Full wwPDB EM Validation Report (i)

Nov 9, 2022 – 05:45 AM JST

PDB ID	:	6IOK
EMDB ID	:	EMD-9695
Title	:	Cryo-EM structure of multidrug efflux pump MexAB-OprM (0 degree state)
Authors	:	Tsutsumi, K.; Yonehara, R.; Nakagawa, A.; Yamashita, E.
Deposited on	:	2018-10-30
Resolution	:	3.64 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:

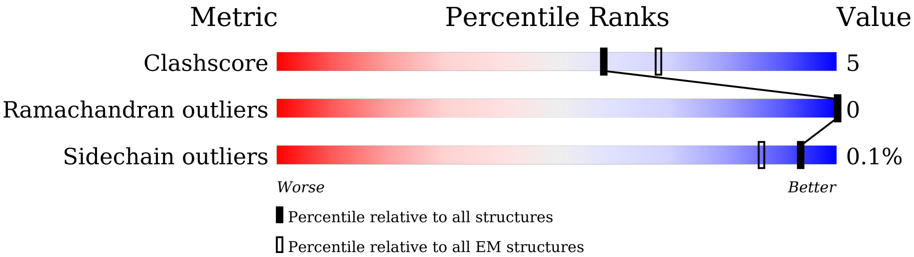
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.64 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	I	362	76% 15% 9%
1	J	362	79% 13% 8%
1	K	362	• 77% 13% • 9%
1	L	362	81% 11% 8%
1	M	362	• 82% 9% 9%
1	N	362	80% 12% 8%
2	A	474	• 84% 12% •
2	B	474	• 85% 11% •

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Mol	Chain	Length	Quality of chain
2	C	474	• 85% 11% •
3	E	1054	• 85% 13% •
3	F	1054	5% 85% 13% •
3	G	1054	• 84% 13% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 49014 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 Multidrug resistance protein MexA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	329	Total 2505	C 1565	N 448	O 490	S 2	0	0
1	J	333	Total 2538	C 1585	N 455	O 496	S 2	0	0
1	K	331	Total 2518	C 1572	N 451	O 493	S 2	0	0
1	L	334	Total 2543	C 1588	N 456	O 497	S 2	0	0
1	M	331	Total 2522	C 1575	N 452	O 493	S 2	0	0
1	N	334	Total 2542	C 1588	N 456	O 496	S 2	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	GLY	-	expression tag	UNP P52477
I	0	ALA	-	expression tag	UNP P52477
I	1	MET	-	expression tag	UNP P52477
J	-1	GLY	-	expression tag	UNP P52477
J	0	ALA	-	expression tag	UNP P52477
J	1	MET	-	expression tag	UNP P52477
K	-1	GLY	-	expression tag	UNP P52477
K	0	ALA	-	expression tag	UNP P52477
K	1	MET	-	expression tag	UNP P52477
L	-1	GLY	-	expression tag	UNP P52477
L	0	ALA	-	expression tag	UNP P52477
L	1	MET	-	expression tag	UNP P52477
M	-1	GLY	-	expression tag	UNP P52477
M	0	ALA	-	expression tag	UNP P52477
M	1	MET	-	expression tag	UNP P52477
N	-1	GLY	-	expression tag	UNP P52477
N	0	ALA	-	expression tag	UNP P52477
N	1	MET	-	expression tag	UNP P52477

- Molecule 2 is a protein called Outer membrane protein OprM.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	455	Total 3486	C 2182	N 621	O 680	S 3	0	0
2	B	455	Total 3486	C 2182	N 621	O 680	S 3	0	0
2	C	455	Total 3486	C 2182	N 621	O 680	S 3	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	HIS	-	expression tag	UNP Q51487
A	470	HIS	-	expression tag	UNP Q51487
A	471	HIS	-	expression tag	UNP Q51487
A	472	HIS	-	expression tag	UNP Q51487
A	473	HIS	-	expression tag	UNP Q51487
A	474	HIS	-	expression tag	UNP Q51487
B	469	HIS	-	expression tag	UNP Q51487
B	470	HIS	-	expression tag	UNP Q51487
B	471	HIS	-	expression tag	UNP Q51487
B	472	HIS	-	expression tag	UNP Q51487
B	473	HIS	-	expression tag	UNP Q51487
B	474	HIS	-	expression tag	UNP Q51487
C	469	HIS	-	expression tag	UNP Q51487
C	470	HIS	-	expression tag	UNP Q51487
C	471	HIS	-	expression tag	UNP Q51487
C	472	HIS	-	expression tag	UNP Q51487
C	473	HIS	-	expression tag	UNP Q51487
C	474	HIS	-	expression tag	UNP Q51487

- Molecule 3 is a protein called Multidrug resistance protein MexB.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	1024	Total 7764	C 4998	N 1289	O 1437	S 40	0	0
3	G	1030	Total 7812	C 5027	N 1298	O 1447	S 40	0	0
3	E	1030	Total 7812	C 5027	N 1298	O 1447	S 40	0	0

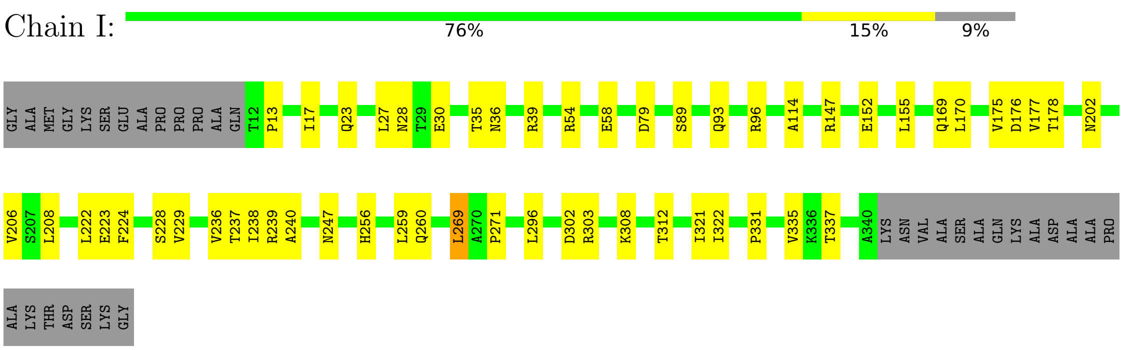
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1047	LEU	-	expression tag	UNP P52002
F	1048	GLU	-	expression tag	UNP P52002
F	1049	HIS	-	expression tag	UNP P52002
F	1050	HIS	-	expression tag	UNP P52002
F	1051	HIS	-	expression tag	UNP P52002
F	1052	HIS	-	expression tag	UNP P52002
F	1053	HIS	-	expression tag	UNP P52002
F	1054	HIS	-	expression tag	UNP P52002
G	1047	LEU	-	expression tag	UNP P52002
G	1048	GLU	-	expression tag	UNP P52002
G	1049	HIS	-	expression tag	UNP P52002
G	1050	HIS	-	expression tag	UNP P52002
G	1051	HIS	-	expression tag	UNP P52002
G	1052	HIS	-	expression tag	UNP P52002
G	1053	HIS	-	expression tag	UNP P52002
G	1054	HIS	-	expression tag	UNP P52002
E	1047	LEU	-	expression tag	UNP P52002
E	1048	GLU	-	expression tag	UNP P52002
E	1049	HIS	-	expression tag	UNP P52002
E	1050	HIS	-	expression tag	UNP P52002
E	1051	HIS	-	expression tag	UNP P52002
E	1052	HIS	-	expression tag	UNP P52002
E	1053	HIS	-	expression tag	UNP P52002
E	1054	HIS	-	expression tag	UNP P52002

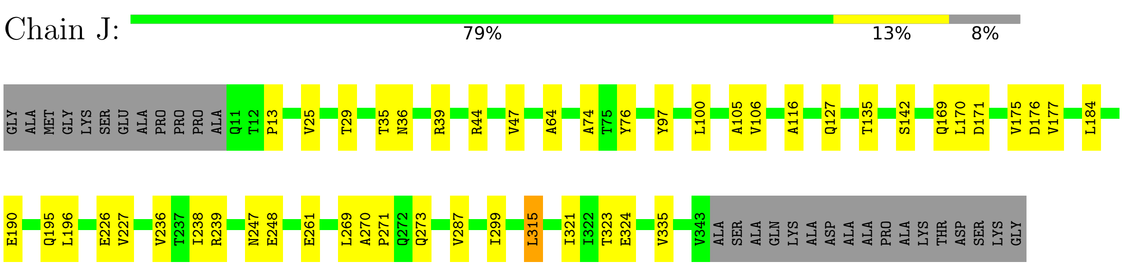
3 Residue-property plots

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.

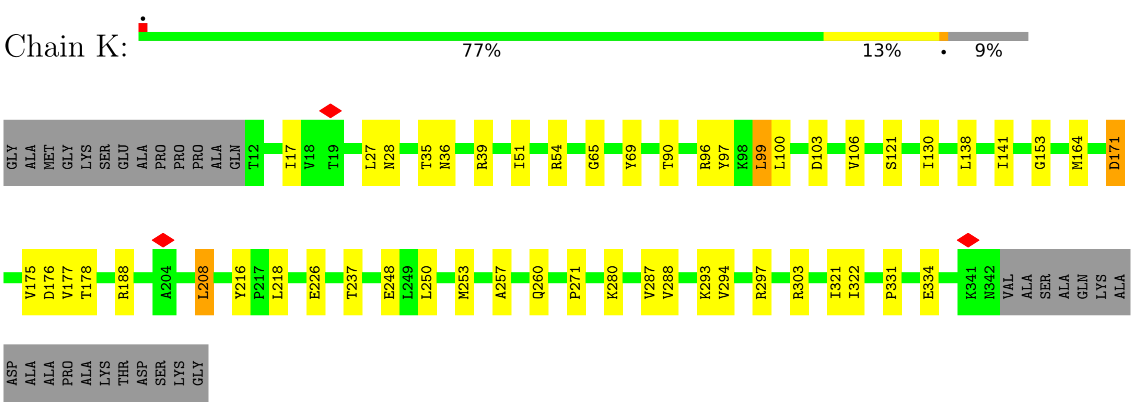
• Molecule 1: Multidrug resistance protein MexA



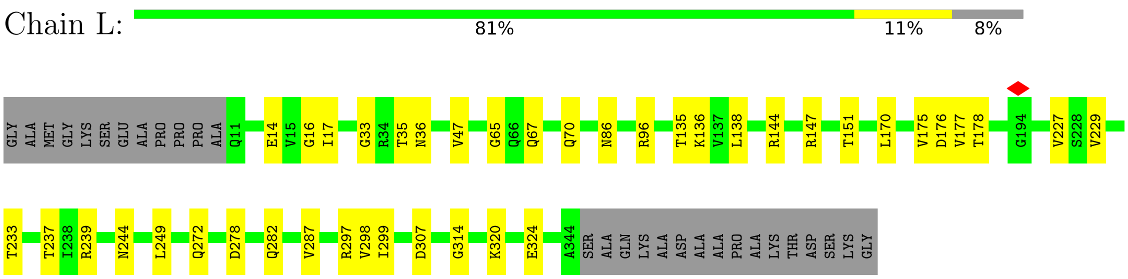
• Molecule 1: Multidrug resistance protein MexA



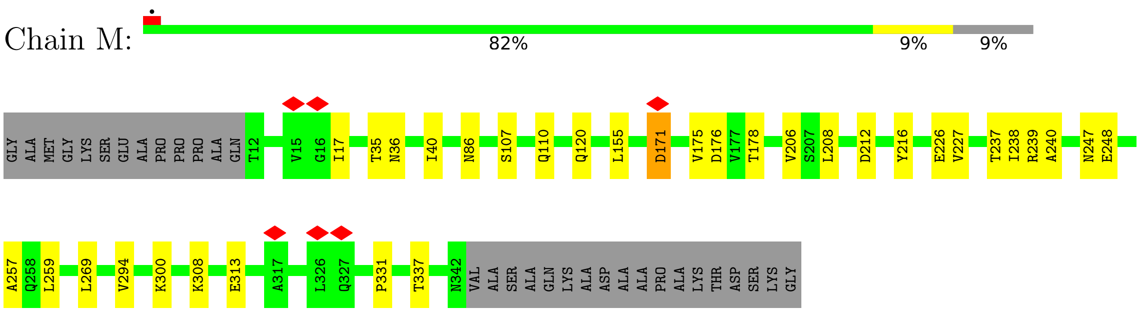
• Molecule 1: Multidrug resistance protein MexA



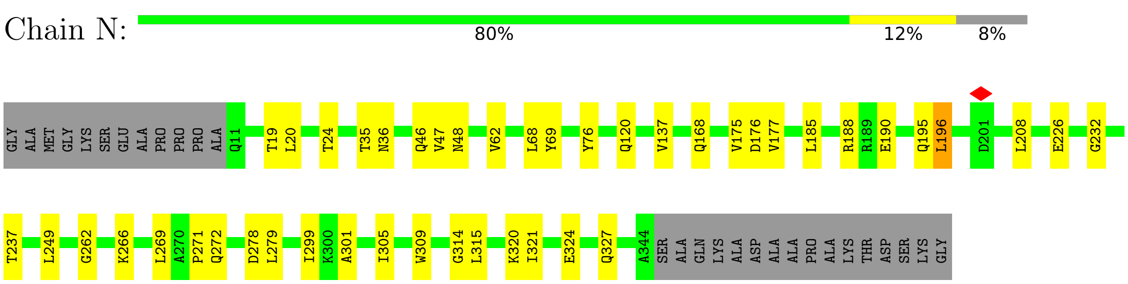
• Molecule 1: Multidrug resistance protein MexA



