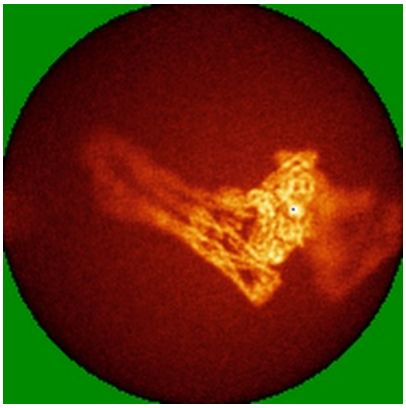


Y

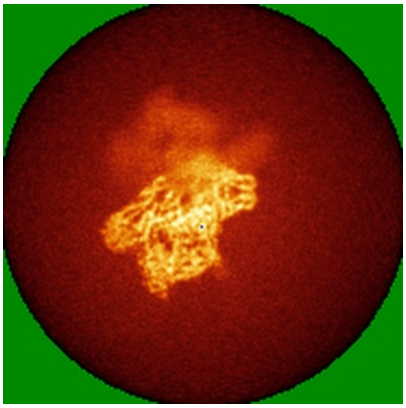


Z

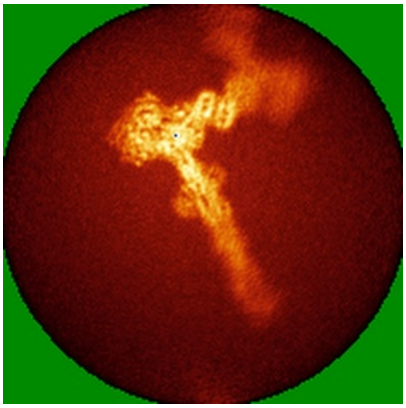
6.4.2 Raw map



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

6.5.2 Raw map

X Y Z

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

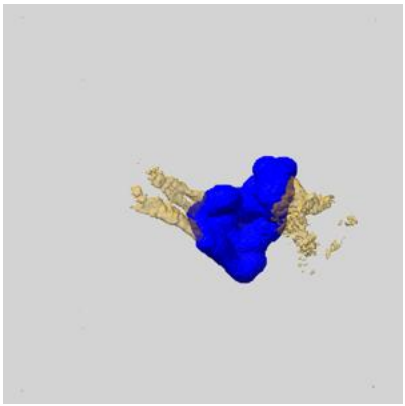
6.6 Mask visualisation (i)

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

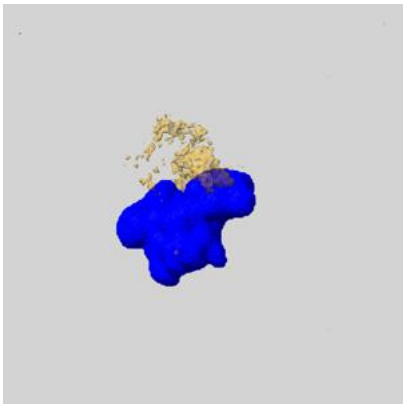
A mask typically either:

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

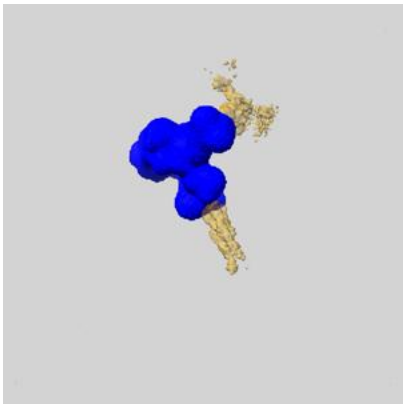
6.6.1 emd_51445_msk_1.map (i)



