Full wwPDB EM Validation Report (i)

Mar 3, 2024 – 07:40 AM EST

PDB ID	:	6BX3
EMDB ID	:	EMD-7303
Title	:	Structure of histone H3k4 methyltransferase
Authors	:	Skiniotis, G.; Qu, Q.H.
Deposited on	:	2017-12-16
Resolution	:	4.30 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 (i) 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 (i)) were used in the production of this report:

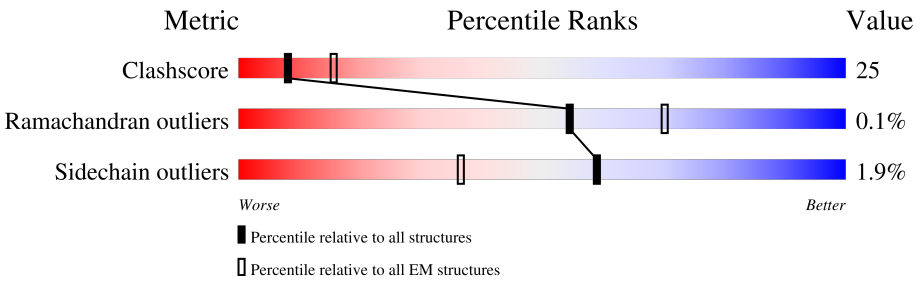
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.30 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

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	E	278	• 50% 18% • 31%
2	K	417	5% 35% 14% • 49%
3	M	42	12% 64% 36%
3	N	42	12% 62% 31% • 5%
4	F	237	8% 61% 29% 9%
5	B	412	10% 56% 39% • •
6	A	314	6% 68% 30% •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10456 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 Histone-lysine N-methyltransferase, H3 lysine-4 specific.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	192	1432	904	255	266	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	843	VAL	ILE	conflict	UNP A6ZT27

- Molecule 2 is a protein called COMPASS component BRE2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	K	211	1520	954	252	309	5	0	0

- Molecule 3 is a protein called COMPASS component SDC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	M	42	328	207	60	60	1	0	0
3	N	40	304	194	54	55	1	0	0

- Molecule 4 is a protein called COMPASS component SPP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	215	1526	951	257	309	9	0	0

- Molecule 5 is a protein called COMPASS component SWD1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	399	3050	1950	512	577	11	0	0

- Molecule 6 is a protein called COMPASS component SWD3.

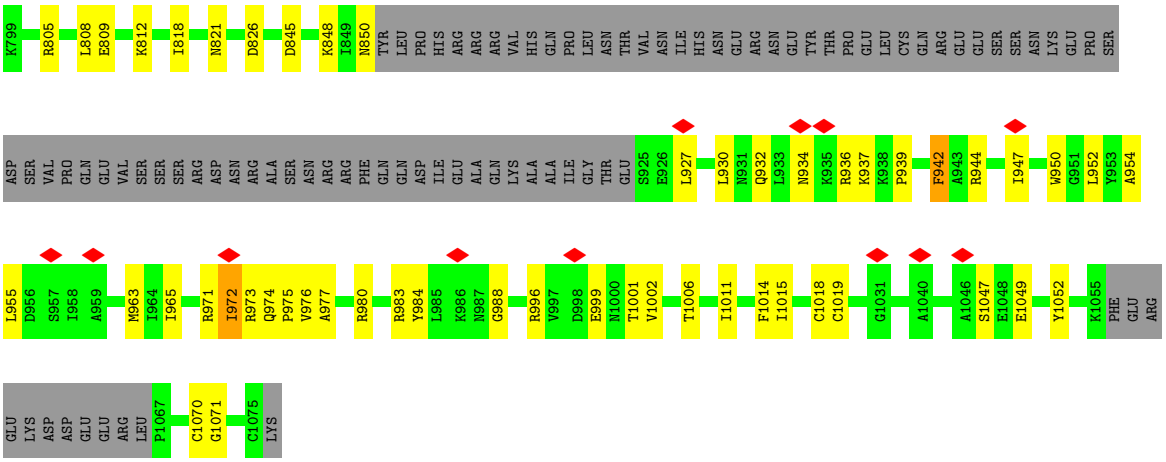
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	314	2296	1448	396	439	13	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

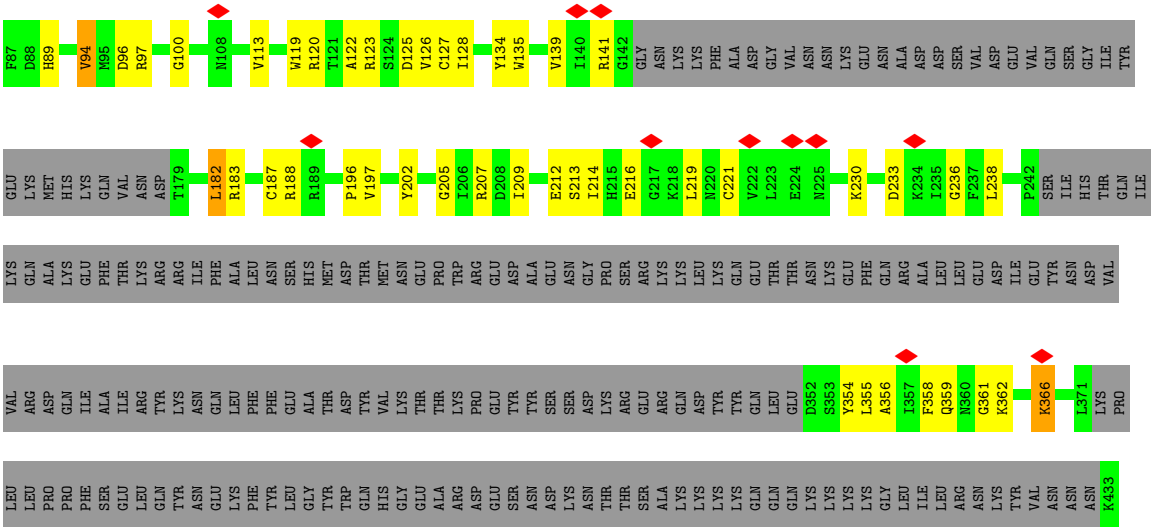
- Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-4 specific

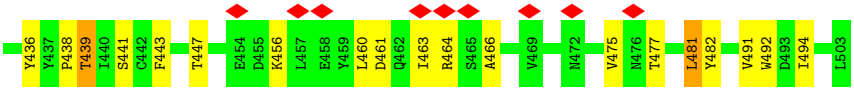
Chain E:



- Molecule 2: COMPASS component BRE2

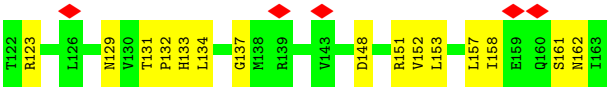
Chain K:





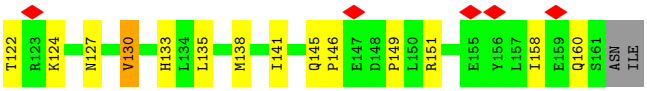
- Molecule 3: COMPASS component SDC1

Chain M:



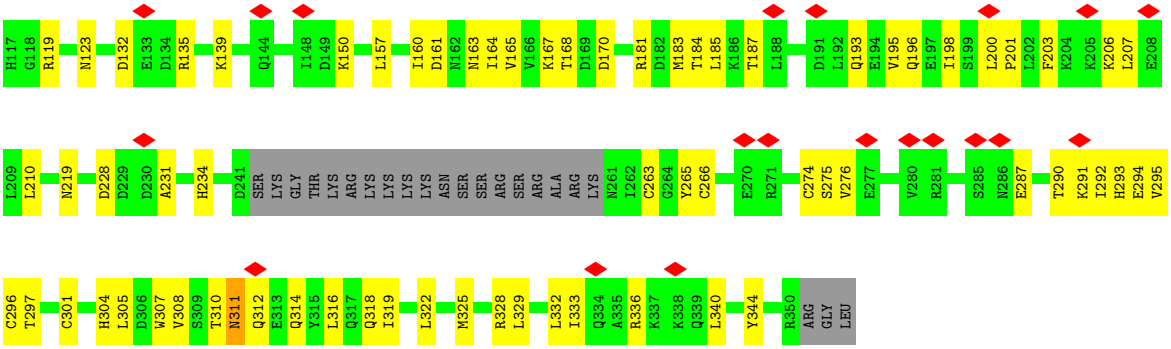
- Molecule 3: COMPASS component SDC1

Chain N:



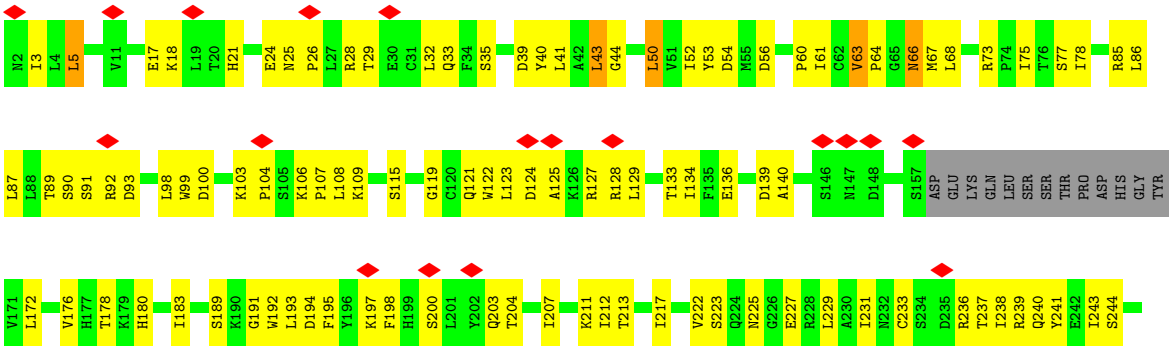
- Molecule 4: COMPASS component SPP1

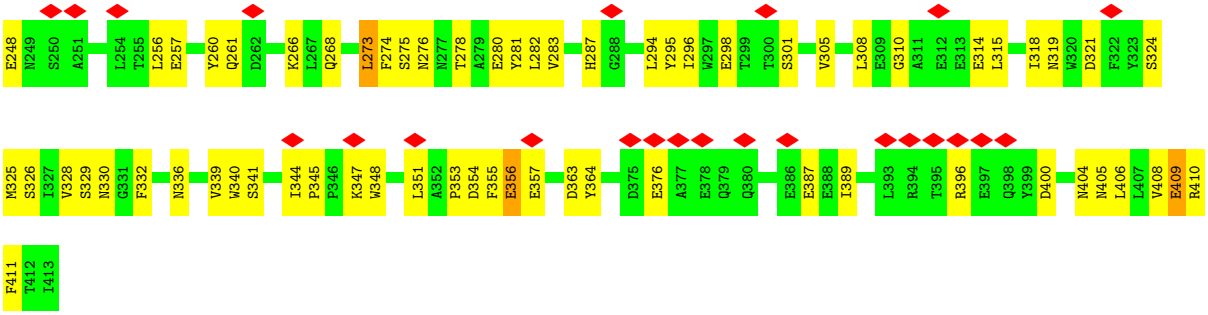
Chain F:



- Molecule 5: COMPASS component SWD1

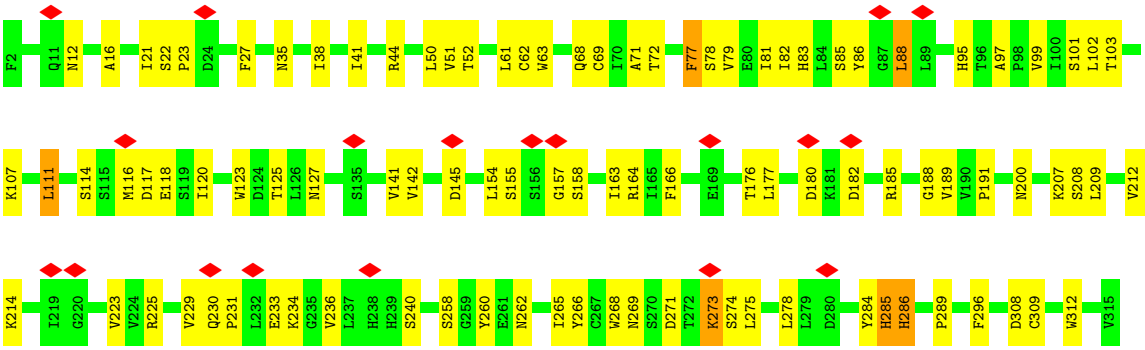
Chain B:





- Molecule 6: COMPASS component SWD3

Chain A:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	163539	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	50000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.948	Depositor
Minimum map value	-0.354	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	312.0, 312.0, 312.0	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	E	0.37	0/1452	0.69	1/1958 (0.1%)
2	K	0.39	0/1547	0.76	1/2103 (0.0%)
3	M	0.36	0/333	0.67	0/453
3	N	0.34	0/309	0.63	0/422
4	F	0.35	0/1546	0.67	0/2110
5	B	0.43	0/3124	0.76	3/4273 (0.1%)
6	A	0.42	0/2347	0.73	2/3200 (0.1%)
All	All	0.40	0/10658	0.72	7/14519 (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	E	0	2
2	K	0	1
3	M	0	1
4	F	0	2
5	B	0	7
6	A	0	5
All	All	0	18

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	182	LEU	CA-CB-CG	6.54	130.35	115.30
5	B	356	GLU	N-CA-C	-6.15	94.40	111.00
5	B	50	LEU	CA-CB-CG	5.39	127.70	115.30
6	A	111	LEU	CA-CB-CG	5.26	127.39	115.30
5	B	273	LEU	CB-CG-CD2	-5.19	102.18	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	972	ILE	N-CA-C	5.16	124.94	111.00
6	A	88	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	180	ASP	Peptide
6	A	285	HIS	Peptide
6	A	286	HIS	Peptide
6	A	77	PHE	Peptide
6	A	78	SER	Peptide
5	B	197	LYS	Peptide
5	B	21	HIS	Peptide
5	B	3	ILE	Peptide
5	B	396	ARG	Peptide
5	B	400	ASP	Peptide
5	B	5	LEU	Peptide
5	B	66	ASN	Peptide
1	E	947	ILE	Peptide
1	E	999	GLU	Peptide
4	F	181	ARG	Peptide
4	F	305	LEU	Peptide
2	K	94	VAL	Peptide
3	M	148	ASP	Peptide

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	E	1432	0	1389	71	0
2	K	1520	0	1304	51	0
3	M	328	0	329	12	0
3	N	304	0	304	13	0
4	F	1526	0	1263	99	0
5	B	3050	0	2839	163	0
6	A	2296	0	2135	125	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10456	0	9563	494	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 25.