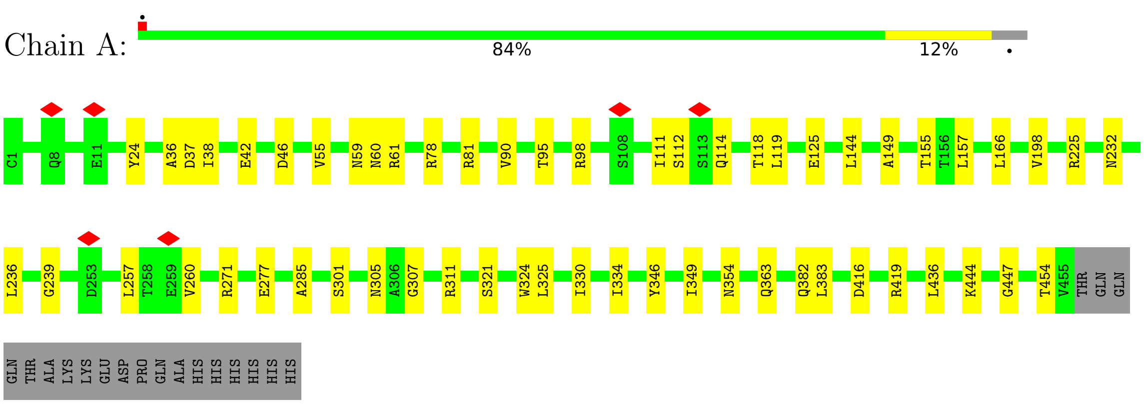
• Molecule 1: Multidrug resistance protein MexA



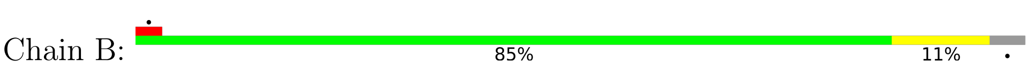
• Molecule 1: Multidrug resistance protein MexA

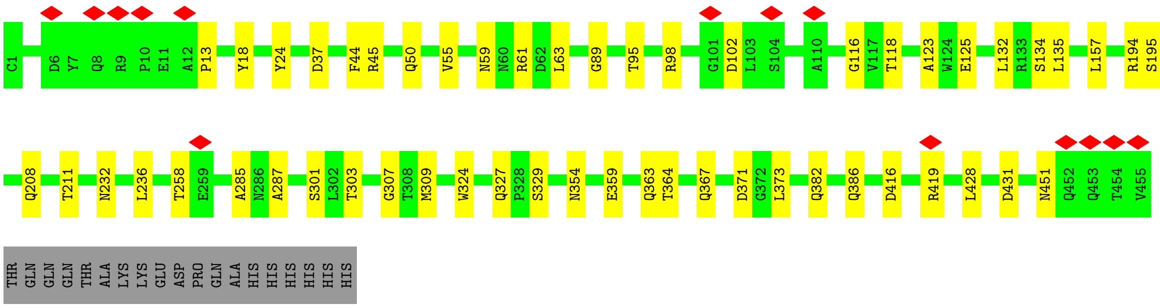


• Molecule 2: Outer membrane protein OprM



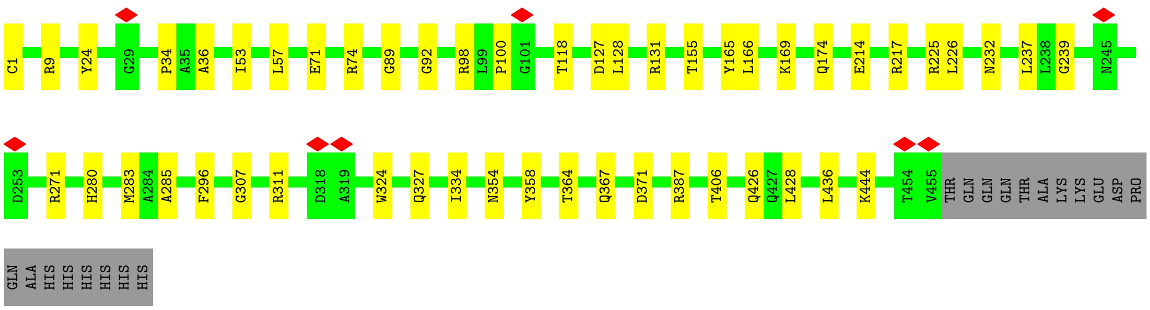
• Molecule 2: Outer membrane protein OprM





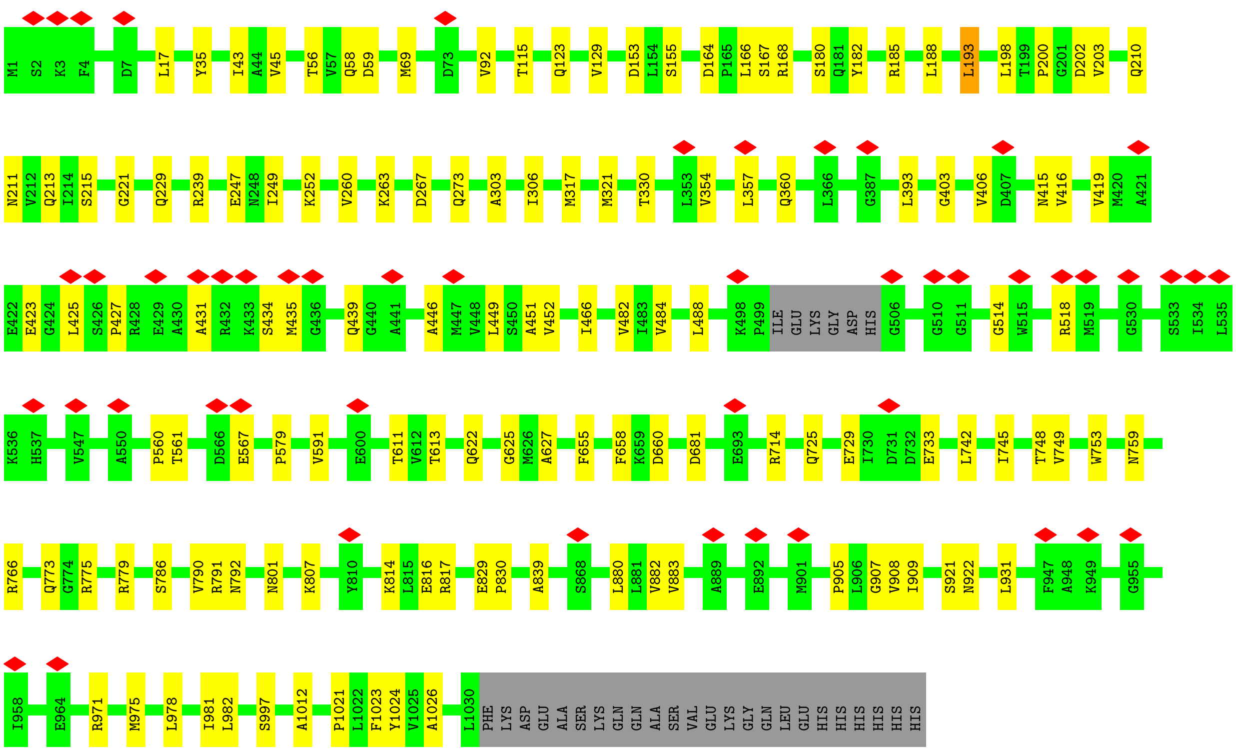
• Molecule 2: Outer membrane protein OprM

Chain C:



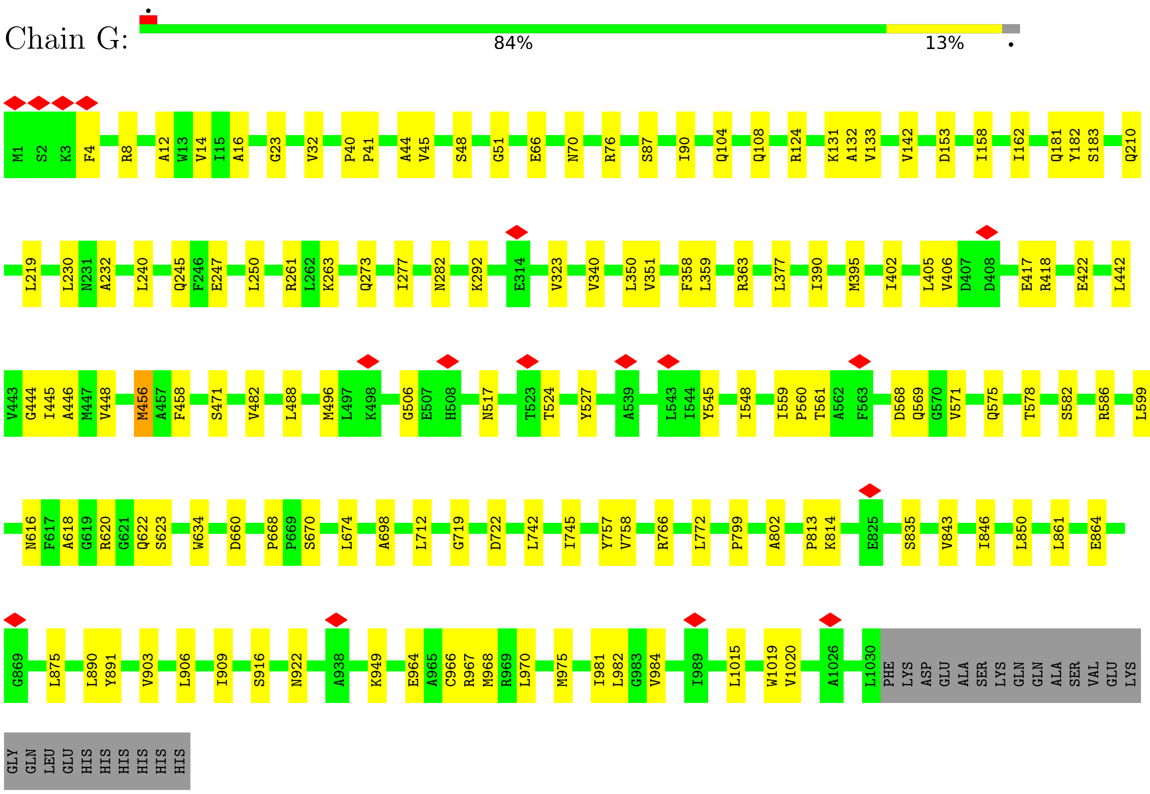
• Molecule 3: Multidrug resistance protein MexB

Chain F:



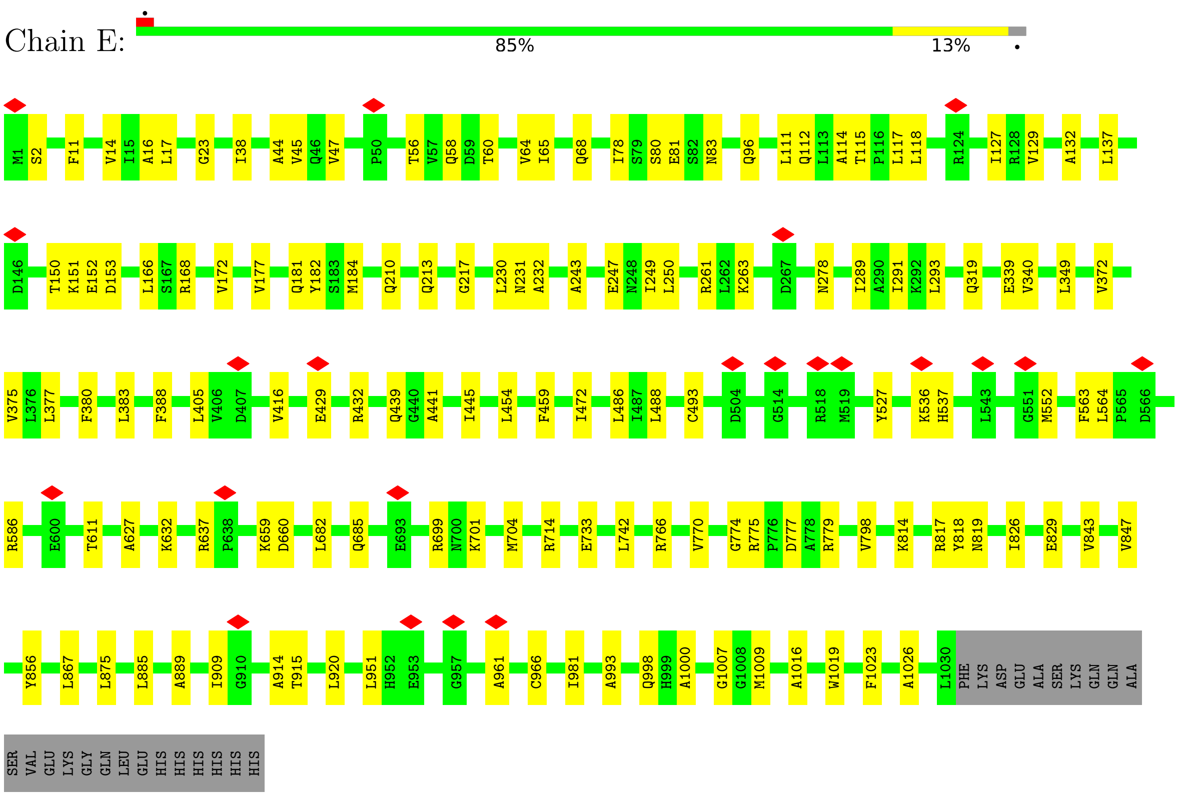
• Molecule 3: Multidrug resistance protein MexB