X



Y

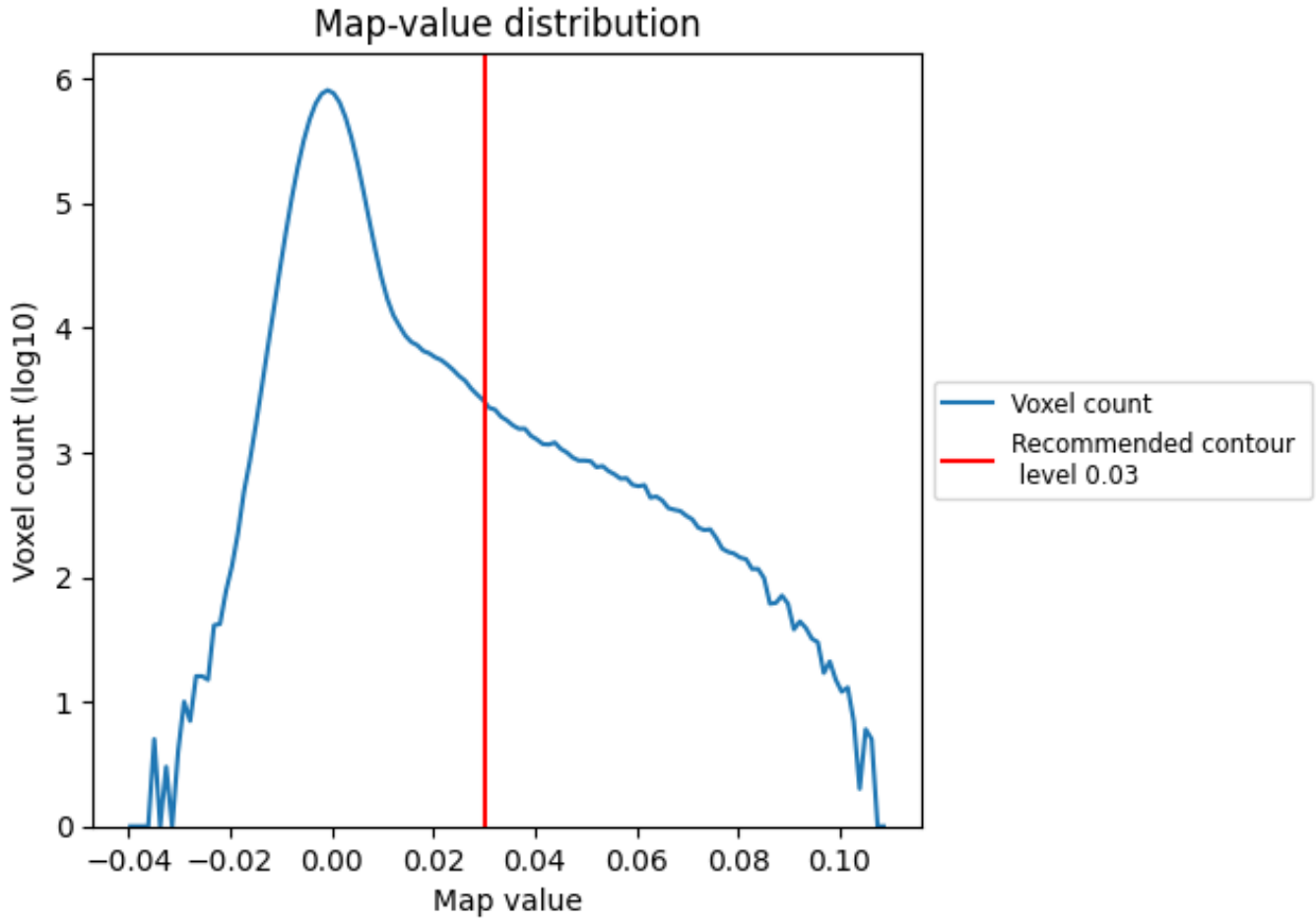


Z

7 Map analysis

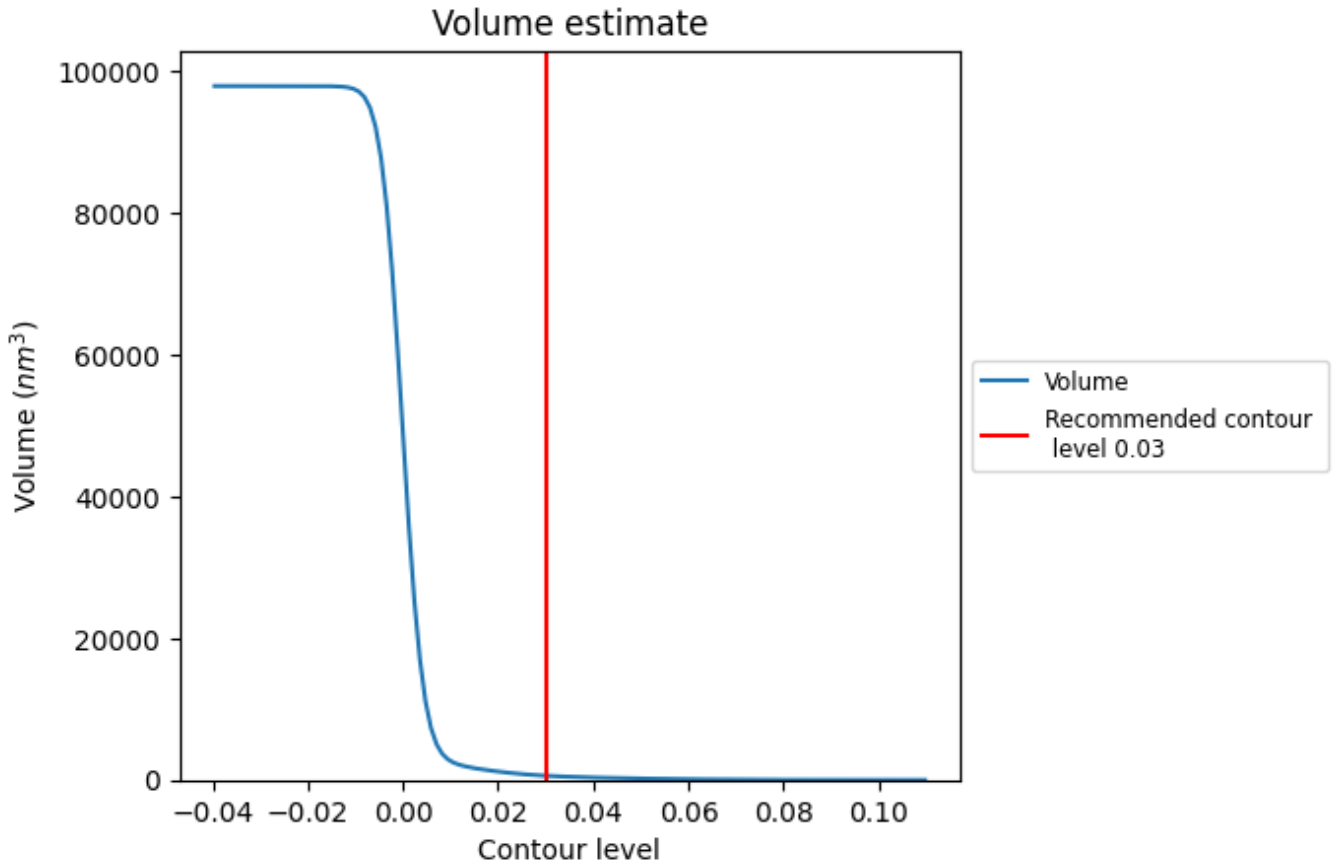
This section contains the results of statistical analysis of the map.

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.