All (494) 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)
4:F:297:THR:HG23	4:F:304:HIS:CE1	1.40	1.54
4:F:297:THR:CG2	4:F:304:HIS:CE1	1.95	1.49
6:A:22:SER:HB3	6:A:63:TRP:CZ3	1.65	1.31
2:K:126:VAL:CG2	2:K:481:LEU:HD12	1.60	1.31
4:F:276:VAL:HG23	4:F:292:ILE:CD1	1.63	1.28
2:K:126:VAL:HG21	2:K:481:LEU:CD1	1.62	1.28
4:F:263:CYS:CB	4:F:297:THR:HG21	1.66	1.26
2:K:122:ALA:O	2:K:439:THR:HG21	1.33	1.26
6:A:22:SER:HB3	6:A:63:TRP:CE3	1.72	1.24
4:F:263:CYS:O	4:F:297:THR:OG1	1.52	1.24
6:A:22:SER:CB	6:A:63:TRP:CE3	2.21	1.23
4:F:297:THR:HG23	4:F:304:HIS:NE2	1.58	1.19
6:A:229:VAL:HG22	6:A:231:PRO:CD	1.72	1.19
2:K:96:ASP:O	2:K:123:ARG:CB	1.92	1.16
4:F:185:LEU:HB2	4:F:193:GLN:HE22	1.09	1.16
5:B:108:LEU:O	5:B:109:LYS:HD3	1.44	1.15
4:F:297:THR:HG22	4:F:301:CYS:SG	1.86	1.15
5:B:61:ILE:CG2	5:B:406:LEU:HD11	1.75	1.15
4:F:297:THR:HG22	4:F:304:HIS:CE1	1.82	1.13
4:F:185:LEU:CB	4:F:193:GLN:HE22	1.62	1.13
4:F:276:VAL:CG2	4:F:292:ILE:HD13	1.76	1.13
4:F:263:CYS:HB3	4:F:297:THR:CG2	1.79	1.12
1:E:1014:PHE:HE1	5:B:351:LEU:CG	1.62	1.11
2:K:122:ALA:O	2:K:439:THR:CG2	1.99	1.11
6:A:164:ARG:HH11	6:A:176:THR:HG21	1.03	1.10
1:E:1014:PHE:CE1	5:B:351:LEU:HD12	1.86	1.10
6:A:229:VAL:CG2	6:A:231:PRO:HD2	1.82	1.10
5:B:63:VAL:H	5:B:64:PRO:HD2	1.15	1.09
6:A:79:VAL:HG23	6:A:99:VAL:HG11	1.35	1.06
1:E:1014:PHE:CD1	5:B:351:LEU:HD12	1.91	1.05
5:B:63:VAL:N	5:B:64:PRO:HD2	1.70	1.04
4:F:263:CYS:HB3	4:F:297:THR:HG21	1.05	1.03
5:B:61:ILE:HG21	5:B:406:LEU:HD11	1.06	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:100:ASP:CB	5:B:108:LEU:HD11	1.89	1.01
4:F:297:THR:CG2	4:F:304:HIS:HE1	1.46	1.00
1:E:973:ARG:HG2	1:E:975:PRO:HD2	1.44	1.00
4:F:185:LEU:HB2	4:F:193:GLN:NE2	1.77	0.98
6:A:62:CYS:SG	6:A:102:LEU:C	2.42	0.98
4:F:200:LEU:HD21	4:F:340:LEU:CD2	1.92	0.98
5:B:63:VAL:H	5:B:64:PRO:CD	1.78	0.97
4:F:263:CYS:SG	4:F:297:THR:HG21	2.05	0.96
1:E:973:ARG:CG	1:E:975:PRO:HD2	1.95	0.96
1:E:1014:PHE:HE1	5:B:351:LEU:CD1	1.77	0.96
4:F:287:GLU:HG3	4:F:291:LYS:HD3	1.48	0.96
1:E:1014:PHE:HE1	5:B:351:LEU:HG	1.31	0.95
1:E:1014:PHE:CE1	5:B:351:LEU:CD1	2.49	0.95
6:A:22:SER:CB	6:A:63:TRP:CZ3	2.41	0.95
6:A:229:VAL:HG22	6:A:231:PRO:HD2	0.94	0.94
5:B:103:LYS:CB	5:B:104:PRO:CD	2.46	0.94
5:B:353:PRO:HA	6:A:176:THR:OG1	1.67	0.94
4:F:297:THR:CG2	4:F:301:CYS:SG	2.56	0.93
6:A:164:ARG:NH1	6:A:176:THR:HG21	1.83	0.93
4:F:265:TYR:H	4:F:295:VAL:HB	1.33	0.93
6:A:22:SER:CA	6:A:63:TRP:CD2	2.53	0.92
1:E:952:LEU:HD11	1:E:1014:PHE:HB3	1.49	0.91
4:F:265:TYR:CB	4:F:296:CYS:H	1.82	0.91
6:A:22:SER:HB3	6:A:63:TRP:CH2	2.04	0.91
6:A:79:VAL:CG2	6:A:99:VAL:HG11	2.00	0.91
6:A:22:SER:HA	6:A:63:TRP:CG	2.06	0.91
1:E:1014:PHE:CE1	5:B:351:LEU:CG	2.54	0.88
6:A:22:SER:HA	6:A:63:TRP:CD2	2.08	0.88
5:B:139:ASP:O	5:B:172:LEU:CD2	2.20	0.88
1:E:1014:PHE:CE1	5:B:351:LEU:HG	2.10	0.87
1:E:973:ARG:O	1:E:977:ALA:HB3	1.73	0.87
4:F:200:LEU:HD21	4:F:340:LEU:CG	2.06	0.86
6:A:22:SER:OG	6:A:63:TRP:CE3	2.27	0.86
5:B:61:ILE:HG21	5:B:406:LEU:CD1	2.00	0.86
6:A:164:ARG:HH11	6:A:176:THR:CG2	1.87	0.84
6:A:22:SER:HB3	6:A:63:TRP:CD2	2.13	0.83
5:B:139:ASP:O	5:B:172:LEU:HD22	1.77	0.83
5:B:63:VAL:N	5:B:64:PRO:CD	2.36	0.82
4:F:200:LEU:HD21	4:F:340:LEU:HG	1.62	0.82
6:A:23:PRO:HD2	6:A:63:TRP:HB3	1.59	0.82
6:A:62:CYS:SG	6:A:102:LEU:HB2	2.20	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:61:ILE:CG2	5:B:406:LEU:CD1	2.58	0.80
6:A:22:SER:CB	6:A:63:TRP:CD2	2.64	0.80
6:A:23:PRO:HD2	6:A:63:TRP:CG	2.17	0.79
6:A:234:LYS:O	6:A:234:LYS:HD3	1.83	0.79
2:K:126:VAL:HG21	2:K:481:LEU:HD12	0.81	0.78
5:B:139:ASP:C	5:B:172:LEU:HD22	2.03	0.78
2:K:122:ALA:O	2:K:439:THR:CB	2.31	0.78
6:A:23:PRO:HD2	6:A:63:TRP:CB	2.13	0.78
6:A:233:GLU:O	6:A:236:VAL:HG12	1.84	0.78
5:B:17:GLU:CB	5:B:296:ILE:HD13	2.14	0.77
2:K:182:LEU:HD22	2:K:447:THR:H	1.49	0.76
4:F:297:THR:CB	4:F:301:CYS:SG	2.73	0.76
2:K:125:ASP:C	2:K:482:TYR:HE1	1.89	0.76
5:B:238:ILE:HG13	5:B:261:GLN:HE21	1.48	0.75
2:K:122:ALA:C	2:K:439:THR:HG21	2.05	0.75
4:F:297:THR:HG23	4:F:304:HIS:HE2	1.49	0.75
6:A:164:ARG:HD3	6:A:176:THR:HG22	1.70	0.74
1:E:973:ARG:HG2	1:E:975:PRO:CD	2.18	0.74
4:F:292:ILE:HD12	4:F:292:ILE:O	1.86	0.74
6:A:62:CYS:SG	6:A:102:LEU:CB	2.76	0.73
6:A:62:CYS:SG	6:A:102:LEU:O	2.47	0.73
1:E:1015:ILE:CG2	1:E:1052:TYR:HD1	2.00	0.73
4:F:276:VAL:HG23	4:F:292:ILE:HD13	0.80	0.73
6:A:23:PRO:HD2	6:A:63:TRP:CD1	2.24	0.73
4:F:200:LEU:HD21	4:F:340:LEU:HD21	1.67	0.73
4:F:263:CYS:HB3	4:F:297:THR:CB	2.18	0.72
1:E:1015:ILE:HG22	1:E:1052:TYR:HD1	1.56	0.71
4:F:297:THR:CG2	4:F:304:HIS:NE2	2.29	0.71
5:B:103:LYS:CB	5:B:104:PRO:HD2	2.20	0.71
5:B:409:GLU:HA	5:B:409:GLU:OE2	1.88	0.71
5:B:108:LEU:C	5:B:109:LYS:HD3	2.10	0.71
5:B:17:GLU:HB3	5:B:296:ILE:HD13	1.73	0.70
1:E:1014:PHE:HD1	5:B:351:LEU:HD12	1.55	0.70
5:B:103:LYS:CB	5:B:104:PRO:HD3	2.20	0.69
6:A:23:PRO:CD	6:A:63:TRP:CD1	2.74	0.69
4:F:275:SER:O	4:F:293:HIS:N	2.25	0.69
6:A:229:VAL:HG22	6:A:231:PRO:CG	2.21	0.69
6:A:27:PHE:O	6:A:63:TRP:CH2	2.46	0.69
4:F:265:TYR:O	4:F:308:VAL:HG21	1.92	0.69
5:B:296:ILE:O	5:B:296:ILE:HG22	1.91	0.69
6:A:27:PHE:HB3	6:A:63:TRP:HH2	1.57	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:122:ALA:O	2:K:439:THR:OG1	2.11	0.69
5:B:52:ILE:CG2	5:B:63:VAL:HG22	2.23	0.68
6:A:23:PRO:N	6:A:63:TRP:CD1	2.62	0.68
4:F:265:TYR:CB	4:F:296:CYS:N	2.55	0.68
5:B:139:ASP:O	5:B:172:LEU:HD23	1.92	0.68
5:B:52:ILE:HG21	5:B:63:VAL:HG22	1.74	0.68
1:E:972:ILE:O	1:E:1001:THR:HA	1.94	0.67
5:B:281:TYR:HB3	5:B:296:ILE:HG23	1.75	0.67
4:F:292:ILE:HD12	4:F:292:ILE:C	2.15	0.67
1:E:973:ARG:CD	1:E:975:PRO:HD2	2.25	0.67
5:B:345:PRO:HG2	5:B:347:LYS:HE3	1.76	0.67
4:F:185:LEU:HB3	4:F:193:GLN:HE22	1.56	0.67
5:B:281:TYR:HD1	5:B:296:ILE:HG22	1.60	0.67
4:F:297:THR:HB	4:F:301:CYS:SG	2.35	0.66
2:K:126:VAL:CG2	2:K:481:LEU:CD1	2.44	0.66
4:F:184:THR:HB	4:F:196:GLN:NE2	2.09	0.66
6:A:22:SER:CA	6:A:63:TRP:CE3	2.77	0.66
5:B:25:ASN:CB	5:B:26:PRO:HD2	2.26	0.66
4:F:336:ARG:NH1	6:A:85:SER:OG	2.28	0.66
5:B:192:TRP:H	5:B:211:LYS:HG2	1.62	0.65
1:E:952:LEU:HD11	1:E:1014:PHE:CB	2.22	0.65
6:A:230:GLN:N	6:A:231:PRO:HD2	2.11	0.65
5:B:140:ALA:HA	5:B:172:LEU:HD21	1.77	0.65
1:E:952:LEU:CD1	1:E:1014:PHE:HB3	2.27	0.64
6:A:22:SER:C	6:A:63:TRP:CE2	2.70	0.64
6:A:22:SER:O	6:A:63:TRP:CE2	2.50	0.64
6:A:27:PHE:CB	6:A:63:TRP:HH2	2.09	0.64
1:E:973:ARG:O	1:E:977:ALA:CB	2.44	0.64
5:B:283:VAL:HA	5:B:295:TYR:O	1.98	0.64
1:E:848:LYS:HG2	6:A:117:ASP:HB3	1.79	0.63
1:E:1015:ILE:CG2	1:E:1052:TYR:CD1	2.82	0.63
6:A:229:VAL:CG2	6:A:231:PRO:CD	2.60	0.63
2:K:183:ARG:HH22	2:K:214:ILE:HG13	1.64	0.63
5:B:180:HIS:CD2	5:B:183:ILE:HD12	2.33	0.63
6:A:234:LYS:HD3	6:A:234:LYS:C	2.18	0.63
5:B:123:LEU:HB2	5:B:129:LEU:HB3	1.80	0.62
5:B:140:ALA:HA	5:B:172:LEU:CD2	2.29	0.62
5:B:18:LYS:HB2	5:B:341:SER:HA	1.82	0.62
6:A:79:VAL:HG22	6:A:99:VAL:HG21	1.80	0.62
3:M:162:ASN:HA	3:N:151:ARG:HH12	1.65	0.62
4:F:310:THR:HG22	4:F:310:THR:O	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:263:CYS:HG	4:F:304:HIS:HE2	1.48	0.62
5:B:195:PHE:HB2	5:B:207:ILE:HD11	1.80	0.62
5:B:212:ILE:HG22	5:B:213:THR:HG23	1.81	0.61
1:E:932:GLN:NE2	1:E:963:MET:O	2.33	0.61
2:K:126:VAL:HG22	2:K:127:CYS:N	2.15	0.61
5:B:310:GLY:H	5:B:340:TRP:HH2	1.49	0.61
6:A:269:ASN:ND2	6:A:274:SER:OG	2.33	0.61
2:K:128:ILE:HB	2:K:436:TYR:HB2	1.83	0.61
5:B:225:ASN:ND2	5:B:278:THR:OG1	2.33	0.61
1:E:973:ARG:NH1	1:E:976:VAL:HG21	2.16	0.61
5:B:44:GLY:HA2	5:B:50:LEU:HA	1.82	0.61
6:A:164:ARG:CD	6:A:176:THR:HG22	2.30	0.61
2:K:238:LEU:HB3	2:K:354:TYR:HB3	1.82	0.60
5:B:318:ILE:HG13	5:B:329:SER:HB2	1.83	0.60
5:B:405:ASN:ND2	6:A:107:LYS:O	2.34	0.60
5:B:408:VAL:O	5:B:408:VAL:HG13	1.99	0.60
2:K:491:VAL:HA	2:K:494:ILE:HD12	1.83	0.60
5:B:53:TYR:HE1	5:B:60:PRO:HD3	1.66	0.60
5:B:294:LEU:HD21	5:B:315:LEU:HD11	1.82	0.60
1:E:1018:CYS:SG	1:E:1019:CYS:N	2.74	0.60
2:K:359:GLN:N	2:K:362:LYS:O	2.35	0.60
2:K:460:LEU:HG	2:K:463:ILE:HD12	1.83	0.60
1:E:942:PHE:HD1	1:E:942:PHE:H	1.48	0.60
2:K:207:ARG:NH1	2:K:212:GLU:OE1	2.35	0.60
5:B:115:SER:OG	5:B:134:ILE:HG23	2.02	0.60
5:B:17:GLU:HB2	5:B:296:ILE:CD1	2.31	0.60
4:F:276:VAL:CG2	4:F:292:ILE:CD1	2.57	0.59
5:B:281:TYR:CD1	5:B:296:ILE:CG2	2.85	0.59
6:A:22:SER:C	6:A:63:TRP:CD2	2.75	0.59
1:E:937:LYS:HD2	1:E:937:LYS:O	2.02	0.59
4:F:318:GLN:HE22	5:B:68:LEU:HA	1.67	0.59
6:A:154:LEU:HB3	6:A:166:PHE:HB2	1.83	0.59
2:K:207:ARG:HG2	2:K:209:ILE:H	1.68	0.59
4:F:195:VAL:HG12	4:F:195:VAL:O	2.01	0.59
6:A:69:CYS:HA	6:A:83:HIS:HA	1.85	0.59
1:E:1014:PHE:CE1	5:B:351:LEU:HB2	2.38	0.59
3:M:133:HIS:HB3	3:M:157:LEU:HD22	1.85	0.58
5:B:119:GLY:N	5:B:133:THR:OG1	2.35	0.58
2:K:139:VAL:HG22	2:K:182:LEU:HD11	1.86	0.58
2:K:94:VAL:O	2:K:97:ARG:NH1	2.35	0.58
2:K:463:ILE:HG22	2:K:464:ARG:HG2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:336:ARG:HH12	6:A:85:SER:HG	1.51	0.58
5:B:344:ILE:HG13	5:B:345:PRO:HD2	1.85	0.58
2:K:126:VAL:CG2	2:K:127:CYS:N	2.66	0.58
6:A:51:VAL:HB	6:A:82:ILE:HD13	1.85	0.58
5:B:106:LYS:O	5:B:107:PRO:C	2.40	0.58
5:B:217:ILE:HG22	5:B:233:CYS:HA	1.86	0.58
4:F:200:LEU:CD2	4:F:340:LEU:HD21	2.34	0.58
5:B:408:VAL:HG22	5:B:410:ARG:HG2	1.86	0.58
6:A:111:LEU:HG	6:A:123:TRP:HB2	1.85	0.57
1:E:1015:ILE:HG22	1:E:1052:TYR:CD1	2.39	0.57
3:M:158:ILE:HG12	3:N:151:ARG:HA	1.86	0.57
5:B:17:GLU:CB	5:B:296:ILE:CD1	2.80	0.57
4:F:203:PHE:HA	4:F:206:LYS:HG2	1.85	0.57
5:B:29:THR:HG21	5:B:43:LEU:HB2	1.85	0.57
1:E:1011:ILE:O	1:E:1011:ILE:HG12	2.05	0.57
5:B:115:SER:OG	5:B:134:ILE:CG2	2.53	0.57
1:E:850:ASN:OD1	1:E:944:ARG:NH1	2.38	0.56
4:F:297:THR:HG22	4:F:301:CYS:HG	1.67	0.56
1:E:1014:PHE:HE1	5:B:351:LEU:CB	2.18	0.56
5:B:321:ASP:OD2	5:B:324:SER:OG	2.22	0.56
2:K:183:ARG:HH12	2:K:207:ARG:HE	1.53	0.56
2:K:100:GLY:HA3	2:K:113:VAL:HG13	1.87	0.56
6:A:229:VAL:CG2	6:A:231:PRO:CG	2.83	0.56
5:B:61:ILE:HG22	5:B:406:LEU:HD11	1.81	0.56
6:A:95:HIS:NE2	6:A:114:SER:O	2.38	0.56
5:B:134:ILE:HG22	5:B:136:GLU:H	1.71	0.56
3:M:131:THR:HG22	3:M:134:LEU:HD12	1.86	0.56
3:N:146:PRO:HG2	3:N:149:PRO:HA	1.88	0.56
6:A:41:ILE:HG22	6:A:44:ARG:H	1.71	0.56
6:A:97:ALA:HB1	6:A:116:MET:HB3	1.87	0.55
1:E:1006:THR:HA	5:B:355:PHE:HE1	1.72	0.55
5:B:40:TYR:OH	5:B:404:ASN:O	2.20	0.55
4:F:263:CYS:SG	4:F:297:THR:CG2	2.88	0.55
6:A:164:ARG:HD3	6:A:176:THR:CG2	2.37	0.55
1:E:973:ARG:NH1	1:E:976:VAL:CG2	2.70	0.55
5:B:35:SER:OG	5:B:39:ASP:N	2.38	0.55
5:B:119:GLY:H	5:B:133:THR:HG1	1.54	0.55
1:E:942:PHE:CD1	1:E:942:PHE:N	2.71	0.55
1:E:1006:THR:HA	5:B:355:PHE:CE1	2.42	0.54
6:A:22:SER:CA	6:A:63:TRP:CG	2.81	0.54
3:N:133:HIS:HB3	3:N:160:GLN:HE22	1.71	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:973:ARG:HD2	1:E:975:PRO:HD2	1.88	0.54
5:B:32:LEU:HG	5:B:43:LEU:HB3	1.90	0.54
6:A:83:HIS:HB2	6:A:86:TYR:HB2	1.90	0.54
6:A:284:TYR:O	6:A:285:HIS:ND1	2.40	0.54
4:F:119:ARG:O	4:F:123:ASN:ND2	2.40	0.54
6:A:22:SER:HB3	6:A:63:TRP:CZ2	2.43	0.54
6:A:79:VAL:HG11	6:A:102:LEU:HD21	1.89	0.54
5:B:73:ARG:HB3	5:B:92:ARG:HB2	1.90	0.54
6:A:62:CYS:SG	6:A:103:THR:N	2.81	0.54
5:B:354:ASP:O	5:B:356:GLU:HG3	2.08	0.54
5:B:244:SER:OG	5:B:248:GLU:O	2.27	0.53
1:E:950:TRP:CG	5:B:351:LEU:HD13	2.43	0.53
5:B:321:ASP:OD1	5:B:326:SER:N	2.35	0.53
6:A:23:PRO:CD	6:A:63:TRP:CG	2.91	0.53
4:F:167:LYS:HA	4:F:170:ASP:HB2	1.89	0.53
6:A:22:SER:HA	6:A:63:TRP:CB	2.38	0.53
5:B:61:ILE:HG22	5:B:406:LEU:CD1	2.36	0.53
5:B:276:ASN:ND2	5:B:325:MET:SD	2.82	0.53