Chain G:



- Molecule 3: Multidrug resistance protein MexB

Chain E:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37971	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	40	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	113.052	Depositor
Minimum map value	-88.440	Depositor
Average map value	0.023	Depositor
Map value standard deviation	3.031	Depositor
Recommended contour level	6.1	Depositor
Map size (Å)	350.0, 350.0, 350.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.875, 0.875, 0.875	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	I	0.35	0/2536	0.61	2/3442 (0.1%)
1	J	0.36	0/2569	0.62	1/3486 (0.0%)
1	K	0.35	0/2549	0.61	2/3460 (0.1%)
1	L	0.35	0/2574	0.62	0/3493
1	M	0.35	0/2553	0.61	0/3464
1	N	0.35	0/2573	0.63	4/3491 (0.1%)
2	A	0.33	0/3542	0.61	1/4818 (0.0%)
2	B	0.33	0/3542	0.61	0/4818
2	C	0.33	0/3542	0.59	0/4818
3	E	0.35	0/7971	0.61	5/10833 (0.0%)
3	F	0.34	0/7921	0.61	3/10765 (0.0%)
3	G	0.34	0/7971	0.61	2/10833 (0.0%)
All	All	0.34	0/49843	0.61	20/67721 (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	J	0	1
1	K	0	1
1	M	0	1
All	All	0	3