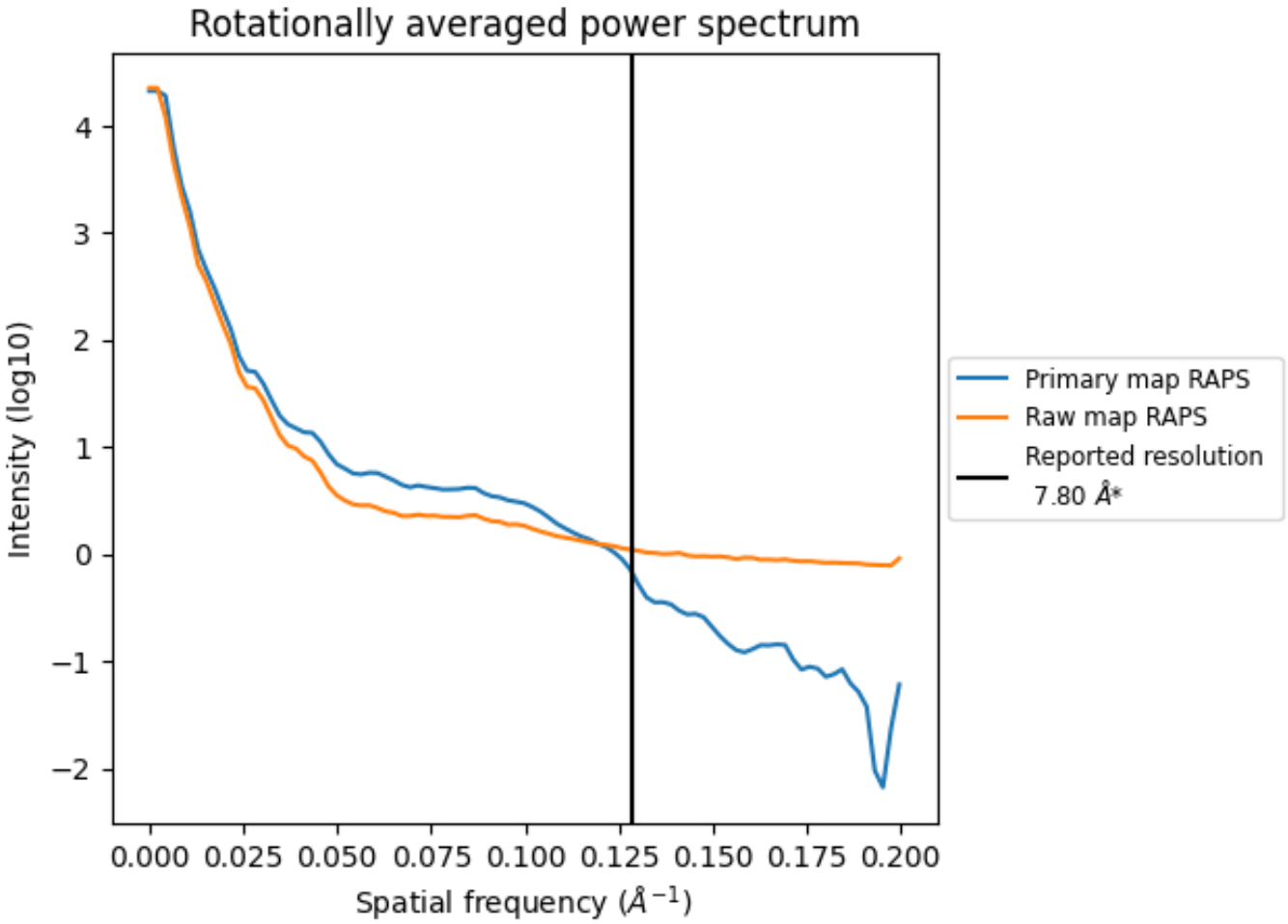
7.2 Volume estimate



The volume at the recommended contour level is 599 nm^3; this corresponds to an approximate mass of 541 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)