1:E:1014:PHE:CE1	5:B:351:LEU:CB	2.92	0.53
3:M:151:ARG:HA	3:N:158:ILE:HG12	1.91	0.53
4:F:164:ILE:O	4:F:167:LYS:N	2.42	0.53
6:A:22:SER:HB3	6:A:63:TRP:CE2	2.43	0.53
5:B:178:THR:OG1	5:B:180:HIS:O	2.26	0.53
5:B:180:HIS:HD2	5:B:183:ILE:HD12	1.72	0.53
6:A:285:HIS:CD2	6:A:312:TRP:HE1	2.27	0.53
5:B:98:LEU:HD23	5:B:108:LEU:HB2	1.89	0.53
4:F:200:LEU:CD2	4:F:340:LEU:CD2	2.78	0.52
6:A:214:LYS:HE3	6:A:223:VAL:HG21	1.90	0.52
1:E:973:ARG:CG	1:E:974:GLN:N	2.72	0.52
5:B:121:GLN:HE22	5:B:176:VAL:HG23	1.74	0.52
2:K:202:TYR:HA	2:K:216:GLU:HG2	1.91	0.52
6:A:240:SER:HB3	6:A:262:ASN:HD21	1.74	0.52
2:K:196:PRO:HG3	2:K:443:PHE:HZ	1.74	0.52
1:E:980:ARG:NH1	5:B:364:TYR:OH	2.43	0.52
4:F:307:TRP:O	4:F:311:ASN:HB2	2.08	0.52
6:A:22:SER:OG	6:A:63:TRP:CZ3	2.55	0.52
5:B:193:LEU:HD12	5:B:212:ILE:HD12	1.91	0.52
6:A:182:ASP:HB2	6:A:188:GLY:HA2	1.91	0.52
1:E:927:LEU:HD23	1:E:930:LEU:HD12	1.92	0.52
1:E:1015:ILE:N	1:E:1015:ILE:HD13	2.23	0.52
5:B:240:GLN:HG3	5:B:257:GLU:HB2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:328:ARG:HH12	5:B:410:ARG:HA	1.75	0.51
6:A:163:ILE:N	6:A:177:LEU:O	2.42	0.51
5:B:223:SER:OG	5:B:227:GLU:N	2.39	0.51
5:B:52:ILE:HG21	5:B:63:VAL:CG2	2.39	0.51
1:E:1070:CYS:SG	1:E:1071:GLY:N	2.83	0.51
5:B:298:GLU:OE1	5:B:301:SER:N	2.44	0.51
5:B:353:PRO:HA	6:A:176:THR:HG1	1.74	0.51
1:E:845:ASP:OD1	1:E:845:ASP:N	2.44	0.51
1:E:821:ASN:HA	6:A:77:PHE:HB3	1.92	0.51
5:B:24:GLU:O	5:B:336:ASN:ND2	2.44	0.51
5:B:275:SER:OG	5:B:276:ASN:N	2.43	0.51
2:K:134:TYR:H	2:K:477:THR:HG22	1.75	0.50
5:B:91:SER:HB2	5:B:93:ASP:HB2	1.92	0.50
5:B:387:GLU:O	6:A:225:ARG:NH1	2.44	0.50
6:A:262:ASN:H	6:A:289:PRO:HA	1.76	0.50
4:F:266:CYS:HA	4:F:308:VAL:CG2	2.42	0.50
1:E:932:GLN:OE1	1:E:936:ARG:NH1	2.45	0.50
4:F:185:LEU:HB2	4:F:193:GLN:CD	2.29	0.50
2:K:141:ARG:H	2:K:447:THR:HB	1.75	0.50
6:A:101:SER:H	6:A:114:SER:HB2	1.77	0.50
6:A:142:VAL:N	6:A:157:GLY:O	2.44	0.50
6:A:16:ALA:HB2	6:A:309:CYS:H	1.77	0.50
1:E:952:LEU:HD21	1:E:1014:PHE:HB3	1.93	0.50
5:B:238:ILE:HB	5:B:260:TYR:HB2	1.93	0.50
5:B:287:HIS:HE1	5:B:315:LEU:HG	1.76	0.50
2:K:492:TRP:HE1	3:N:135:LEU:HD21	1.76	0.50
6:A:258:SER:OG	6:A:266:TYR:N	2.45	0.50
5:B:86:LEU:HD21	5:B:127:ARG:HE	1.77	0.50
5:B:239:ARG:HD3	5:B:256:LEU:HD11	1.92	0.50
5:B:87:LEU:HB3	5:B:99:TRP:HB2	1.94	0.49
2:K:456:LYS:H	2:K:460:LEU:HD12	1.77	0.49
5:B:87:LEU:N	5:B:99:TRP:O	2.44	0.49
2:K:139:VAL:HB	2:K:230:LYS:HA	1.93	0.49
6:A:62:CYS:SG	6:A:103:THR:HA	2.53	0.49
5:B:287:HIS:CE1	5:B:315:LEU:H	2.31	0.49
6:A:191:PRO:O	6:A:209:LEU:N	2.46	0.49
4:F:198:ILE:O	4:F:201:PRO:HD3	2.13	0.49
5:B:217:ILE:HG21	5:B:231:ILE:HD11	1.95	0.49
6:A:82:ILE:HB	6:A:88:LEU:HD12	1.94	0.49
4:F:150:LYS:O	4:F:150:LYS:HG3	2.11	0.49
5:B:108:LEU:HB3	5:B:109:LYS:NZ	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1015:ILE:HG21	1:E:1052:TYR:HD1	1.76	0.49
5:B:85:ARG:NH2	5:B:404:ASN:O	2.42	0.49
4:F:297:THR:HG22	4:F:304:HIS:HE1	1.34	0.49
5:B:268:GLN:NE2	5:B:287:HIS:O	2.45	0.49
2:K:183:ARG:N	2:K:441:SER:OG	2.42	0.49
4:F:206:LYS:HG3	4:F:207:LEU:HG	1.95	0.49
4:F:265:TYR:CB	4:F:296:CYS:HB3	2.43	0.49
3:N:127:ASN:HA	3:N:130:VAL:HG12	1.95	0.48
6:A:285:HIS:CG	6:A:312:TRP:HE1	2.32	0.48
4:F:311:ASN:O	4:F:314:GLN:N	2.42	0.48
4:F:161:ASP:HA	4:F:168:THR:HG21	1.96	0.48
5:B:229:LEU:HB2	5:B:241:TYR:HB2	1.94	0.48
4:F:185:LEU:HG	4:F:344:TYR:HE2	1.79	0.48
5:B:198:PHE:HB2	5:B:204:THR:HG21	1.96	0.48
6:A:145:ASP:H	6:A:155:SER:HG	1.54	0.48
5:B:63:VAL:O	5:B:66:ASN:OD1	2.31	0.48
6:A:260:TYR:HB3	6:A:265:ILE:HA	1.95	0.48
5:B:296:ILE:O	5:B:305:VAL:HB	2.14	0.48
6:A:27:PHE:CB	6:A:63:TRP:CH2	2.93	0.48
5:B:357:GLU:O	5:B:357:GLU:HG3	2.14	0.48
1:E:980:ARG:HA	1:E:983:ARG:HE	1.79	0.47
5:B:56:ASP:N	5:B:56:ASP:OD1	2.47	0.47
2:K:187:CYS:SG	2:K:188:ARG:N	2.86	0.47
6:A:22:SER:HA	6:A:63:TRP:CE3	2.46	0.47
6:A:229:VAL:CG2	6:A:231:PRO:HG2	2.45	0.47
2:K:236:GLY:H	2:K:356:ALA:HB3	1.79	0.47
6:A:189:VAL:HG13	6:A:191:PRO:HD3	1.95	0.47
1:E:808:LEU:O	1:E:812:LYS:N	2.48	0.47
4:F:185:LEU:CB	4:F:193:GLN:NE2	2.46	0.47
4:F:185:LEU:HB3	4:F:187:THR:HG23	1.96	0.47
4:F:307:TRP:NE1	4:F:311:ASN:HA	2.29	0.47
6:A:22:SER:C	6:A:63:TRP:CG	2.88	0.47
5:B:53:TYR:CE1	5:B:60:PRO:HD3	2.49	0.47
4:F:157:LEU:HA	4:F:160:ILE:HG22	1.97	0.47
4:F:165:VAL:O	4:F:168:THR:OG1	2.31	0.47
5:B:314:GLU:O	5:B:332:PHE:N	2.42	0.47
6:A:22:SER:HA	6:A:63:TRP:HB2	1.97	0.47
6:A:230:GLN:N	6:A:231:PRO:CD	2.78	0.47
1:E:984:TYR:OH	1:E:1006:THR:OG1	2.28	0.47
5:B:194:ASP:OD1	5:B:195:PHE:N	2.47	0.47
6:A:27:PHE:HB2	6:A:63:TRP:CH2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:826:ASP:OD1	1:E:826:ASP:N	2.48	0.46
2:K:219:LEU:N	5:B:376:GLU:OE2	2.48	0.46
6:A:22:SER:C	6:A:63:TRP:CD1	2.88	0.46
4:F:265:TYR:C	4:F:308:VAL:HG21	2.36	0.46
6:A:27:PHE:O	6:A:63:TRP:CZ3	2.68	0.46
5:B:18:LYS:HD2	5:B:341:SER:HA	1.96	0.46
5:B:100:ASP:CB	5:B:108:LEU:CD1	2.79	0.46
4:F:263:CYS:SG	4:F:304:HIS:NE2	2.79	0.46
5:B:273:LEU:HD21	5:B:319:ASN:HA	1.98	0.46
6:A:225:ARG:NH2	6:A:271:ASP:OD1	2.49	0.46
2:K:188:ARG:HG3	2:K:202:TYR:CE2	2.50	0.46
3:M:137:GLY:HA3	3:M:157:LEU:HD11	1.98	0.46
1:E:973:ARG:HG2	1:E:974:GLN:N	2.30	0.46
4:F:207:LEU:HD22	4:F:210:LEU:HB2	1.96	0.46
3:M:132:PRO:HG2	3:M:133:HIS:CD2	2.51	0.46
1:E:965:ILE:O	1:E:965:ILE:HG23	2.16	0.46
5:B:125:ALA:HB3	5:B:129:LEU:HD12	1.97	0.46
1:E:965:ILE:HG21	1:E:1011:ILE:HG21	1.98	0.46
1:E:973:ARG:CG	1:E:975:PRO:CD	2.81	0.46
3:N:122:THR:OG1	3:N:124:LYS:NZ	2.40	0.46
5:B:281:TYR:HD1	5:B:296:ILE:CG2	2.19	0.46
3:M:151:ARG:HG3	3:N:158:ILE:HA	1.97	0.46
5:B:108:LEU:O	5:B:109:LYS:CD	2.38	0.46
6:A:68:GLN:HE21	6:A:86:TYR:HE2	1.64	0.46
4:F:263:CYS:HG	4:F:297:THR:HG21	1.78	0.45
5:B:32:LEU:HD23	5:B:41:LEU:HD21	1.98	0.45
1:E:1015:ILE:HG21	1:E:1052:TYR:CD1	2.50	0.45
4:F:290:THR:HB	4:F:294:GLU:HA	1.98	0.45
6:A:61:LEU:HG	6:A:72:THR:HG22	1.99	0.45
5:B:328:VAL:HG12	5:B:339:VAL:HG22	1.99	0.45
6:A:12:ASN:ND2	6:A:308:ASP:O	2.45	0.45
5:B:33:GLN:OE1	5:B:319:ASN:ND2	2.50	0.45
6:A:273:LYS:H	6:A:273:LYS:HD2	1.81	0.45
6:A:285:HIS:CE1	6:A:286:HIS:HB2	2.51	0.45
2:K:354:TYR:HA	2:K:366:LYS:HB2	1.97	0.45
6:A:182:ASP:HA	6:A:189:VAL:HG12	1.98	0.45
6:A:185:ARG:HH22	6:A:236:VAL:HG23	1.82	0.45
2:K:461:ASP:O	2:K:466:ALA:N	2.48	0.45
4:F:135:ARG:O	4:F:139:LYS:N	2.48	0.44
4:F:263:CYS:HG	4:F:297:THR:CG2	2.30	0.44
5:B:411:PHE:O	5:B:411:PHE:CD2	2.70	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:114:SER:HA	6:A:120:ILE:HG22	1.98	0.44
5:B:278:THR:HB	5:B:280:GLU:HG3	1.99	0.44
5:B:344:ILE:CG1	5:B:345:PRO:HD2	2.46	0.44
4:F:297:THR:CG2	4:F:304:HIS:HE2	2.16	0.44
5:B:78:ILE:HG22	5:B:89:THR:HA	1.99	0.44
5:B:274:PHE:HD1	5:B:282:LEU:HD13	1.82	0.44
4:F:311:ASN:O	4:F:312:GLN:C	2.55	0.44
6:A:182:ASP:OD1	6:A:182:ASP:N	2.50	0.44
1:E:950:TRP:CD2	5:B:351:LEU:HD13	2.53	0.44
5:B:122:TRP:HB3	5:B:124:ASP:H	1.81	0.44
6:A:118:GLU:HA	6:A:141:VAL:HG23	1.99	0.44
3:M:152:VAL:HG23	3:M:153:LEU:HD22	1.99	0.44
6:A:234:LYS:C	6:A:234:LYS:CD	2.85	0.44
4:F:266:CYS:HA	4:F:308:VAL:HG22	1.99	0.44
3:M:161:SER:O	3:N:151:ARG:NH2	2.42	0.43
5:B:24:GLU:HB3	5:B:25:ASN:H	1.69	0.43
5:B:54:ASP:OD1	5:B:54:ASP:N	2.50	0.43
4:F:187:THR:OG1	4:F:193:GLN:NE2	2.42	0.43
4:F:200:LEU:HD11	4:F:340:LEU:HG	2.00	0.43
1:E:942:PHE:HB3	5:B:351:LEU:HD11	2.00	0.43
1:E:954:ALA:O	1:E:1047:SER:N	2.50	0.43
3:M:129:ASN:HD21	3:N:145:GLN:HE22	1.65	0.43
4:F:132:ASP:N	4:F:163:ASN:O	2.38	0.43
4:F:184:THR:HB	4:F:196:GLN:HE22	1.81	0.43
4:F:203:PHE:HE1	4:F:207:LEU:HD12	1.84	0.43
4:F:228:ASP:HA	4:F:231:ALA:HB3	1.99	0.43
5:B:296:ILE:O	5:B:305:VAL:CG2	2.67	0.43
6:A:266:TYR:HA	6:A:278:LEU:HD13	2.00	0.43
5:B:233:CYS:SG	5:B:237:THR:OG1	2.67	0.43
5:B:348:TRP:HA	5:B:348:TRP:CE3	2.53	0.43
6:A:208:SER:HG	6:A:212:VAL:H	1.61	0.43
1:E:971:ARG:O	1:E:1002:VAL:O	2.36	0.43
5:B:351:LEU:HD23	5:B:351:LEU:N	2.34	0.43
1:E:973:ARG:HH11	1:E:976:VAL:CG2	2.31	0.43
2:K:119:TRP:HB3	2:K:120:ARG:H	1.60	0.43
3:N:138:MET:HA	3:N:141:ILE:HG22	2.00	0.43
6:A:141:VAL:HA	6:A:158:SER:HA	2.00	0.43
6:A:207:LYS:HA	6:A:213:VAL:HG12	2.00	0.43
2:K:358:PHE:CE2	2:K:361:GLY:HA2	2.53	0.43
4:F:203:PHE:CG	4:F:336:ARG:HG2	2.54	0.43
5:B:192:TRP:HD1	5:B:211:LYS:HB3	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:307:TRP:HA	4:F:307:TRP:CE3	2.52	0.43
5:B:189:SER:N	5:B:191:GLY:O	2.52	0.43
5:B:229:LEU:HD11	5:B:243:ILE:HA	2.00	0.43
2:K:135:TRP:CZ2	2:K:438:PRO:HB2	2.54	0.42
4:F:325:MET:O	4:F:329:LEU:HB2	2.18	0.42
1:E:952:LEU:H	1:E:1049:GLU:HG2	1.84	0.42
5:B:363:ASP:N	5:B:363:ASP:OD1	2.52	0.42
4:F:265:TYR:N	4:F:295:VAL:HB	2.16	0.42
1:E:952:LEU:HD21	1:E:1014:PHE:HD1	1.84	0.42
5:B:75:ILE:HD13	5:B:78:ILE:HG23	2.02	0.42
6:A:38:ILE:HG13	6:A:50:LEU:HB3	2.01	0.42
4:F:203:PHE:CE1	4:F:207:LEU:HD12	2.54	0.42
5:B:389:ILE:O	6:A:200:ASN:ND2	2.49	0.42
2:K:213:SER:OG	2:K:221:CYS:O	2.33	0.41
4:F:332:LEU:HD11	6:A:86:TYR:HE1	1.85	0.41
2:K:475:VAL:HA	2:K:477:THR:HG23	2.02	0.41
6:A:35:ASN:HA	6:A:52:THR:HG22	2.02	0.41
4:F:312:GLN:O	4:F:316:LEU:N	2.48	0.41
2:K:89:HIS:CE1	3:M:123:ARG:H	2.38	0.41
5:B:5:LEU:HD22	5:B:5:LEU:HA	1.92	0.41
2:K:197:VAL:HG11	2:K:205:GLY:HA3	2.02	0.41
2:K:233:ASP:HA	2:K:359:GLN:HA	2.02	0.41
5:B:29:THR:OG1	5:B:330:ASN:ND2	2.49	0.41
6:A:21:ILE:HG12	6:A:296:PHE:H	1.86	0.41
4:F:234:HIS:ND1	4:F:274:CYS:SG	2.91	0.41
6:A:72:THR:O	6:A:79:VAL:HG13	2.20	0.41
1:E:805:ARG:O	1:E:809:GLU:N	2.49	0.41
1:E:818:ILE:HA	1:E:821:ASN:HB2	2.01	0.41
4:F:263:CYS:CB	4:F:297:THR:CG2	2.57	0.41
5:B:200:SER:HA	5:B:203:GLN:HA	2.02	0.41
5:B:29:THR:H	5:B:330:ASN:HD21	1.68	0.41
5:B:77:SER:N	5:B:90:SER:OG	2.42	0.41
5:B:231:ILE:HG22	5:B:239:ARG:H	1.86	0.41
6:A:111:LEU:HD23	6:A:125:THR:HG22	2.03	0.41
1:E:939:PRO:O	1:E:955:LEU:N	2.39	0.40
1:E:984:TYR:O	1:E:988:GLY:N	2.53	0.40
4:F:297:THR:CA	4:F:301:CYS:SG	3.09	0.40
6:A:71:ALA:HB2	6:A:81:ILE:HG12	2.03	0.40
2:K:481:LEU:HD22	2:K:481:LEU:HA	1.93	0.40
4:F:203:PHE:HZ	4:F:333:ILE:HG12	1.84	0.40
4:F:319:ILE:HA	4:F:322:LEU:HB2	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:491:VAL:HG21	3:N:138:MET:HG3	2.04	0.40
5:B:178:THR:HA	5:B:222:VAL:HG11	2.02	0.40
6:A:225:ARG:NE	6:A:271:ASP:HA	2.36	0.40
4:F:287:GLU:HB2	4:F:291:LYS:HE3	2.03	0.40
5:B:63:VAL:CG2	5:B:64:PRO:HD3	2.51	0.40
5:B:233:CYS:HB2	5:B:237:THR:H	1.86	0.40
6:A:268:TRP:HE1	6:A:275:LEU:HD23	1.85	0.40
1:E:973:ARG:HH11	1:E:976:VAL:HG21	1.83	0.40
4:F:311:ASN:C	4:F:311:ASN:HD22	2.24	0.40
5:B:308:LEU:HD13	5:B:340:TRP:CE2	2.56	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	E	186/278 (67%)	151 (81%)	35 (19%)	0	100	100
2	K	203/417 (49%)	152 (75%)	51 (25%)	0	100	100
3	M	40/42 (95%)	34 (85%)	6 (15%)	0	100	100
3	N	38/42 (90%)	33 (87%)	5 (13%)	0	100	100
4	F	211/237 (89%)	184 (87%)	27 (13%)	0	100	100
5	B	395/412 (96%)	318 (80%)	76 (19%)	1 (0%)	41	76
6	A	312/314 (99%)	252 (81%)	60 (19%)	0	100	100
All	All	1385/1742 (80%)	1124 (81%)	260 (19%)	1 (0%)	54	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	63	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	E	141/246 (57%)	138 (98%)	3 (2%)	53	72
2	K	140/371 (38%)	136 (97%)	4 (3%)	42	64
3	M	35/38 (92%)	35 (100%)	0	100	100
3	N	32/38 (84%)	31 (97%)	1 (3%)	40	63
4	F	135/222 (61%)	132 (98%)	3 (2%)	52	71
5	B	315/374 (84%)	308 (98%)	7 (2%)	52	71
6	A	238/278 (86%)	236 (99%)	2 (1%)	81	89
All	All	1036/1567 (66%)	1016 (98%)	20 (2%)	59	75