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	454	LEU	CA-CB-CG	6.44	130.12	115.30
1	K	99	LEU	CA-CB-CG	6.26	129.70	115.30
2	A	144	LEU	CA-CB-CG	5.96	129.00	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	249	LEU	C-N-CA	5.73	136.03	121.70
1	N	249	LEU	CA-CB-CG	5.69	128.39	115.30
1	J	315	LEU	CA-CB-CG	5.61	128.21	115.30
3	F	193	LEU	CA-CB-CG	5.59	128.15	115.30
3	E	349	LEU	CA-CB-CG	5.53	128.01	115.30
3	G	772	LEU	CA-CB-CG	5.48	127.91	115.30
3	E	166	LEU	CA-CB-CG	5.45	127.83	115.30
3	F	17	LEU	CA-CB-CG	5.43	127.79	115.30
1	N	208	LEU	CA-CB-CG	5.26	127.41	115.30
3	E	867	LEU	CA-CB-CG	5.25	127.37	115.30
3	G	456	MET	CA-CB-CG	5.17	122.09	113.30
3	E	17	LEU	CA-CB-CG	5.14	127.12	115.30
3	F	59	ASP	CB-CG-OD1	5.12	122.90	118.30
1	I	208	LEU	CA-CB-CG	5.09	127.01	115.30
1	N	196	LEU	CA-CB-CG	5.08	126.98	115.30
1	K	208	LEU	CA-CB-CG	5.07	126.97	115.30
1	I	269	LEU	C-N-CA	5.03	134.27	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	171	ASP	Peptide
1	K	171	ASP	Peptide
1	M	171	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2505	0	2554	36	0
1	J	2538	0	2589	45	0
1	K	2518	0	2562	35	0
1	L	2543	0	2595	29	0
1	M	2522	0	2573	29	0
1	N	2542	0	2595	27	0
2	A	3486	0	3466	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3486	0	3466	38	0
2	C	3486	0	3466	33	0
3	E	7812	0	7944	82	0
3	F	7764	0	7899	80	0
3	G	7812	0	7944	82	0
All	All	49014	0	49653	485	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 (485) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:190:GLU:OE2	1:J:195:GLN:CG	1.83	1.27
1:J:190:GLU:OE2	1:J:195:GLN:HG3	1.02	1.18
1:J:170:LEU:HD11	1:J:247:ASN:ND2	1.82	0.94
1:J:190:GLU:CD	1:J:195:GLN:HG3	1.92	0.89
1:M:238:ILE:HG22	1:M:239:ARG:H	1.39	0.85
2:B:18:TYR:CD2	2:B:373:LEU:HD11	2.11	0.85
1:M:238:ILE:HG22	1:M:239:ARG:N	1.94	0.80
1:J:238:ILE:HG22	1:J:239:ARG:N	1.98	0.78
3:F:971:ARG:O	3:F:975:MET:HB2	1.91	0.70
1:J:170:LEU:HD11	1:J:247:ASN:HD22	1.58	0.69
1:J:47:VAL:HG11	1:J:135:THR:HG22	1.75	0.67
1:J:238:ILE:CG2	1:J:239:ARG:N	2.58	0.66
1:N:271:PRO:HD2	1:N:321:ILE:HD11	1.77	0.66
1:M:35:THR:HG22	1:M:175:VAL:HG22	1.78	0.65
3:E:429:GLU:HA	3:E:432:ARG:HG2	1.79	0.65
2:C:71:GLU:OE1	2:C:74:ARG:NH2	2.30	0.65
1:J:190:GLU:OE2	1:J:195:GLN:CD	2.28	0.65
1:J:190:GLU:CD	1:J:195:GLN:CG	2.48	0.65
3:G:340:VAL:HG21	3:G:395:MET:HB3	1.77	0.65
1:I:178:THR:HG22	1:I:237:THR:HG22	1.80	0.64
3:F:180:SER:HB2	3:F:273:GLN:HG2	1.80	0.64
3:G:418:ARG:NH1	3:G:968:MET:SD	2.71	0.64
2:A:382:GLN:OE1	2:C:225:ARG:NH2	2.30	0.63
1:J:36:ASN:ND2	1:J:176:ASP:OD2	2.31	0.63
3:G:23:GLY:HA3	3:G:377:LEU:HB3	1.79	0.63
3:G:351:VAL:HG21	3:G:406:VAL:HG21	1.81	0.63
1:K:271:PRO:HD2	1:K:321:ILE:HD11	1.81	0.63
2:B:285:ALA:HB2	2:B:354:ASN:HD22	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:58:GLN:HE21	3:E:817:ARG:HD2	1.63	0.63
1:J:13:PRO:HG2	1:J:335:VAL:HG12	1.81	0.63
1:K:216:TYR:CE2	1:K:218:LEU:HB2	2.34	0.63
2:B:123:ALA:H	2:B:303:THR:HG22	1.63	0.63
1:L:47:VAL:HG11	1:L:135:THR:HG22	1.81	0.63
1:M:216:TYR:CE1	1:M:248:GLU:OE1	2.52	0.62
1:J:238:ILE:CG2	1:J:239:ARG:H	2.11	0.62
1:J:35:THR:HG22	1:J:175:VAL:HG22	1.80	0.62
1:J:170:LEU:HD11	1:J:247:ASN:HD21	1.61	0.62
2:B:18:TYR:CD2	2:B:373:LEU:CD1	2.81	0.62
1:I:36:ASN:ND2	1:I:176:ASP:OD2	2.32	0.61
1:K:216:TYR:HE1	1:K:248:GLU:OE1	1.82	0.61
1:M:238:ILE:CG2	1:M:239:ARG:H	2.10	0.61
2:B:301:SER:HG	2:B:329:SER:HG	1.48	0.61
2:B:95:THR:HG22	2:C:327:GLN:HG2	1.82	0.61
3:G:240:LEU:HD12	3:G:245:GLN:HB3	1.81	0.60
3:E:23:GLY:HA3	3:E:377:LEU:HB3	1.83	0.60
3:E:527:TYR:OH	3:E:966:CYS:SG	2.59	0.60
1:I:202:ASN:O	1:I:260:GLN:NE2	2.33	0.60
1:N:24:THR:HG22	1:N:266:LYS:H	1.67	0.60
2:A:225:ARG:NH1	2:B:382:GLN:OE1	2.34	0.60
1:I:96:ARG:HG3	2:A:198:VAL:HG12	1.83	0.60
2:A:257:LEU:HD23	2:A:436:LEU:HD22	1.84	0.60
2:A:95:THR:OG1	2:A:114:GLN:NE2	2.34	0.60
3:G:445:ILE:HA	3:G:448:VAL:HG12	1.83	0.59
1:I:155:LEU:HD23	1:J:44:ARG:HE	1.67	0.59
1:K:36:ASN:ND2	1:K:176:ASP:OD2	2.34	0.59
3:F:198:LEU:HA	3:F:791:ARG:HH21	1.67	0.59
3:E:181:GLN:OE1	3:E:766:ARG:NH1	2.35	0.59
1:I:271:PRO:HD2	1:I:321:ILE:HD11	1.83	0.59
2:A:305:ASN:HB2	2:A:325:LEU:HB3	1.84	0.59
2:A:416:ASP:OD1	2:A:419:ARG:NH2	2.36	0.59
1:M:155:LEU:HD11	1:N:46:GLN:HB2	1.85	0.59
1:N:36:ASN:ND2	1:N:176:ASP:OD2	2.37	0.58
1:N:299:ILE:HG21	1:N:315:LEU:HG	1.85	0.58
1:M:238:ILE:CG2	1:M:239:ARG:N	2.65	0.58
3:F:185:ARG:NH2	3:F:773:GLN:OE1	2.35	0.58
3:E:340:VAL:HG22	3:E:998:GLN:HE21	1.68	0.58
1:L:299:ILE:HG22	1:L:314:GLY:HA3	1.86	0.58
1:M:36:ASN:ND2	1:M:176:ASP:OD2	2.35	0.58
1:J:170:LEU:HD12	1:J:170:LEU:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:104:GLN:OE1	3:G:131:LYS:NZ	2.37	0.58
2:B:37:ASP:HA	2:B:451:ASN:HD21	1.68	0.57
3:F:210:GLN:HG3	3:F:249:ILE:HG23	1.85	0.57
3:F:561:THR:HA	3:F:922:ASN:HB3	1.86	0.57
2:A:149:ALA:HB2	2:A:277:GLU:HG3	1.86	0.57
3:F:168:ARG:NH2	3:G:66:GLU:O	2.38	0.57
3:G:261:ARG:NH2	3:E:733:GLU:OE2	2.36	0.57
1:K:103:ASP:OD2	2:B:194:ARG:NH1	2.38	0.57
2:C:9:ARG:NH2	2:C:358:TYR:OH	2.37	0.57
2:C:214:GLU:OE2	2:C:217:ARG:NH2	2.35	0.57
2:C:367:GLN:NE2	2:C:371:ASP:OD2	2.38	0.57
3:E:699:ARG:HG3	3:E:826:ILE:HD11	1.86	0.57
3:E:184:MET:HB3	3:E:770:VAL:HG12	1.86	0.56
1:J:287:VAL:HG22	1:J:321:ILE:HG22	1.87	0.56
3:G:158:ILE:HA	3:G:162:ILE:HG12	1.88	0.56
3:G:418:ARG:NH2	3:G:422:GLU:OE2	2.38	0.56
3:F:742:LEU:HD23	3:F:745:ILE:HD12	1.87	0.56
3:E:16:ALA:HB2	3:E:488:LEU:HD22	1.85	0.56
3:E:774:GLY:O	3:E:779:ARG:NH1	2.39	0.56
1:N:19:THR:HG22	1:N:320:LYS:HG2	1.86	0.56
1:L:35:THR:HG22	1:L:175:VAL:HG22	1.87	0.56
3:F:221:GLY:HA2	3:G:622:GLN:HE22	1.70	0.56
3:F:814:LYS:NZ	3:F:816:GLU:OE2	2.38	0.56
1:N:232:GLY:O	3:F:792:ASN:ND2	2.39	0.56
3:F:423:GLU:HB3	3:F:425:LEU:HD13	1.87	0.56
3:G:14:VAL:HG11	3:E:889:ALA:HB2	1.88	0.56
3:F:714:ARG:NE	3:F:829:GLU:OE2	2.39	0.56
1:L:178:THR:HG22	1:L:237:THR:HG22	1.87	0.56
3:G:569:GLN:NE2	3:G:670:SER:O	2.38	0.56
2:A:285:ALA:HB2	2:A:354:ASN:HD22	1.72	0.55
1:I:35:THR:HG22	1:I:175:VAL:HG22	1.87	0.55
1:M:17:ILE:HD13	1:M:337:THR:HB	1.88	0.55
2:B:44:PHE:O	2:B:50:GLN:NE2	2.38	0.55
3:G:843:VAL:HA	3:G:846:ILE:HG22	1.89	0.55
3:E:111:LEU:HD11	3:E:127:ILE:HD11	1.89	0.55
3:E:247:GLU:HG3	3:E:263:LYS:HG2	1.88	0.55
3:G:456:MET:SD	3:G:471:SER:OG	2.64	0.55
1:J:238:ILE:HG22	1:J:239:ARG:H	1.66	0.55
1:N:35:THR:HG22	1:N:175:VAL:HG22	1.89	0.55
3:E:632:LYS:O	3:E:637:ARG:NH1	2.37	0.55
2:B:367:GLN:NE2	2:B:371:ASP:OD2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:167:SER:OG	3:G:70:ASN:ND2	2.40	0.55
3:F:213:GLN:HB2	3:F:239:ARG:HG3	1.88	0.55
2:A:61:ARG:NH2	2:B:359:GLU:OE2	2.40	0.54
2:B:134:SER:OG	2:B:287:ALA:O	2.25	0.54
3:G:181:GLN:OE1	3:G:766:ARG:NH1	2.41	0.54
1:L:272:GLN:HG2	3:G:230:LEU:HB3	1.89	0.54
1:N:324:GLU:HB2	3:F:660:ASP:HA	1.88	0.54
2:A:349:ILE:HD11	2:C:71:GLU:HG3	1.90	0.54
3:G:4:PHE:HA	3:G:8:ARG:HH11	1.72	0.54
1:J:324:GLU:HG2	3:G:660:ASP:HB3	1.89	0.54
1:M:178:THR:HG22	1:M:237:THR:HG22	1.90	0.54
1:L:282:GLN:HE21	1:L:298:VAL:HG11	1.73	0.54
3:F:446:ALA:HB2	3:F:482:VAL:HG21	1.89	0.54
3:F:775:ARG:O	3:F:779:ARG:NH1	2.41	0.54
3:G:282:ASN:HD22	3:G:599:LEU:HD11	1.72	0.54
1:L:36:ASN:ND2	1:L:176:ASP:OD2	2.32	0.54
2:B:55:VAL:HG13	2:B:59:ASN:HD22	1.73	0.54
3:E:45:VAL:HG22	3:E:129:VAL:HG22	1.90	0.54
3:E:685:GLN:HE21	3:E:818:TYR:HD2	1.55	0.54
2:A:37:ASP:OD1	2:A:271:ARG:NH2	2.41	0.53
3:E:775:ARG:NH2	3:E:777:ASP:OD2	2.41	0.53
1:L:67:GLN:HG3	1:L:136:LYS:HB2	1.89	0.53
1:I:17:ILE:HG12	1:I:322:ILE:HG13	1.90	0.53
1:J:97:TYR:HE1	1:J:106:VAL:HG21	1.74	0.53
3:E:80:SER:OG	3:E:81:GLU:N	2.41	0.53
1:I:152:GLU:OE2	1:J:39:ARG:NH1	2.41	0.53
2:C:387:ARG:HE	2:C:428:LEU:HD21	1.74	0.53
1:I:30:GLU:OE2	1:I:256:HIS:ND1	2.41	0.53
1:I:152:GLU:HG2	1:J:39:ARG:HD2	1.91	0.53
3:G:618:ALA:O	3:G:814:LYS:NZ	2.38	0.53
3:F:58:GLN:HE21	3:F:817:ARG:HD2	1.73	0.53
2:C:34:PRO:HG2	2:C:271:ARG:HH21	1.74	0.53
3:G:124:ARG:NH2	3:G:758:VAL:O	2.41	0.53
1:K:208:LEU:HA	1:K:257:ALA:HA	1.91	0.52
3:E:151:LYS:HD3	3:E:278:ASN:HB2	1.91	0.52
3:E:951:LEU:HB3	3:E:961:ALA:HB1	1.91	0.52
2:B:63:LEU:HG	2:B:157:LEU:HD13	1.89	0.52
3:G:524:THR:HG22	3:G:970:LEU:HD23	1.91	0.52
3:G:719:GLY:HA2	3:G:814:LYS:HD3	1.91	0.52
3:E:1016:ALA:HA	3:E:1019:TRP:HB2	1.90	0.52
1:J:97:TYR:HD1	1:J:106:VAL:HG11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:170:LEU:CD1	1:J:247:ASN:HD22	2.22	0.52
3:G:571:VAL:HG23	3:G:668:PRO:HG3	1.92	0.52
1:J:74:ALA:HB1	1:K:130:ILE:HD13	1.92	0.52
3:G:76:ARG:NH1	3:G:864:GLU:OE2	2.42	0.52
3:G:799:PRO:HG2	3:G:802:ALA:HB2	1.91	0.52
2:A:363:GLN:NE2	2:C:239:GLY:O	2.43	0.52
3:E:177:VAL:HG22	3:E:289:ILE:HG22	1.92	0.52
1:L:86:ASN:OD1	1:M:120:GLN:NE2	2.43	0.51
2:A:324:TRP:H	2:C:98:ARG:HB3	1.75	0.51
3:F:567:GLU:OE2	3:F:997:SER:OG	2.27	0.51
1:N:190:GLU:OE1	1:N:195:GLN:NE2	2.43	0.51
2:A:98:ARG:HB3	2:B:324:TRP:HB3	1.91	0.51
1:L:324:GLU:HG3	3:E:660:ASP:HB2	1.92	0.51
1:M:206:VAL:HG12	1:M:259:LEU:HA	1.91	0.51
2:A:334:ILE:H	2:C:89:GLY:HA2	1.75	0.51
3:F:215:SER:OG	3:G:51:GLY:O	2.25	0.51
2:B:125:GLU:HA	2:B:301:SER:HA	1.92	0.51
1:K:178:THR:HG22	1:K:237:THR:HG22	1.93	0.51
1:L:96:ARG:HG3	2:C:406:THR:HG22	1.93	0.51
1:L:278:ASP:HB2	1:L:282:GLN:HB3	1.91	0.51
2:C:36:ALA:HB3	2:C:271:ARG:HD2	1.93	0.51
3:F:69:MET:O	3:E:168:ARG:NH1	2.44	0.51
3:G:981:ILE:HA	3:G:984:VAL:HG12	1.93	0.51
1:L:176:ASP:OD1	1:L:239:ARG:NE	2.44	0.51
3:F:357:LEU:O	3:F:360:GLN:NE2	2.44	0.51
1:I:27:LEU:HD22	1:I:303:ARG:HH11	1.74	0.51
1:K:216:TYR:CE1	1:K:248:GLU:OE1	2.63	0.51
1:I:93:GLN:HB3	1:I:114:ALA:HB1	1.93	0.50
2:C:166:LEU:HD13	2:C:436:LEU:HB3	1.93	0.50
3:F:449:LEU:HA	3:F:452:VAL:HG12	1.93	0.50
3:E:38:ILE:O	3:E:96:GLN:NE2	2.44	0.50
1:K:35:THR:HG22	1:K:175:VAL:HG22	1.92	0.50
2:A:90:VAL:HA	2:A:119:LEU:HA	1.94	0.50
3:E:83:ASN:OD1	3:E:814:LYS:NZ	2.40	0.50
3:E:243:ALA:O	3:E:247:GLU:HB2	2.10	0.50
3:E:714:ARG:NH2	3:E:829:GLU:OE1	2.44	0.50
3:E:915:THR:HG23	3:E:920:LEU:HB2	1.94	0.50
2:A:112:SER:OG	2:A:311:ARG:NH1	2.45	0.50
3:G:350:LEU:HD13	3:G:982:LEU:HB3	1.94	0.50
3:G:506:GLY:O	3:G:517:ASN:ND2	2.43	0.50
3:E:372:VAL:HG12	3:E:405:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:17:ILE:HD12	1:I:337:THR:HA	1.93	0.50
2:A:42:GLU:OE1	2:A:454:THR:OG1	2.28	0.50
3:F:415:ASN:ND2	3:F:434:SER:OG	2.44	0.50
3:F:451:ALA:HB1	3:F:882:VAL:HG13	1.93	0.50
1:K:177:VAL:HG11	1:K:257:ALA:HB3	1.93	0.50
1:M:269:LEU:HB3	1:M:308:LYS:HD3	1.93	0.50
1:N:299:ILE:HG22	1:N:314:GLY:HA3	1.94	0.50
2:A:59:ASN:O	2:A:61:ARG:NH1	2.44	0.50
3:F:1021:PRO:HA	3:F:1024:TYR:HB3	1.93	0.50
3:G:44:ALA:HB2	3:G:132:ALA:HB2	1.94	0.50
3:G:891:TYR:O	3:G:949:LYS:NZ	2.38	0.50
1:I:296:LEU:HD23	1:I:331:PRO:HG3	1.94	0.49
3:F:753:TRP:HB3	3:E:217:GLY:HA3	1.94	0.49
1:I:228:SER:HB2	1:N:168:GLN:HE22	1.76	0.49
1:K:69:TYR:HE2	1:K:164:MET:HB3	1.77	0.49
3:F:164:ASP:OD2	3:F:766:ARG:NH1	2.45	0.49
3:F:427:PRO:O	3:F:431:ALA:CB	2.60	0.49
3:F:155:SER:OG	3:F:180:SER:N	2.44	0.49
3:F:611:THR:HA	3:F:627:ALA:HA	1.93	0.49
3:G:742:LEU:HD23	3:G:745:ILE:HD12	1.94	0.49
3:E:586:ARG:NH2	3:E:660:ASP:OD1	2.44	0.49
3:F:153:ASP:OD1	3:F:182:TYR:OH	2.24	0.49
3:G:722:ASP:HA	3:G:813:PRO:HD3	1.95	0.49
1:I:147:ARG:NH1	1:J:226:GLU:OE2	2.41	0.49
1:L:287:VAL:HG21	1:L:297:ARG:HE	1.78	0.49
2:A:98:ARG:HD3	2:A:111:ILE:HG13	1.94	0.49
1:J:100:LEU:HD12	1:J:105:ALA:HB3	1.94	0.49
3:F:393:LEU:HD21	3:F:466:ILE:HG23	1.94	0.49
1:K:250:LEU:HD12	1:L:227:VAL:HA	1.95	0.49
3:G:674:LEU:HD23	3:G:861:LEU:HD21	1.95	0.49
1:M:216:TYR:HE1	1:M:248:GLU:OE1	1.94	0.48
3:G:964:GLU:OE2	3:G:967:ARG:NH2	2.44	0.48
1:I:79:ASP:OD1	1:J:127:GLN:NE2	2.45	0.48
1:K:97:TYR:HE1	1:K:106:VAL:HG21	1.79	0.48
3:F:435:MET:O	3:F:439:GLN:HB2	2.14	0.48
3:G:277:ILE:HD11	3:G:620:ARG:HH21	1.78	0.48
1:K:54:ARG:HG3	1:K:69:TYR:HE1	1.78	0.48
1:N:69:TYR:HB2	1:N:137:VAL:HG12	1.96	0.48
3:G:183:SER:OG	3:G:273:GLN:NE2	2.47	0.48
3:E:81:GLU:OE2	3:E:814:LYS:NZ	2.46	0.48
1:N:196:LEU:HD13	1:N:262:GLY:HA3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:53:ILE:O	2:C:57:LEU:HB2	2.13	0.48
2:C:285:ALA:HB2	2:C:354:ASN:HD22	1.78	0.48
1:I:176:ASP:OD1	1:I:239:ARG:NE	2.38	0.48
3:F:202:ASP:OD2	3:F:791:ARG:NH2	2.47	0.48
3:F:613:THR:HA	3:F:625:GLY:HA2	1.95	0.48
3:G:545:TYR:HB2	3:G:1019:TRP:HZ3	1.78	0.48
3:F:880:LEU:HA	3:F:883:VAL:HG12	1.96	0.48