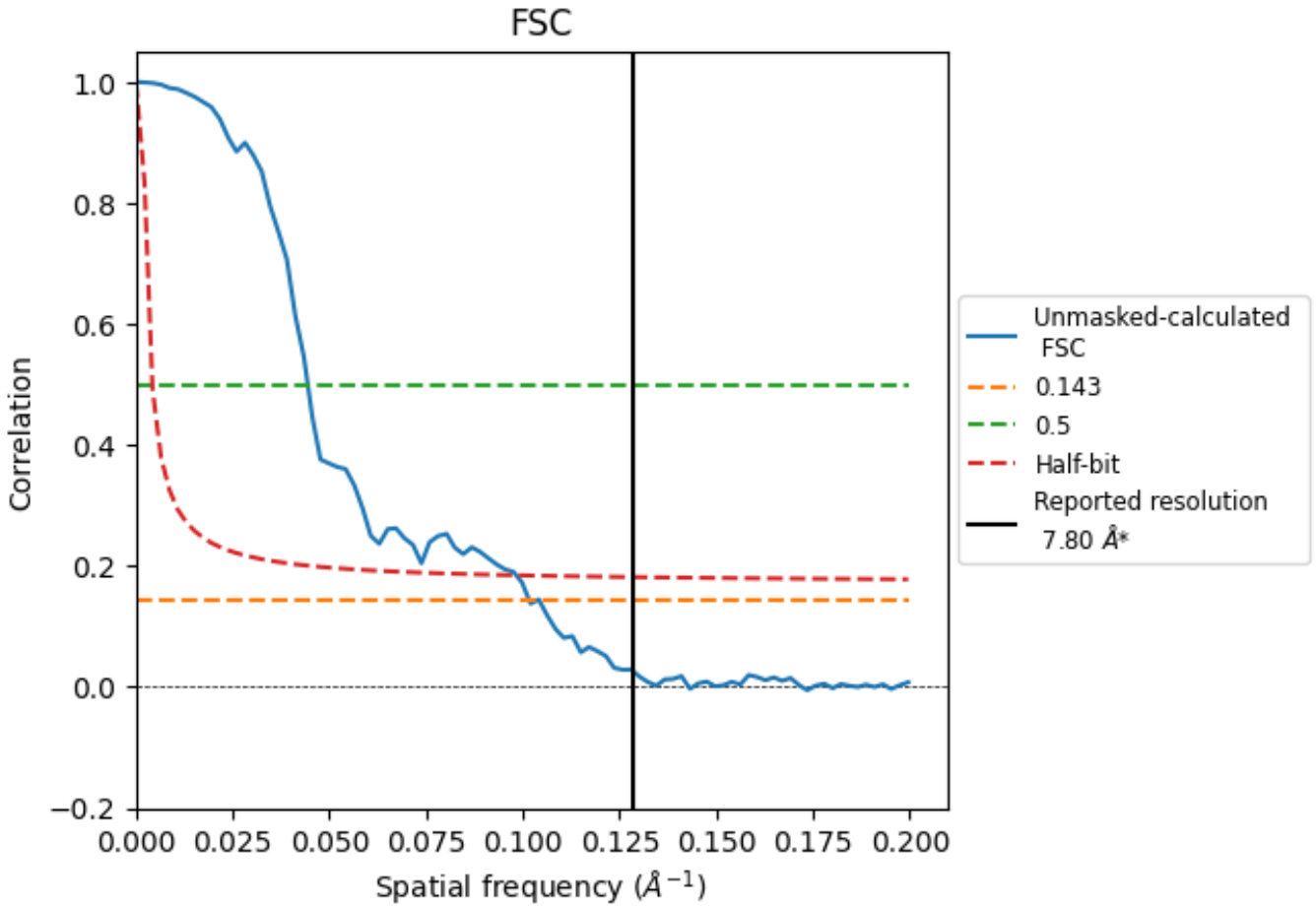


*Reported resolution corresponds to spatial frequency of 0.128 Å^{-1}

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 0.128 Å^{-1}

8.2 Resolution estimates (i)

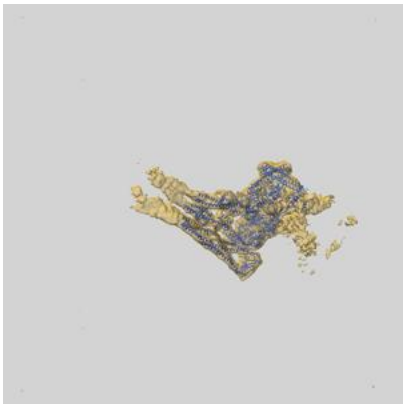
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.84	22.52	10.17

*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 9.84 differs from the reported value 7.8 by more than 10 %

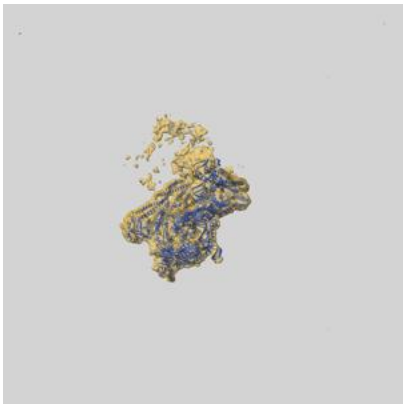
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51445 and PDB model 9GM9. Per-residue inclusion information can be found in section 3 on page 6.