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	934	ASN
1	E	942	PHE
1	E	996	ARG
2	K	355	LEU
2	K	366	LYS
2	K	439	THR
2	K	481	LEU
3	N	130	VAL
4	F	183	MET
4	F	219	ASN
4	F	311	ASN
5	B	28	ARG
5	B	43	LEU
5	B	67	MET
5	B	128	ARG
5	B	236	ARG
5	B	266	LYS
5	B	409	GLU
6	A	127	ASN
6	A	273	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	830	GLN
1	E	934	ASN
1	E	948	HIS
1	E	1022	ASN
3	M	133	HIS
3	N	145	GLN
4	F	123	ASN
4	F	193	GLN
4	F	219	ASN
4	F	311	ASN
4	F	343	GLN
5	B	6	GLN
5	B	66	ASN
5	B	208	HIS
5	B	225	ASN
5	B	287	HIS
6	A	68	GLN
6	A	262	ASN
6	A	269	ASN
6	A	294	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

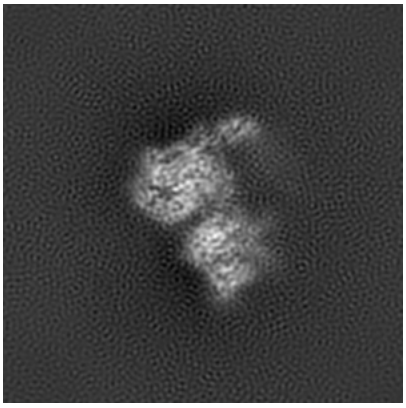
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7303. These allow visual inspection of the internal detail of the map and identification of artifacts.