3:G:578:THR:OG1	3:G:623:SER:O	2.26	0.48
3:E:1023:PHE:HA	3:E:1026:ALA:HB3	1.96	0.48
2:B:232:ASN:ND2	2:C:24:TYR:OH	2.43	0.48
3:F:211:ASN:O	3:F:759:ASN:ND2	2.47	0.48
3:F:830:PRO:HB3	3:F:839:ALA:HB2	1.95	0.48
3:E:682:LEU:HD11	3:E:856:TYR:HB2	1.96	0.48
2:A:232:ASN:ND2	2:B:24:TYR:OH	2.44	0.47
2:B:416:ASP:OD1	2:B:419:ARG:NH1	2.45	0.47
3:G:559:ILE:HD11	3:G:916:SER:HB2	1.96	0.47
3:G:712:LEU:HD21	3:G:843:VAL:HG22	1.96	0.47
3:E:701:LYS:HA	3:E:704:MET:HG2	1.96	0.47
1:K:293:LYS:HB3	1:K:334:GLU:HG3	1.97	0.47
1:M:86:ASN:HB2	1:N:120:GLN:HE21	1.79	0.47
2:B:102:ASP:OD1	2:C:311:ARG:NH1	2.48	0.47
3:G:16:ALA:HB2	3:G:488:LEU:HD22	1.96	0.47
1:L:16:GLY:HA3	1:L:324:GLU:HB3	1.96	0.47
2:A:38:ILE:HD11	2:A:260:VAL:HG22	1.97	0.47
2:A:60:ASN:HD22	2:A:157:LEU:HD21	1.79	0.47
2:C:118:THR:HA	2:C:307:GLY:HA3	1.94	0.47
3:G:446:ALA:HB2	3:G:482:VAL:HG21	1.96	0.47
1:I:177:VAL:O	1:I:238:ILE:N	2.43	0.47
1:K:171:ASP:OD1	1:K:171:ASP:N	2.43	0.47
3:E:153:ASP:OD1	3:E:182:TYR:OH	2.27	0.47
1:J:47:VAL:HG13	1:J:76:TYR:HE2	1.80	0.47
1:J:184:LEU:HD22	1:J:236:VAL:HG21	1.97	0.47
1:M:300:LYS:HE2	1:M:313:GLU:HB3	1.97	0.47
2:A:36:ALA:HB2	2:A:447:GLY:HA3	1.97	0.47
3:F:166:LEU:HD11	3:F:306:ILE:HG23	1.96	0.47
3:G:363:ARG:HB3	3:G:496:MET:HG2	1.97	0.47
3:E:552:MET:HB3	3:E:909:ILE:HB	1.97	0.47
3:E:981:ILE:HD11	3:E:1009:MET:HB3	1.96	0.47
1:I:206:VAL:HG12	1:I:259:LEU:HA	1.97	0.47
1:I:302:ASP:OD2	1:I:312:THR:OG1	2.32	0.47
1:K:97:TYR:HD1	1:K:106:VAL:HG11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:331:PRO:HD2	3:E:319:GLN:HG3	1.97	0.47
3:F:905:PRO:HA	3:F:908:VAL:HG22	1.97	0.47
3:G:358:PHE:HD2	3:G:975:MET:HG2	1.79	0.47
2:A:95:THR:HG22	2:B:327:GLN:HE22	1.80	0.47
2:B:382:GLN:NE2	2:B:431:ASP:OD1	2.47	0.47
3:G:561:THR:HA	3:G:922:ASN:HB3	1.97	0.47
3:G:32:VAL:HG22	3:G:390:ILE:HB	1.96	0.47
1:K:253:MET:HB3	1:L:229:VAL:HG11	1.97	0.46
3:F:435:MET:O	3:F:439:GLN:CB	2.63	0.46
1:K:216:TYR:HE2	1:K:218:LEU:HB2	1.78	0.46
1:M:294:VAL:HG13	1:M:331:PRO:HA	1.98	0.46
2:B:116:GLY:HA3	2:B:309:MET:HG3	1.96	0.46
3:G:548:ILE:HG13	3:G:909:ILE:HG21	1.97	0.46
1:L:147:ARG:HD2	1:M:239:ARG:HH21	1.80	0.46
1:M:171:ASP:OD1	1:M:171:ASP:N	2.38	0.46
3:F:247:GLU:HB3	3:F:263:LYS:HE2	1.96	0.46
3:G:124:ARG:NH2	3:G:757:TYR:O	2.48	0.46
1:J:170:LEU:HD12	1:J:170:LEU:C	2.35	0.46
3:E:250:LEU:HB3	3:E:261:ARG:HD3	1.96	0.46
3:E:439:GLN:HE22	3:E:486:LEU:HD22	1.80	0.46
1:I:238:ILE:HG21	1:I:259:LEU:HD21	1.97	0.46
2:A:78:ARG:HG3	2:A:81:ARG:HH11	1.79	0.46
3:G:48:SER:HA	3:G:87:SER:HA	1.98	0.46
1:I:271:PRO:HA	1:I:308:LYS:HG2	1.98	0.46
2:A:118:THR:HA	2:A:307:GLY:HA3	1.96	0.46
1:K:294:VAL:HG13	1:K:331:PRO:HA	1.98	0.46
3:F:427:PRO:O	3:F:431:ALA:HB2	2.16	0.46
1:J:29:THR:OG1	1:J:261:GLU:OE2	2.33	0.46
1:M:208:LEU:HA	1:M:257:ALA:HA	1.98	0.46
3:F:317:MET:HB3	3:F:321:MET:HB3	1.97	0.46
1:J:273:GLN:HE21	3:F:229:GLN:HE21	1.64	0.45
3:F:193:LEU:HD11	3:F:200:PRO:HD3	1.98	0.45
3:F:725:GLN:HA	3:E:232:ALA:HB1	1.98	0.45
3:G:903:VAL:HG21	3:G:1020:VAL:HG22	1.97	0.45
3:G:219:LEU:HD12	3:G:232:ALA:HB3	1.98	0.45
3:E:380:PHE:HA	3:E:383:LEU:HD12	1.98	0.45
1:L:14:GLU:HG2	3:E:659:LYS:HD3	1.99	0.45
2:B:59:ASN:O	2:B:61:ARG:NH1	2.50	0.45
3:F:729:GLU:OE1	3:F:807:LYS:NZ	2.40	0.45
3:G:142:VAL:HG22	3:G:323:VAL:HG22	1.98	0.45
3:G:527:TYR:HE2	3:G:966:CYS:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:155:THR:HG22	2:C:444:LYS:HG2	1.99	0.45
1:L:151:THR:OG1	1:M:40:ILE:O	2.32	0.45
3:F:43:ILE:HG23	3:F:92:VAL:HB	1.99	0.45
3:E:137:LEU:HD13	3:E:293:LEU:HD23	1.99	0.45
1:J:273:GLN:HB2	1:J:323:THR:HG23	1.99	0.45
1:K:27:LEU:HD22	1:K:303:ARG:HH11	1.82	0.45
1:L:244:ASN:HD22	1:L:249:LEU:HB2	1.82	0.45
2:B:13:PRO:HG3	2:B:359:GLU:HG3	1.99	0.45
2:C:174:GLN:HE22	2:C:426:GLN:HG3	1.82	0.45
1:I:23:GLN:HE21	1:I:269:LEU:HD13	1.81	0.45
1:I:54:ARG:NE	1:I:58:GLU:OE2	2.50	0.45
1:K:90:THR:HG21	1:K:121:SER:HB3	1.99	0.45
2:C:1:CYS:N	2:C:128:LEU:O	2.44	0.45
2:A:236:LEU:HD11	2:B:364:THR:HG22	1.99	0.44
3:F:211:ASN:HB3	3:F:759:ASN:HD21	1.81	0.44
3:F:733:GLU:OE1	3:E:261:ARG:NH2	2.49	0.44
3:E:843:VAL:O	3:E:847:VAL:HB	2.17	0.44
1:M:226:GLU:OE1	1:M:237:THR:OG1	2.35	0.44
2:A:155:THR:HG22	2:A:444:LYS:HG2	1.99	0.44
2:B:208:GLN:HA	2:B:211:THR:HG22	2.00	0.44
1:K:226:GLU:OE1	1:K:237:THR:OG1	2.36	0.44
1:L:65:GLY:HA2	1:L:138:LEU:HD23	1.99	0.44
1:M:107:SER:HB2	1:M:110:GLN:H	1.81	0.44
2:B:98:ARG:HB3	2:C:324:TRP:H	1.82	0.44
3:E:64:VAL:HG21	3:E:117:LEU:HB2	2.00	0.44
3:G:402:ILE:HD13	3:G:405:LEU:HD12	2.00	0.44
2:A:239:GLY:O	2:B:363:GLN:NE2	2.51	0.44
3:F:35:TYR:OH	3:F:567:GLU:OE2	2.35	0.44
3:F:749:VAL:HG22	3:F:753:TRP:HZ3	1.82	0.44
1:J:39:ARG:NH2	1:J:169:GLN:OE1	2.51	0.44
3:E:65:ILE:HD11	3:E:118:LEU:HD11	2.00	0.44
3:E:339:GLU:OE1	3:E:993:ALA:N	2.50	0.44
1:L:272:GLN:NE2	1:L:307:ASP:O	2.41	0.44
1:N:301:ALA:HB1	1:N:309:TRP:HB3	2.00	0.44
3:G:40:PRO:HA	3:G:41:PRO:HD3	1.89	0.44
1:N:62:VAL:HG21	1:N:68:LEU:HD21	2.00	0.43
2:A:90:VAL:HG12	2:A:119:LEU:HB3	2.00	0.43
2:C:127:ASP:OD2	2:C:131:ARG:N	2.45	0.43
3:F:748:THR:HG21	3:F:790:VAL:HG22	1.99	0.43
3:F:1023:PHE:HA	3:F:1026:ALA:HB3	1.99	0.43
3:E:78:ILE:HG23	3:E:819:ASN:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:914:ALA:HB2	3:E:1007:GLY:HA3	1.98	0.43
1:I:247:ASN:HD21	1:J:227:VAL:HG23	1.83	0.43
1:J:299:ILE:HG21	1:J:315:LEU:HD23	1.99	0.43
1:K:28:ASN:HD22	1:K:260:GLN:HB3	1.83	0.43
1:L:233:THR:HA	3:E:798:VAL:HG12	1.99	0.43
2:B:45:ARG:NH1	2:B:258:THR:OG1	2.50	0.43
3:F:303:ALA:HB2	3:F:330:THR:HG21	2.00	0.43
3:G:45:VAL:HB	3:G:90:ILE:HB	2.00	0.43
3:G:250:LEU:HA	3:G:261:ARG:HA	2.00	0.43
3:F:909:ILE:HD13	3:F:909:ILE:HA	1.92	0.43
3:G:108:GLN:HG3	3:E:112:GLN:HG3	1.99	0.43
3:G:446:ALA:HB2	3:G:482:VAL:HG11	2.00	0.43
1:K:65:GLY:HA2	1:K:138:LEU:HD23	2.01	0.43
1:L:17:ILE:HG12	1:L:320:LYS:HD3	2.01	0.43
1:N:175:VAL:HG12	1:N:177:VAL:HG23	2.01	0.43
3:G:458:PHE:HB2	3:G:875:LEU:HD21	2.00	0.43
1:J:248:GLU:HG2	1:K:188:ARG:HH22	1.84	0.43
3:G:247:GLU:HG2	3:G:263:LYS:HG2	1.99	0.43
1:J:25:VAL:HG11	1:J:269:LEU:HD11	2.00	0.43
1:K:280:LYS:HA	3:G:182:TYR:HE2	1.83	0.43
3:E:459:PHE:HE2	3:E:875:LEU:HB2	1.84	0.43
2:A:55:VAL:HG13	2:A:59:ASN:HD22	1.84	0.43
3:E:172:VAL:HG13	3:E:291:ILE:HG23	2.00	0.43
1:L:144:ARG:HG2	1:M:227:VAL:HG21	1.99	0.43
1:N:278:ASP:HB3	1:N:279:LEU:H	1.71	0.43
2:A:321:SER:HA	2:C:100:PRO:HB3	2.00	0.43
3:F:267:ASP:OD1	3:F:267:ASP:N	2.52	0.42
3:E:611:THR:HA	3:E:627:ALA:HA	2.00	0.42
3:F:188:LEU:HD21	3:F:203:VAL:HG11	2.01	0.42
3:F:514:GLY:O	3:F:518:ARG:HG2	2.19	0.42
3:F:655:PHE:HA	3:F:658:PHE:HD2	1.84	0.42
3:E:152:GLU:HB3	3:E:182:TYR:HE1	1.84	0.42
1:L:67:GLN:NE2	1:L:70:GLN:OE1	2.52	0.42
3:G:906:LEU:HB3	3:G:1015:LEU:HD23	2.00	0.42
3:E:11:PHE:HA	3:E:14:VAL:HG12	2.01	0.42
1:J:190:GLU:HG3	1:J:196:LEU:HB2	2.01	0.42
1:M:247:ASN:O	1:N:188:ARG:NH2	2.53	0.42
1:N:272:GLN:HE21	3:E:230:LEU:HB2	1.85	0.42
3:E:416:VAL:HG11	3:E:493:CYS:HB3	2.00	0.42
1:I:39:ARG:HH11	1:I:169:GLN:NE2	2.17	0.42
1:K:17:ILE:HG22	1:K:322:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:349:ILE:CD1	2:C:71:GLU:HG3	2.48	0.42
3:F:591:VAL:HG13	3:F:611:THR:HG21	2.01	0.42
1:N:48:ASN:OD1	1:N:76:TYR:OH	2.38	0.42
3:F:403:GLY:HA2	3:F:406:VAL:HG12	2.01	0.42
3:F:484:VAL:O	3:F:488:LEU:HB3	2.19	0.42
3:F:560:PRO:O	3:F:921:SER:OG	2.35	0.42
3:G:575:GLN:HG3	3:G:616:ASN:HD22	1.84	0.42
1:J:64:ALA:HB2	1:J:142:SER:HB3	2.01	0.42
1:K:287:VAL:HG21	1:K:297:ARG:HH21	1.85	0.42
2:A:346:TYR:HA	2:A:349:ILE:HD12	2.02	0.42
3:G:527:TYR:CE2	3:G:966:CYS:HB3	2.55	0.42
3:G:560:PRO:HB2	3:G:835:SER:HB3	2.01	0.42
3:E:210:GLN:HG3	3:E:249:ILE:HG12	2.01	0.42
1:K:39:ARG:HD3	1:K:141:ILE:HD11	2.02	0.42
1:K:51:ILE:HG23	1:K:153:GLY:H	1.84	0.42
1:N:226:GLU:OE1	1:N:237:THR:OG1	2.37	0.42
2:B:55:VAL:O	2:B:59:ASN:HB2	2.20	0.42
3:E:44:ALA:HB2	3:E:132:ALA:HB2	2.00	0.42
3:E:47:VAL:HG21	3:E:127:ILE:HG22	2.01	0.42
3:E:150:THR:OG1	3:E:151:LYS:N	2.52	0.42
3:E:563:PHE:CD2	3:E:564:LEU:HG	2.55	0.42
2:A:383:LEU:HD23	2:A:383:LEU:HA	1.86	0.41
2:B:89:GLY:HA2	2:C:334:ILE:HG13	2.00	0.41
3:G:444:GLY:HA3	3:G:890:LEU:HD12	2.02	0.41
2:A:46:ASP:N	2:A:46:ASP:OD1	2.54	0.41
2:B:236:LEU:HD11	2:C:364:THR:HG22	2.02	0.41
3:E:56:THR:O	3:E:60:THR:CB	2.68	0.41
3:E:115:THR:HA	3:E:118:LEU:HD12	2.01	0.41
1:M:175:VAL:HB	1:M:240:ALA:HB3	2.01	0.41
2:A:24:TYR:OH	2:C:232:ASN:ND2	2.39	0.41
3:G:12:ALA:HB1	3:G:488:LEU:HA	2.03	0.41
3:G:14:VAL:HG13	3:E:885:LEU:HD12	2.02	0.41
3:E:56:THR:O	3:E:60:THR:HB	2.21	0.41
3:E:375:VAL:HG11	3:E:405:LEU:HD13	2.02	0.41
1:I:229:VAL:HG12	1:I:236:VAL:HG22	2.02	0.41
1:K:288:VAL:HG13	1:K:322:ILE:HD11	2.02	0.41
1:J:175:VAL:HG12	1:J:177:VAL:HG23	2.02	0.41
1:K:97:TYR:CE1	1:K:106:VAL:HG21	2.55	0.41
1:L:33:GLY:HA3	1:L:177:VAL:HA	2.03	0.41
3:F:416:VAL:HA	3:F:419:VAL:HG12	2.01	0.41
3:F:622:GLN:OE1	3:E:231:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:698:ALA:HB1	3:G:850:LEU:HD22	2.01	0.41
3:E:388:PHE:CD2	3:E:472:ILE:HG21	2.55	0.41
1:M:212:ASP:HB2	1:N:185:LEU:HD12	2.02	0.41
2:A:125:GLU:HA	2:A:301:SER:HA	2.02	0.41
3:G:582:SER:OG	3:G:586:ARG:NH1	2.53	0.41
3:E:2:SER:OG	3:E:486:LEU:O	2.32	0.41
3:E:920:LEU:HD13	3:E:1000:ALA:HA	2.02	0.41
1:I:222:LEU:HA	1:I:240:ALA:HA	2.03	0.41
1:J:270:ALA:HA	1:J:271:PRO:HD3	1.93	0.41
1:N:269:LEU:HD21	1:N:305:ILE:HD11	2.02	0.41
2:A:60:ASN:OD1	2:A:61:ARG:N	2.53	0.41
3:F:931:LEU:HD13	3:F:931:LEU:HA	1.95	0.41
3:G:133:VAL:O	3:G:292:LYS:NZ	2.45	0.41
2:B:386:GLN:HB3	2:B:428:LEU:HD23	2.03	0.41
3:F:56:THR:HG23	3:E:213:GLN:HG3	2.03	0.41
3:F:115:THR:O	3:F:123:GLN:NE2	2.53	0.41
1:I:89:SER:HB2	1:J:116:ALA:HB2	2.03	0.41
1:I:223:GLU:HG2	1:I:224:PHE:CD1	2.56	0.41
1:N:20:LEU:HD21	1:N:315:LEU:HD13	2.02	0.41
2:B:118:THR:HA	2:B:307:GLY:HA3	2.02	0.41
2:B:132:LEU:HD13	2:B:135:LEU:HD12	2.02	0.41
3:F:786:SER:OG	3:F:801:ASN:ND2	2.53	0.41
3:G:210:GLN:HG2	3:E:742:LEU:HG	2.02	0.41
1:I:39:ARG:HD2	1:I:169:GLN:HE21	1.86	0.41
1:I:223:GLU:HG2	1:I:224:PHE:HD1	1.86	0.41
1:K:100:LEU:HD11	2:B:195:SER:HA	2.03	0.41
1:N:327:GLN:HE22	3:F:579:PRO:HD3	1.86	0.41
3:F:354:VAL:HG21	3:F:982:LEU:HG	2.02	0.41
1:I:28:ASN:HA	1:I:260:GLN:HA	2.02	0.40
3:G:568:ASP:O	3:G:634:TRP:NE1	2.49	0.40
3:E:441:ALA:O	3:E:445:ILE:HG12	2.21	0.40
1:I:13:PRO:HG2	1:I:335:VAL:HG23	2.02	0.40
2:A:330:ILE:HG13	2:C:92:GLY:H	1.86	0.40
3:F:252:LYS:HG2	3:F:260:VAL:HG22	2.02	0.40
3:G:359:LEU:HD13	3:G:417:GLU:HG3	2.02	0.40
2:C:280:HIS:HA	2:C:283:MET:HG2	2.03	0.40
3:F:45:VAL:HG22	3:F:129:VAL:HG22	2.02	0.40
3:G:153:ASP:OD1	3:G:182:TYR:OH	2.28	0.40
3:G:442:LEU:HA	3:G:445:ILE:HG12	2.02	0.40
3:E:68:GLN:HG3	3:E:114:ALA:HA	2.03	0.40
1:L:170:LEU:HD11	1:M:227:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:536:LYS:HE2	3:E:537:HIS:CE1	2.57	0.40
2:A:166:LEU:HD13	2:A:436:LEU:HB3	2.02	0.40
2:C:165:TYR:CZ	2:C:169:LYS:HD2	2.56	0.40
3:F:681:ASP:N	3:F:681:ASP:OD1	2.55	0.40
3:F:907:GLY:HA2	3:F:1012:ALA:HB2	2.03	0.40
3:F:978:LEU:HA	3:F:981:ILE:HD12	2.02	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	I	327/362 (90%)	302 (92%)	25 (8%)	0	100	100
1	J	331/362 (91%)	307 (93%)	24 (7%)	0	100	100
1	K	329/362 (91%)	306 (93%)	23 (7%)	0	100	100
1	L	332/362 (92%)	307 (92%)	25 (8%)	0	100	100
1	M	329/362 (91%)	310 (94%)	19 (6%)	0	100	100
1	N	332/362 (92%)	310 (93%)	22 (7%)	0	100	100
2	A	453/474 (96%)	442 (98%)	11 (2%)	0	100	100
2	B	453/474 (96%)	444 (98%)	9 (2%)	0	100	100
2	C	453/474 (96%)	434 (96%)	19 (4%)	0	100	100
3	E	1028/1054 (98%)	989 (96%)	39 (4%)	0	100	100
3	F	1020/1054 (97%)	979 (96%)	41 (4%)	0	100	100
3	G	1028/1054 (98%)	990 (96%)	38 (4%)	0	100	100
All	All	6415/6756 (95%)	6120 (95%)	295 (5%)	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	I	266/287 (93%)	265 (100%)	1 (0%)	91	96
1	J	270/287 (94%)	270 (100%)	0	100	100
1	K	267/287 (93%)	265 (99%)	2 (1%)	84	92
1	L	270/287 (94%)	270 (100%)	0	100	100
1	M	268/287 (93%)	268 (100%)	0	100	100
1	N	270/287 (94%)	269 (100%)	1 (0%)	91	96
2	A	358/375 (96%)	358 (100%)	0	100	100
2	B	358/375 (96%)	358 (100%)	0	100	100
2	C	358/375 (96%)	355 (99%)	3 (1%)	81	91
3	E	841/862 (98%)	841 (100%)	0	100	100
3	F	836/862 (97%)	836 (100%)	0	100	100
3	G	841/862 (98%)	841 (100%)	0	100	100
All	All	5203/5433 (96%)	5196 (100%)	7 (0%)	93	98