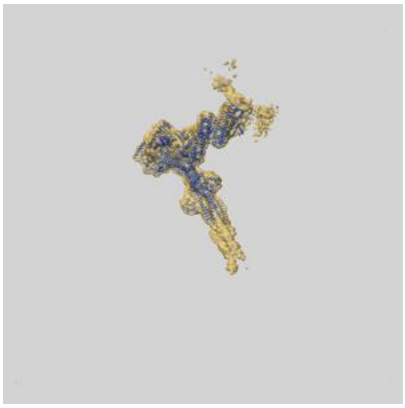
9.1 Map-model overlay



X



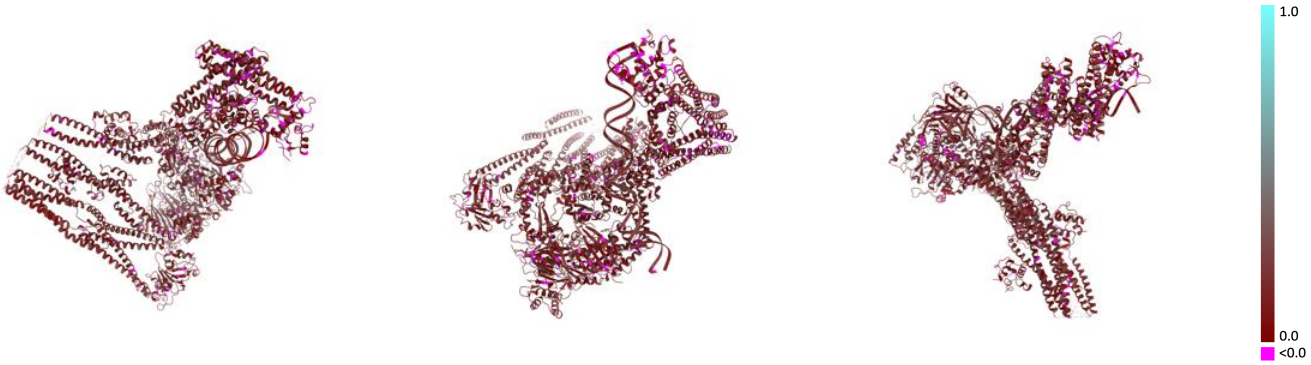
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

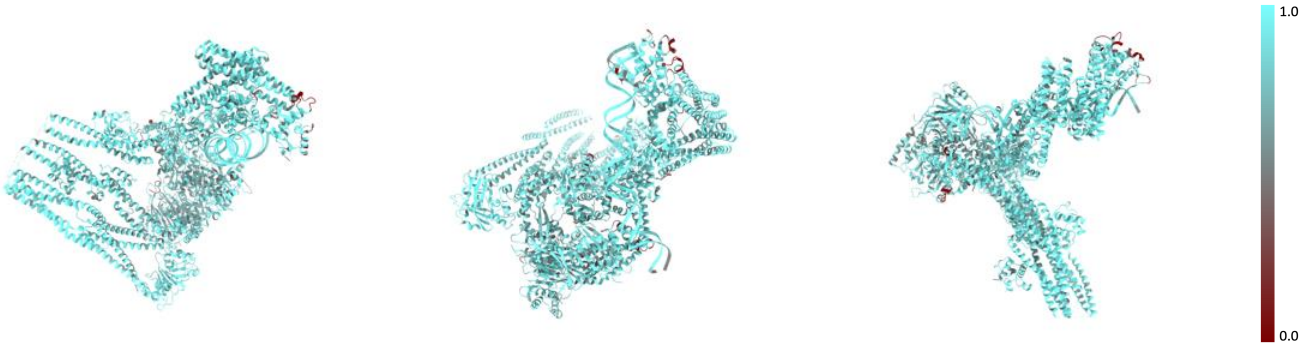
9.2 Q-score mapped to coordinate model (i)



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.