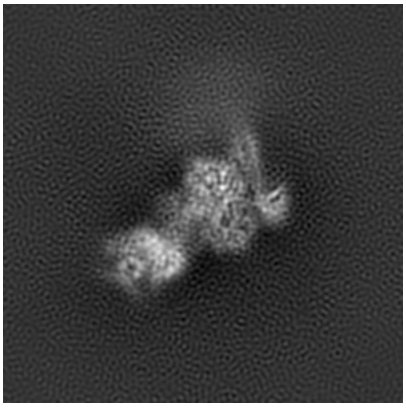
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

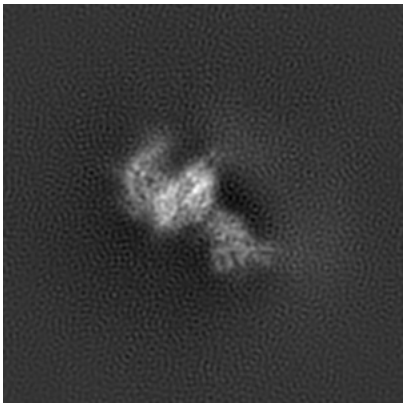
6.1.1 Primary map



X



Y

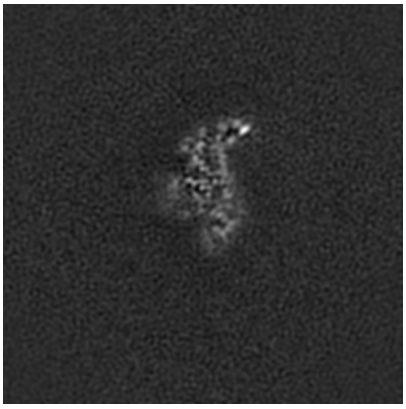


Z

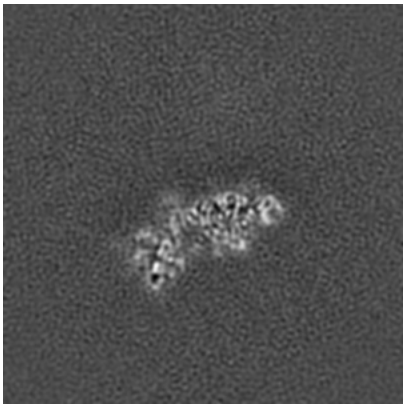
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 156



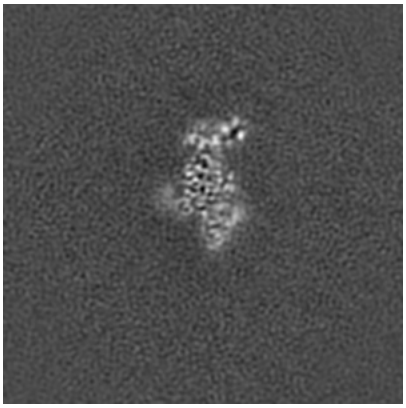
Y Index: 156

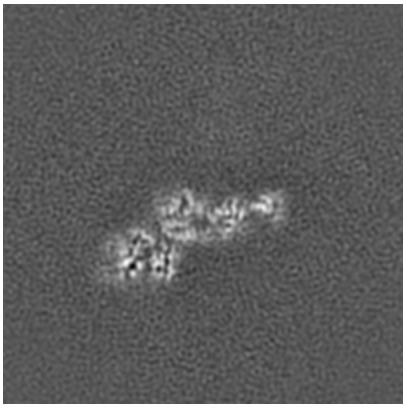
Z Index: 156

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: 151

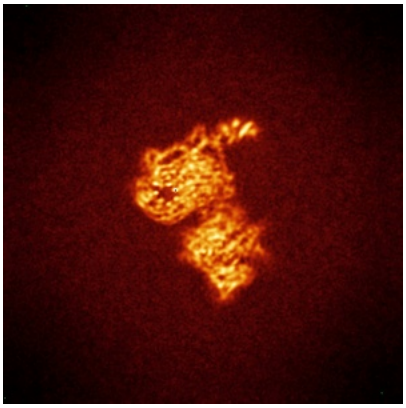

Y Index: 167

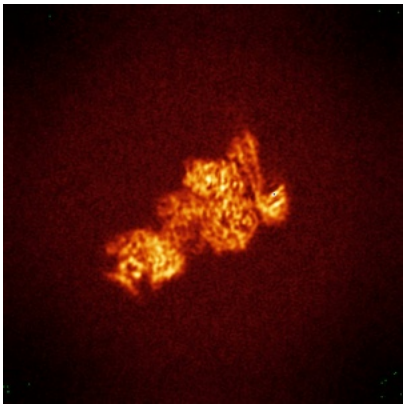
Z Index: 171

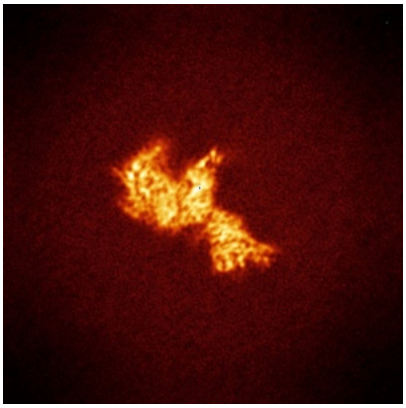
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

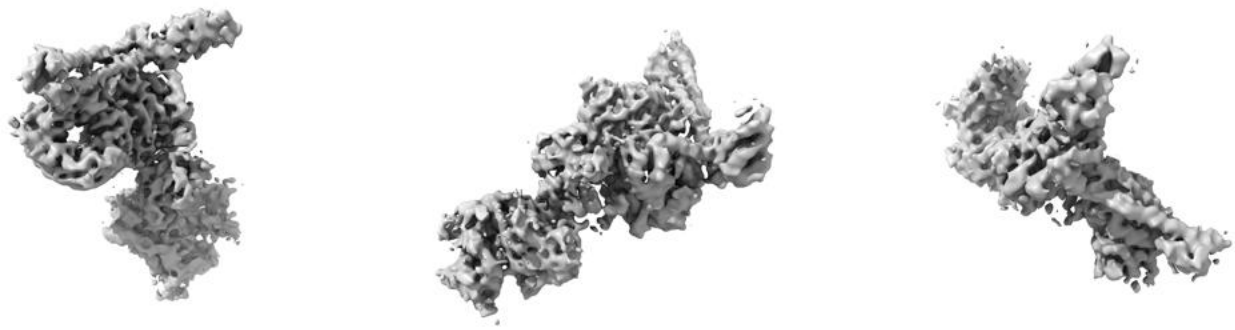

Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

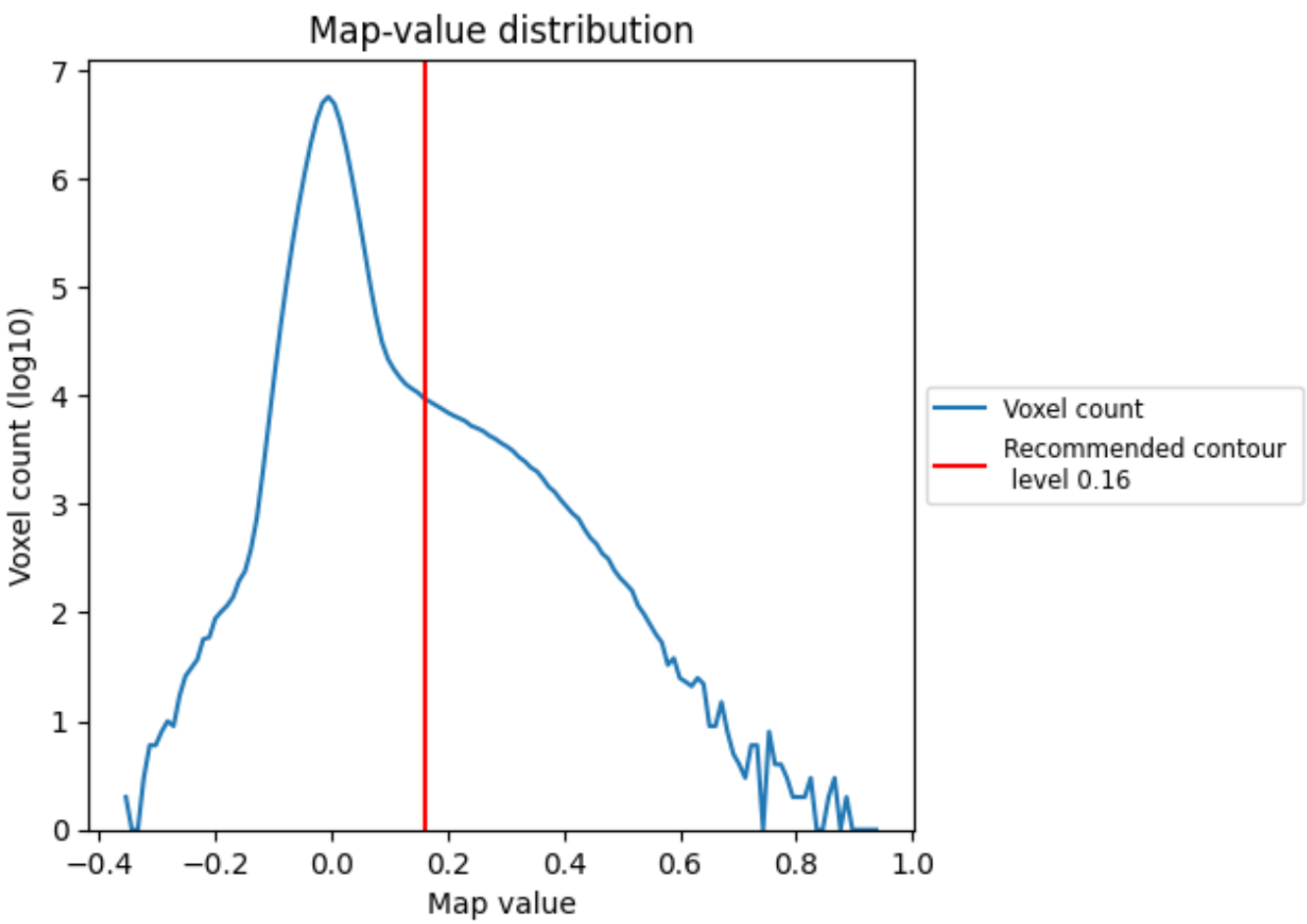
6.6 Mask visualisation (i)