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	170	LEU
1	K	96	ARG
1	K	99	LEU
1	N	47	VAL
2	C	226	LEU
2	C	237	LEU
2	C	296	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	23	GLN
1	I	169	GLN

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Mol	Chain	Res	Type
1	J	247	ASN
1	K	28	ASN
1	K	256	HIS
1	L	46	GLN
1	L	67	GLN
1	L	282	GLN
1	M	46	GLN
1	M	215	GLN
1	M	260	GLN
1	N	120	GLN
1	N	168	GLN
1	N	256	HIS
1	N	272	GLN
2	A	22	GLN
2	A	59	ASN
2	A	114	GLN
2	A	354	ASN
2	B	20	GLN
2	B	59	ASN
2	B	232	ASN
2	B	327	GLN
2	B	354	ASN
2	B	418	GLN
2	C	327	GLN
2	C	354	ASN
2	C	452	GLN
3	F	58	GLN
3	F	229	GLN
3	F	248	ASN
3	F	415	ASN
3	F	508	HIS
3	F	759	ASN
3	F	801	ASN
3	G	70	ASN
3	G	248	ASN
3	G	282	ASN
3	G	685	GLN
3	E	58	GLN
3	E	439	GLN
3	E	469	GLN
3	E	537	HIS
3	E	588	GLN

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Mol	Chain	Res	Type
3	E	998	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)

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)

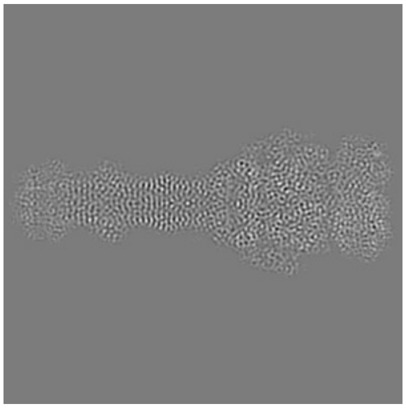
This section contains visualisations of the EMDB entry EMD-9695. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

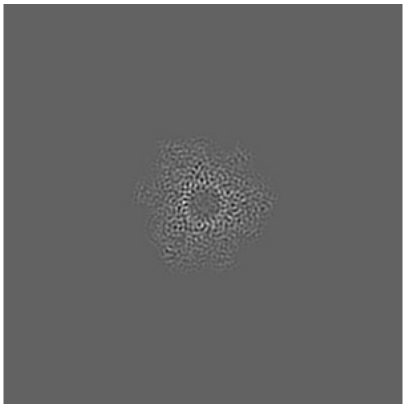
6.1 Orthogonal projections (i)

6.1.1 Primary map

X

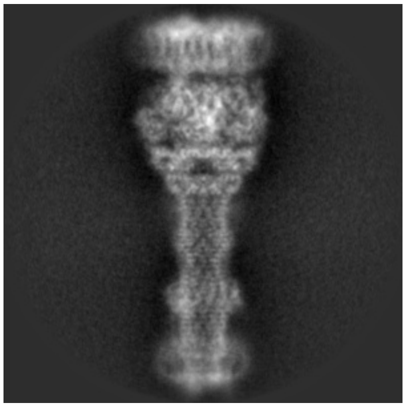


Y

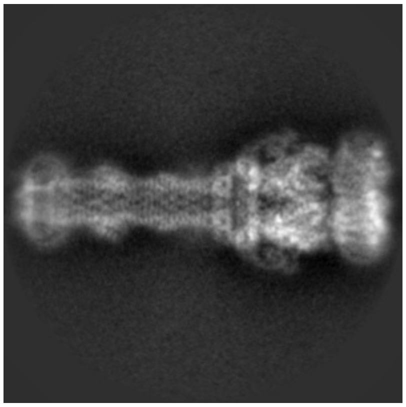


Z

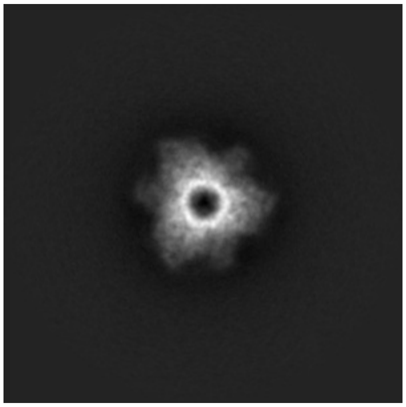
6.1.2 Raw map



X



Y



Z

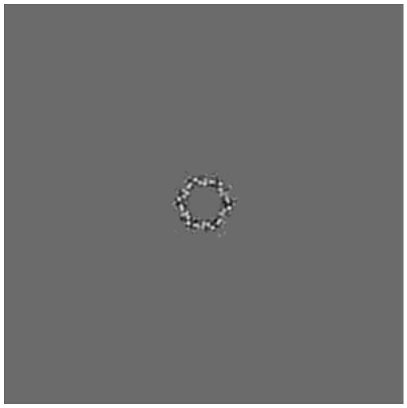
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