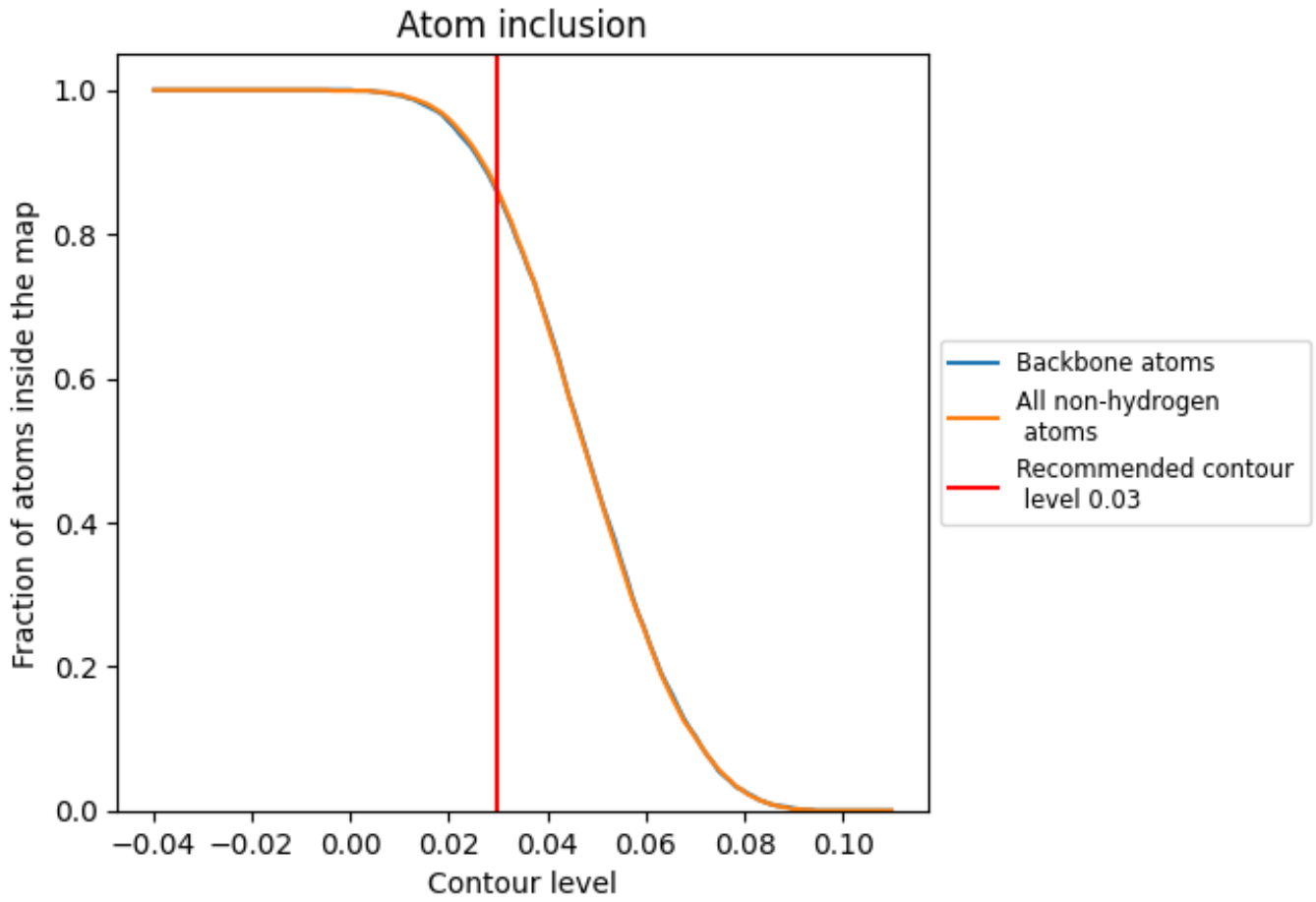
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8600	0.1600
A	0.8620	0.1660
B	0.8630	0.1660
C	0.8710	0.1510
D	0.8780	0.1260
E	0.8790	0.1720
F	0.8410	0.1730
G	0.8840	0.1420
I	0.8900	0.1630
K	0.9290	0.1900
L	0.9260	0.1900
Q	0.8220	0.0900