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

7 Map analysis (i)

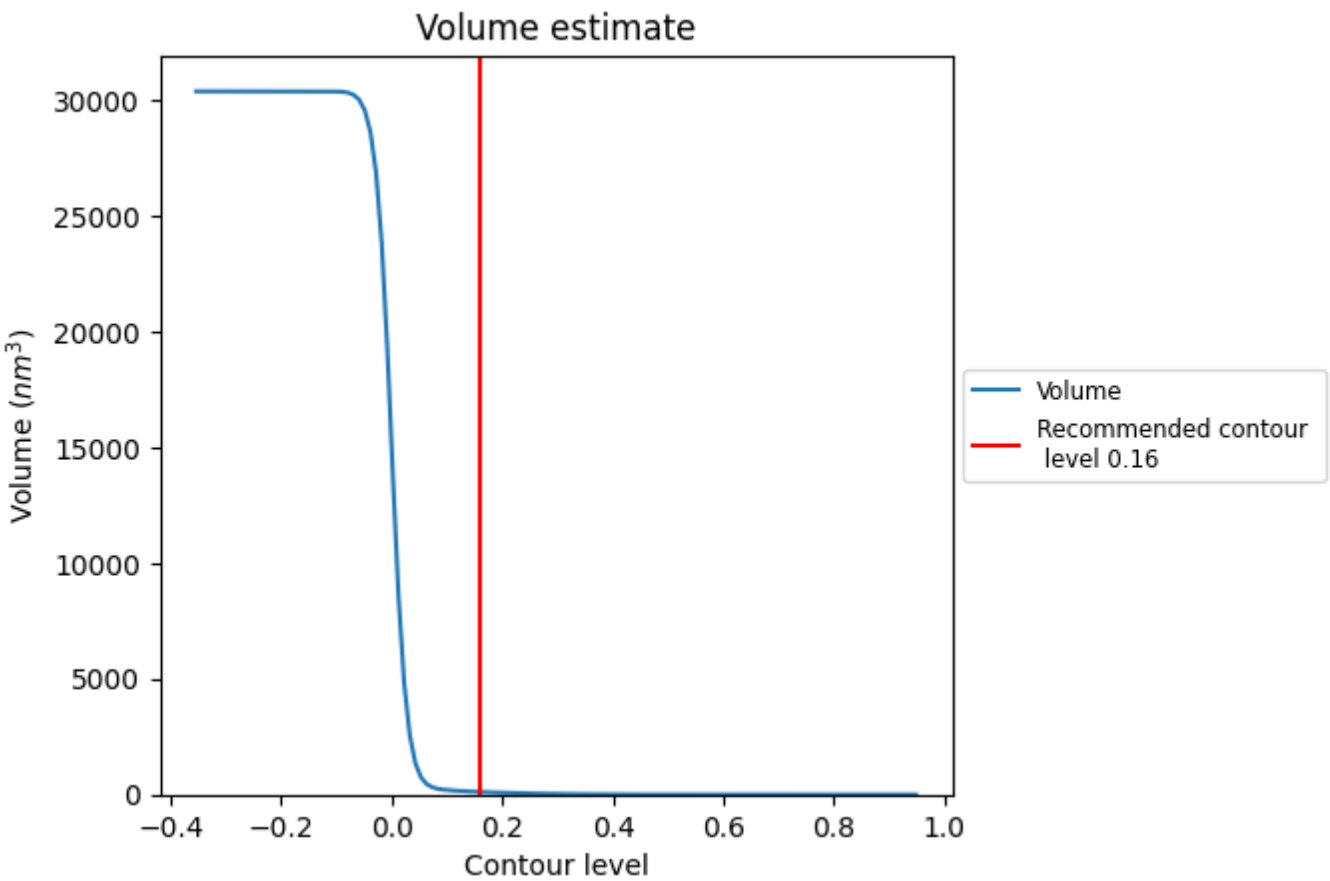
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

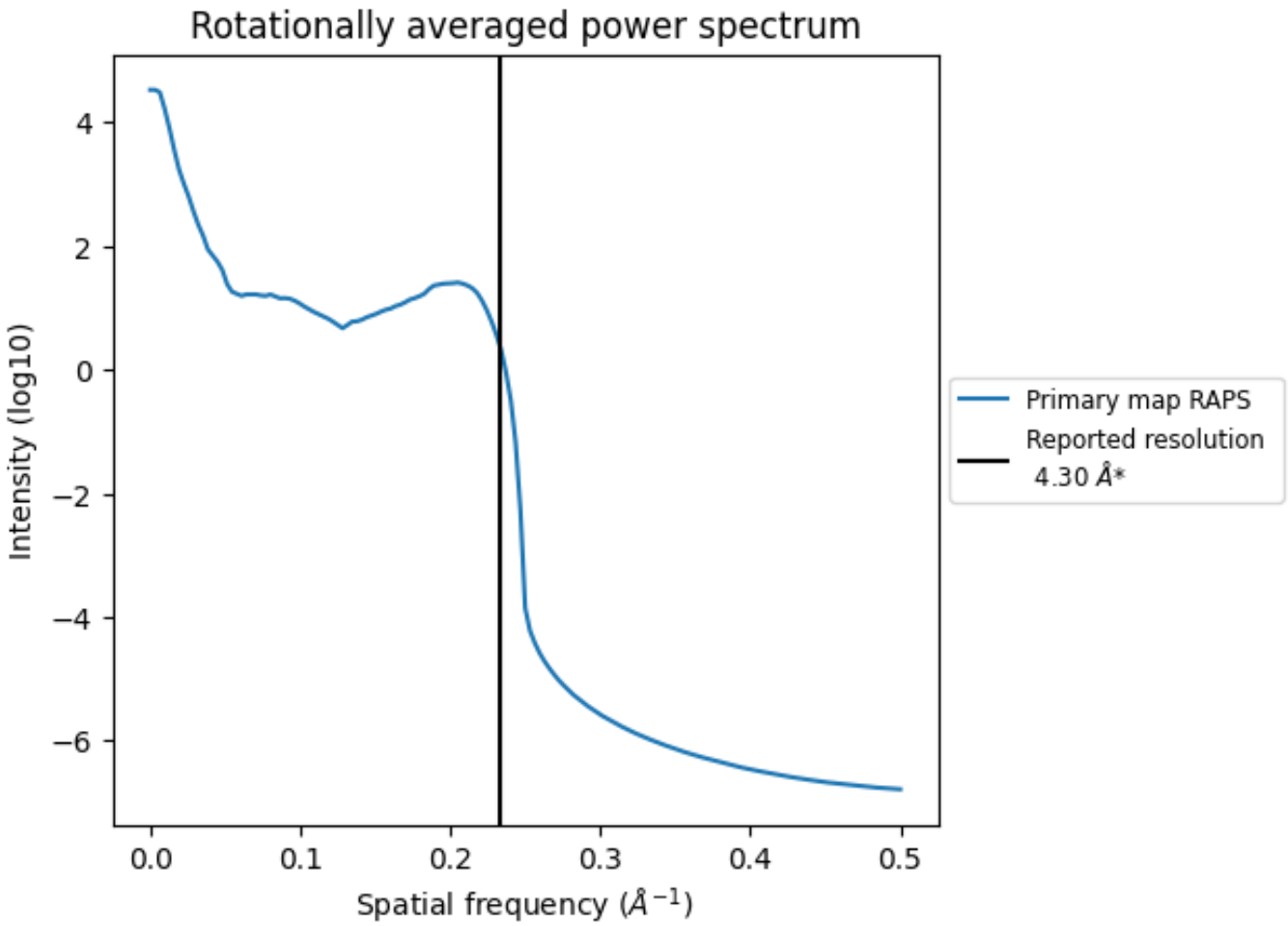
7.2 Volume estimate (i)



The volume at the recommended contour level is 113 nm^3; this corresponds to an approximate mass of 102 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)