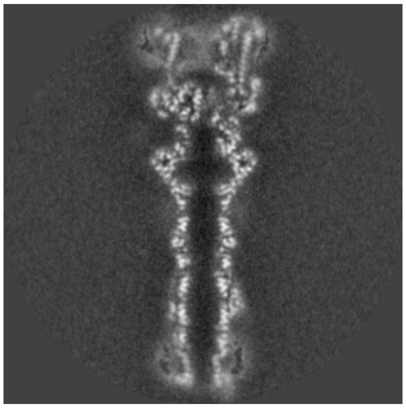
X Index: 200

Y Index: 200

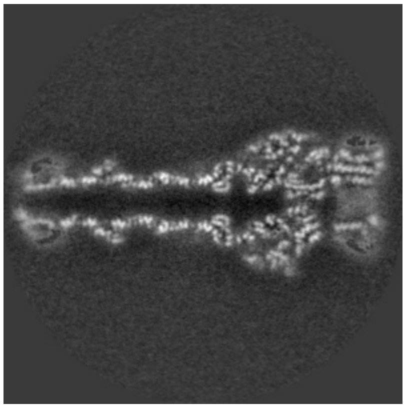


Z Index: 200

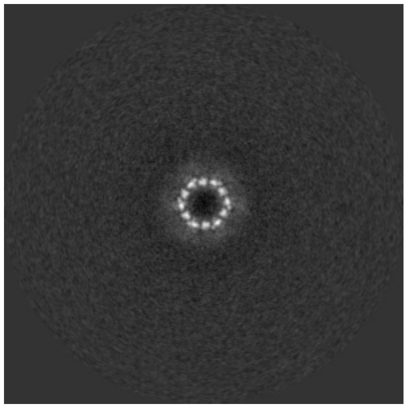
6.2.2 Raw map



X Index: 200



Y Index: 200

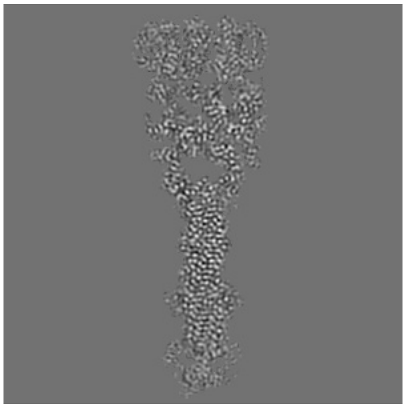


Z Index: 200

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

6.3 Largest variance slices (i)

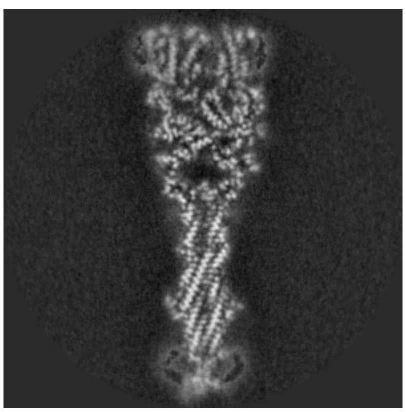
6.3.1 Primary map

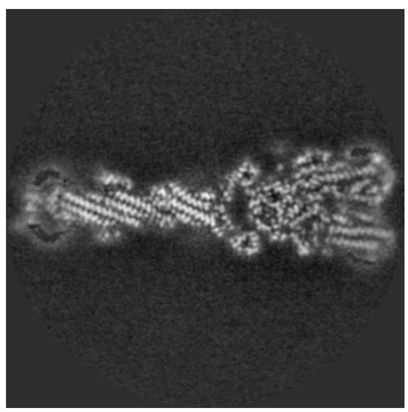

X Index: 182

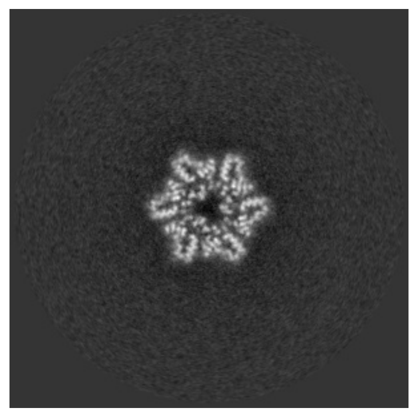

Y Index: 182


Z Index: 272

6.3.2 Raw map


X Index: 184


Y Index: 180

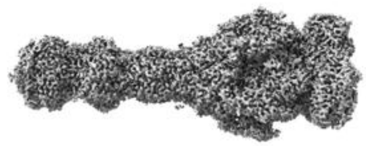

Z Index: 249

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

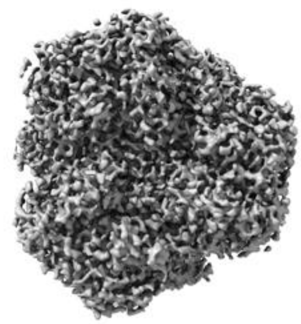
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

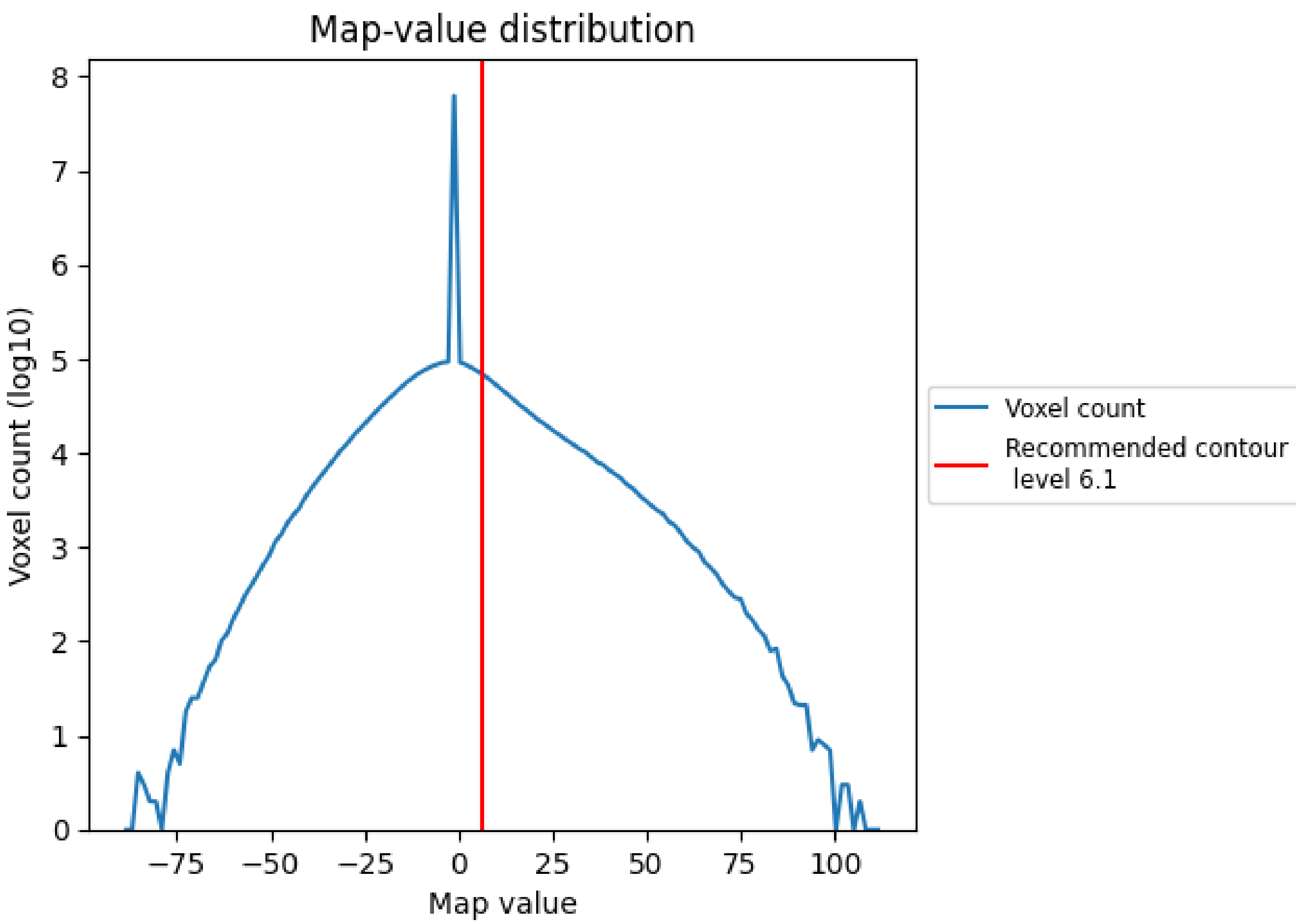
6.5 Mask visualisation (i)

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

7 Map analysis (i)

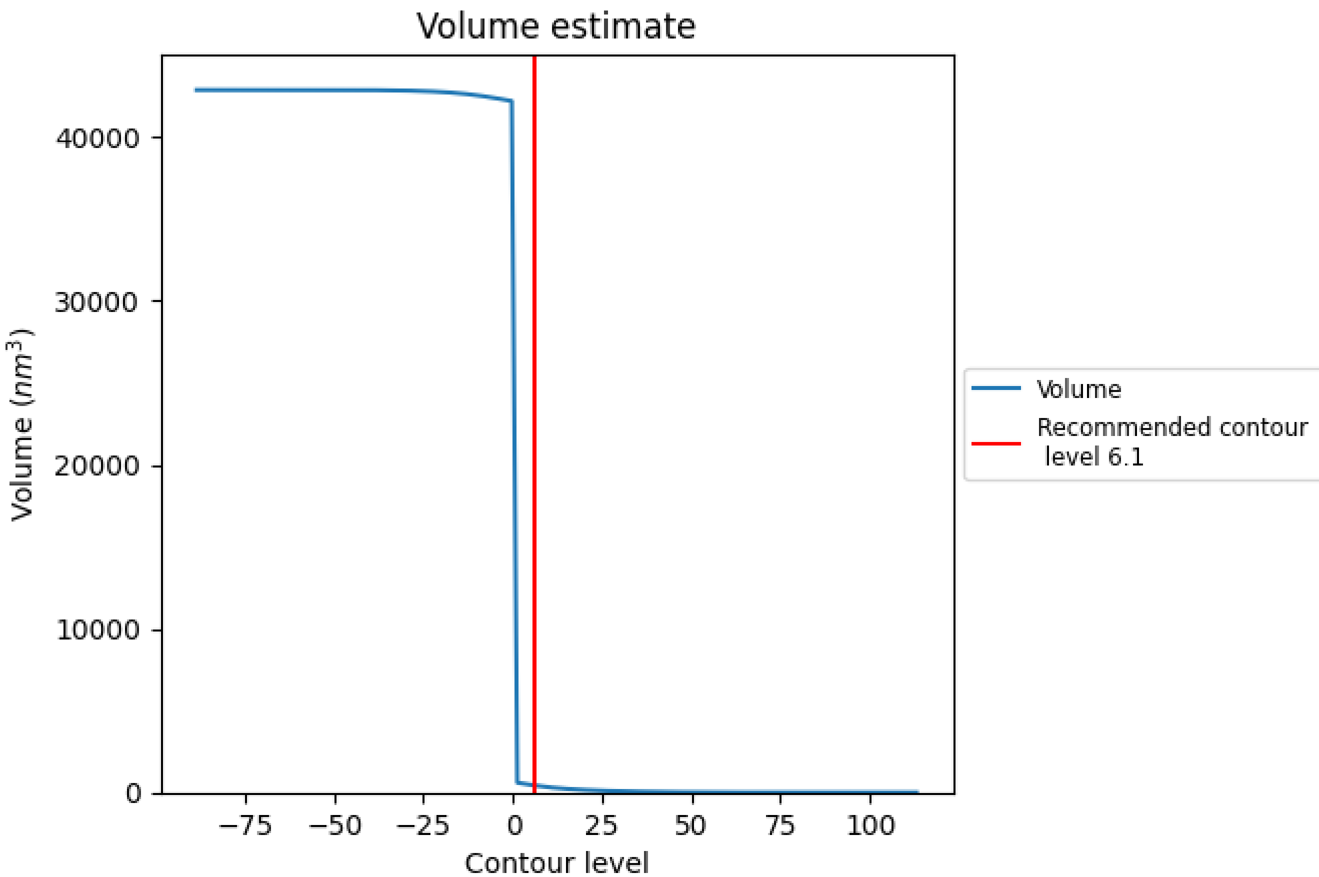
This section contains the results of statistical analysis of the map.

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.