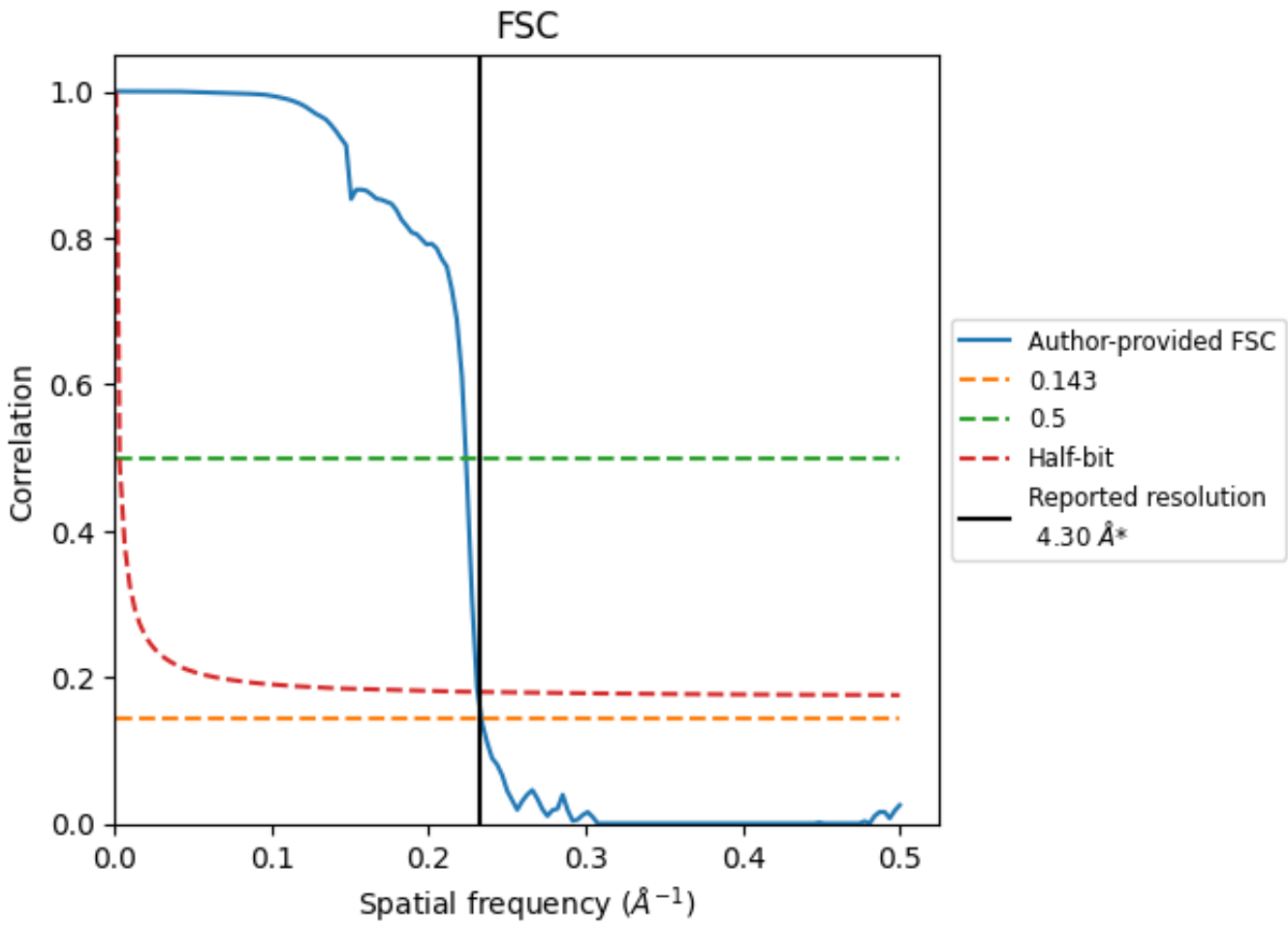


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8.2 Resolution estimates (i)

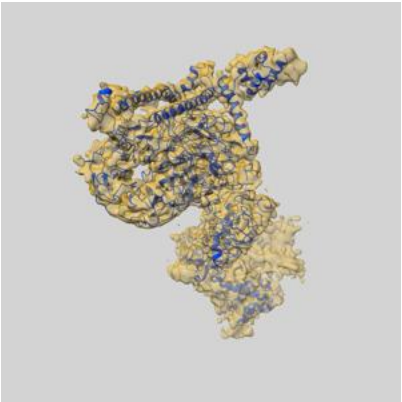
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.28	4.47	4.33
Unmasked-calculated*	-	-	-

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

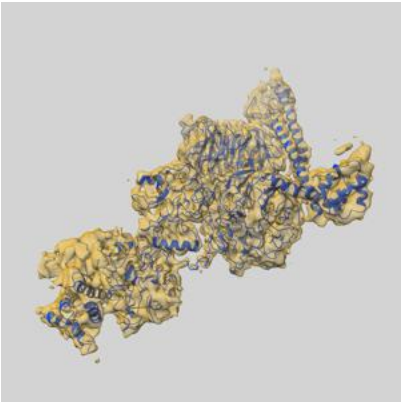
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7303 and PDB model 6BX3. Per-residue inclusion information can be found in section 3 on page 5.

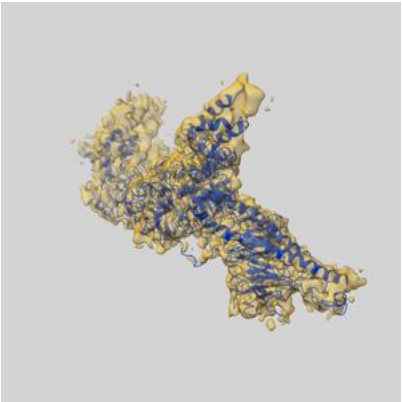
9.1 Map-model overlay (i)



X



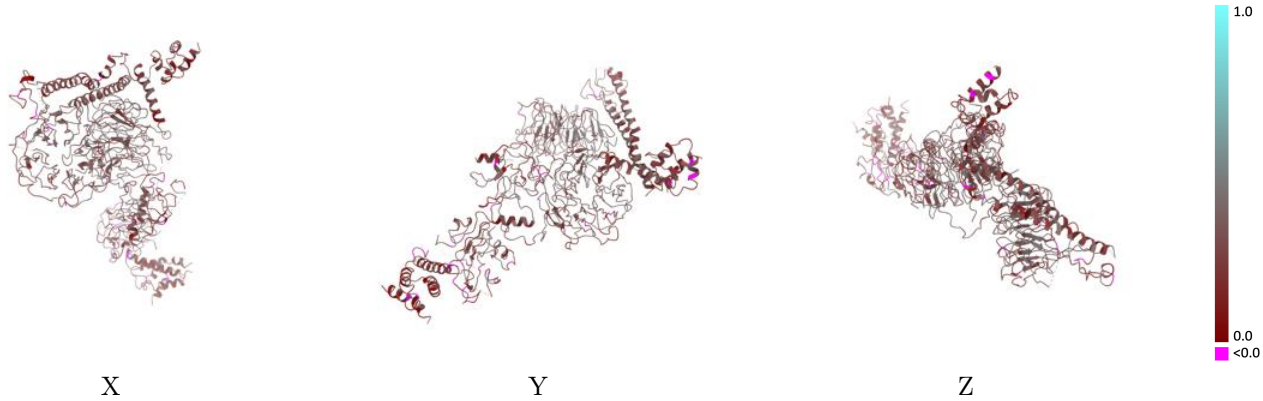
Y



Z

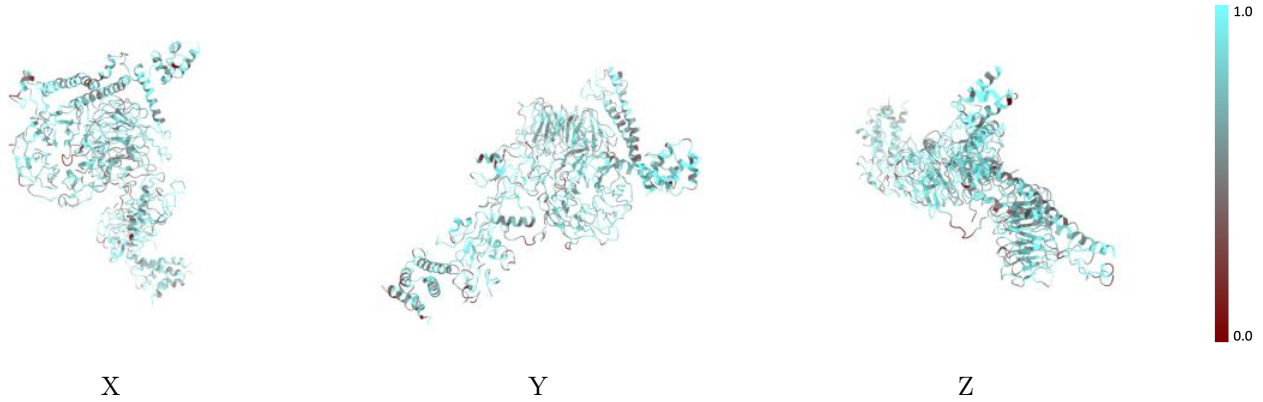
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



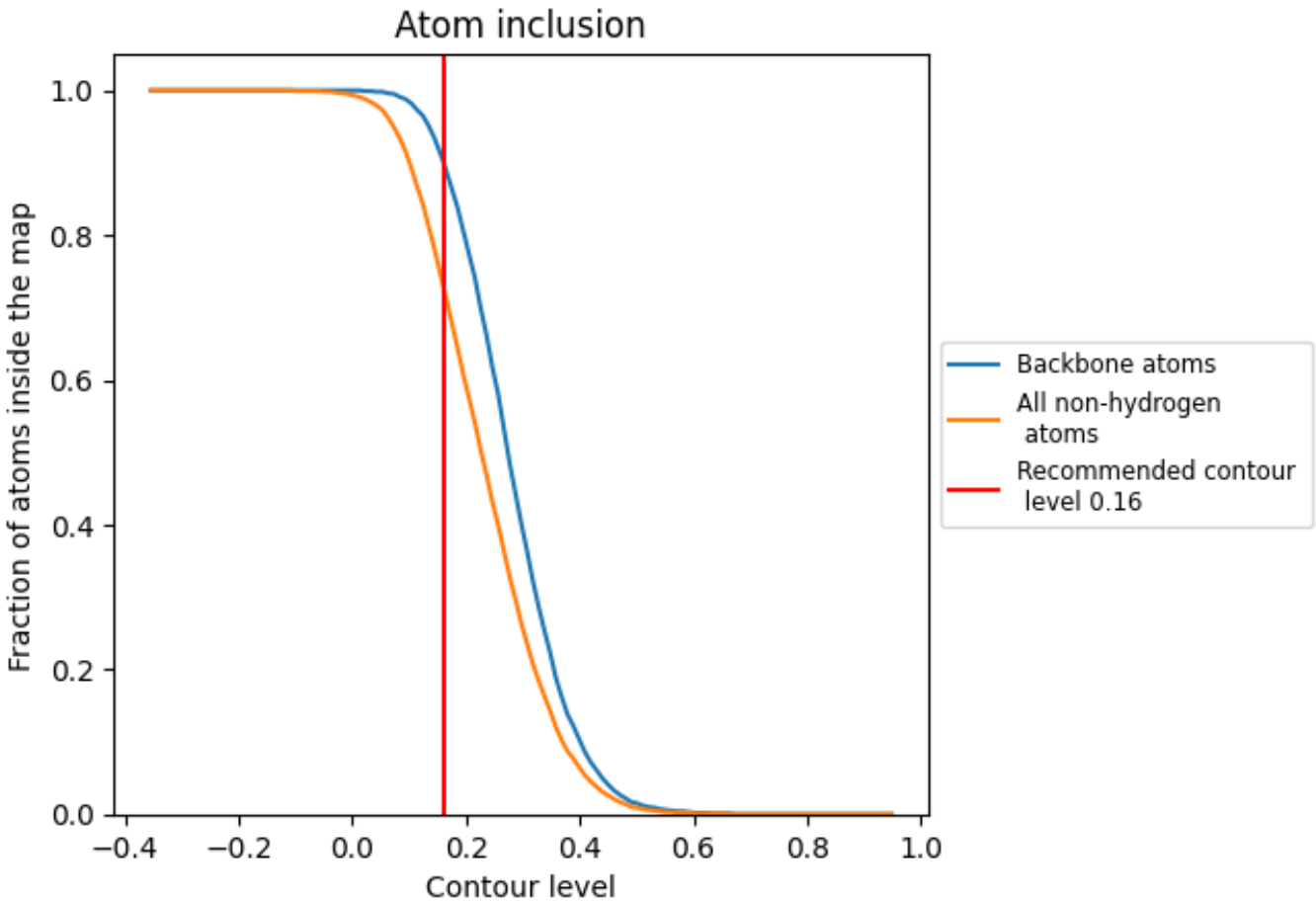
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.16).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7300	0.2970
A	0.7500	0.3360
B	0.6980	0.3310
E	0.7600	0.2930
F	0.7210	0.2640
K	0.7560	0.2540
M	0.7060	0.1820
N	0.6850	0.1840