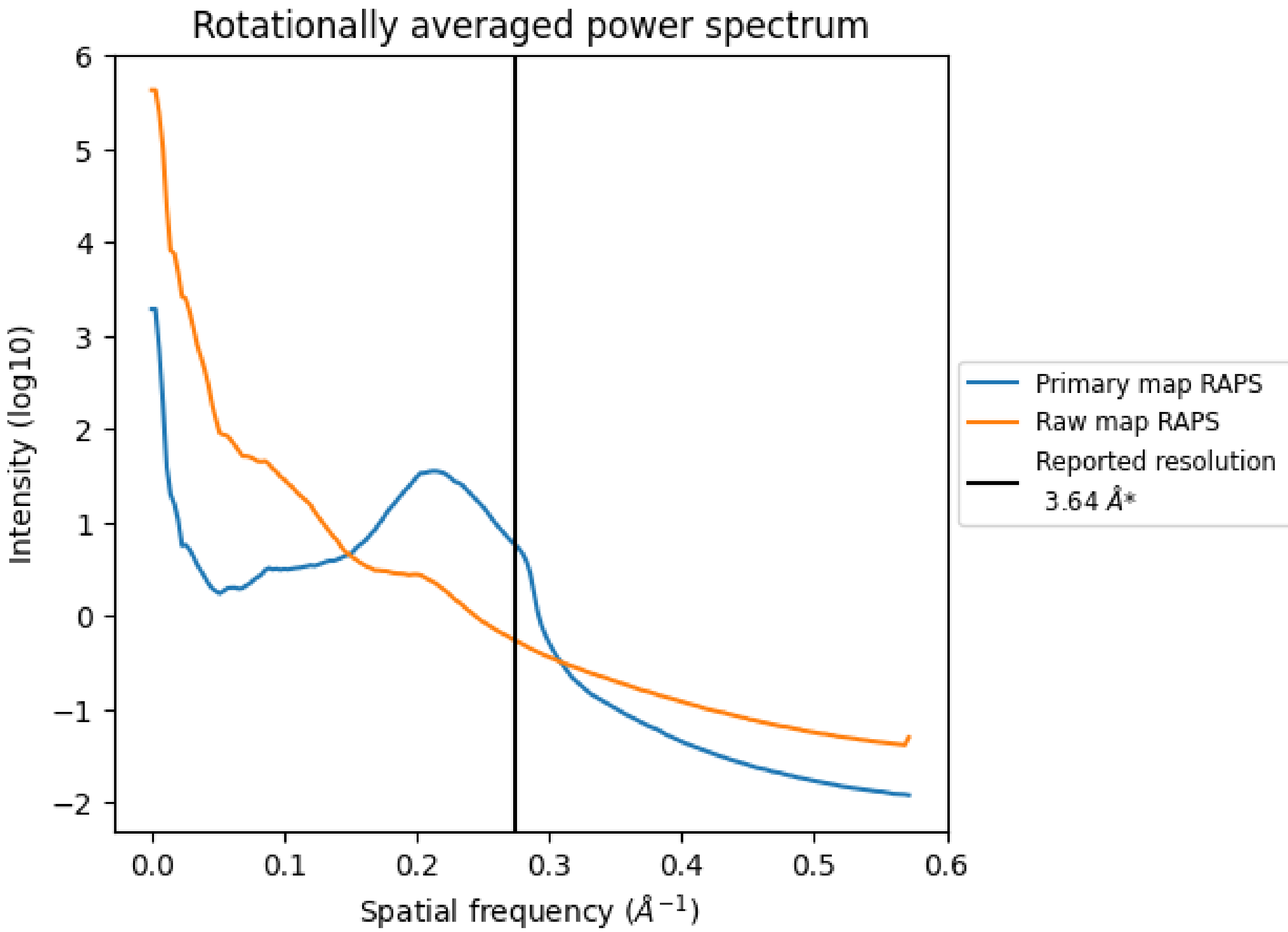
7.2 Volume estimate (i)



The volume at the recommended contour level is 428 nm^3; this corresponds to an approximate mass of 386 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)

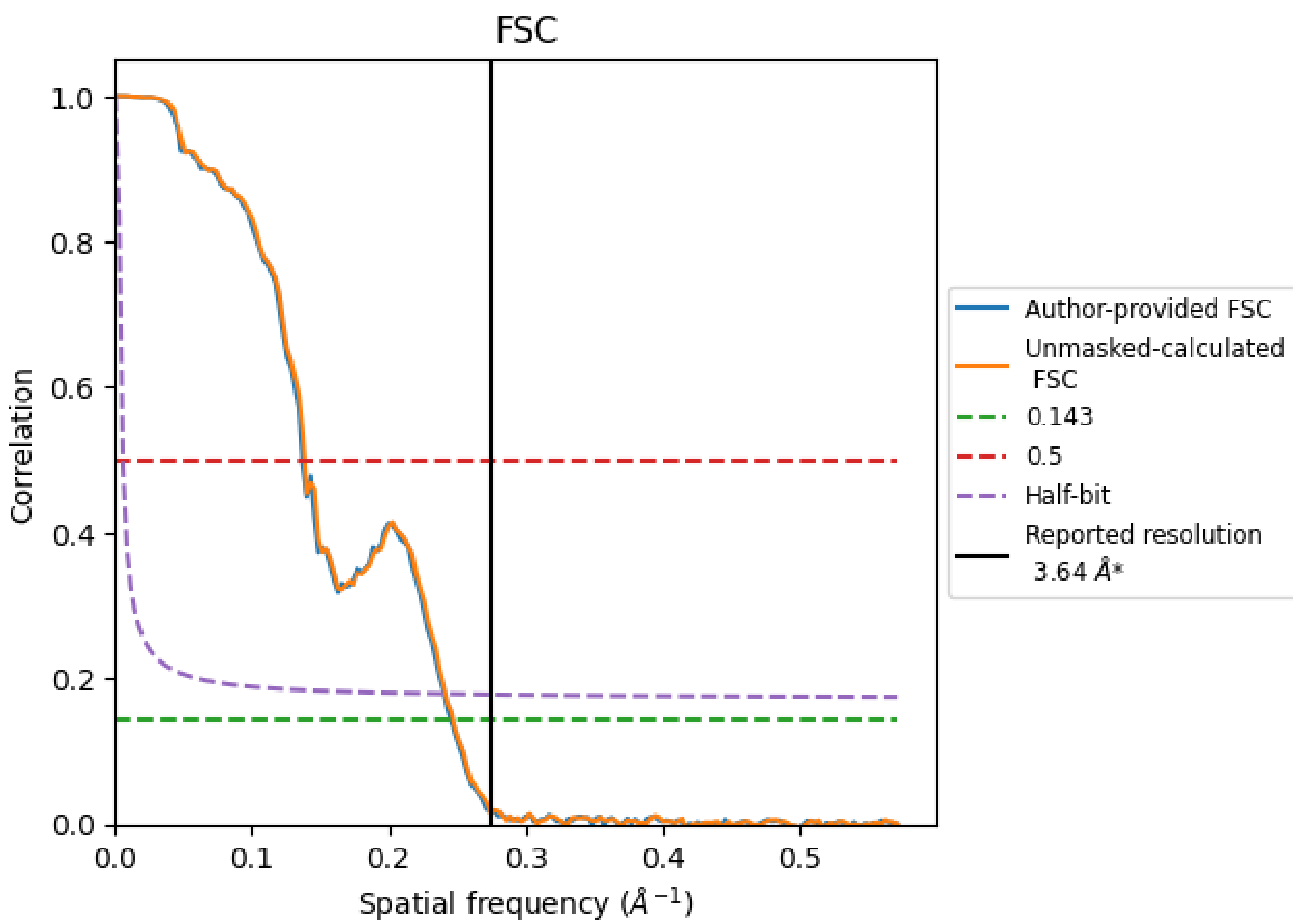


*Reported resolution corresponds to spatial frequency of 0.275 Å^{-1}

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 0.275 $Å^{-1}$

8.2 Resolution estimates (i)

Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.64	-	-
Author-provided FSC curve	4.07	7.31	4.16
Unmasked-calculated*	4.05	7.23	4.14

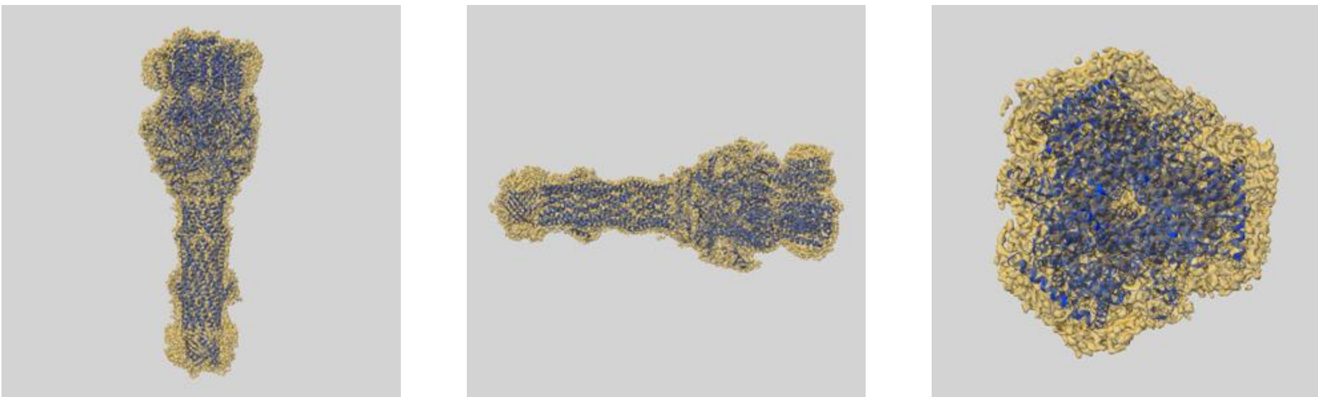
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.07 differs from the reported value 3.64 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.05 differs from the reported value 3.64 by more than 10 %

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9695 and PDB model 6IOK. Per-residue inclusion information can be found in section 3 on page 7.

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 6.1 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

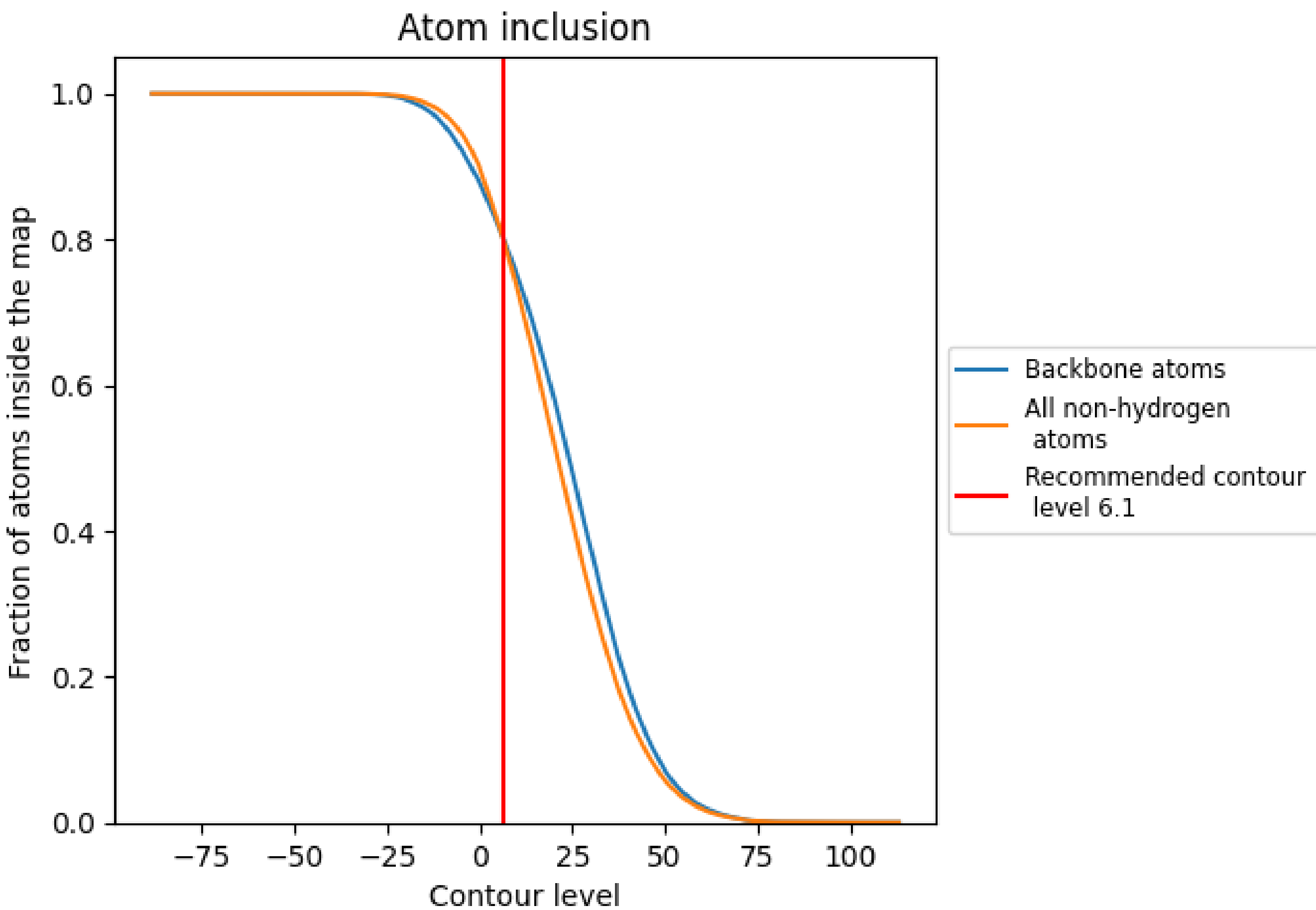
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.1).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 80% 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 (6.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8046	0.4560
A	0.8123	0.4520
B	0.7968	0.4450
C	0.8070	0.4520
E	0.7976	0.4490
F	0.7724	0.4260
G	0.7932	0.4440
I	0.8337	0.4840
J	0.8363	0.4920
K	0.8232	0.4770
L	0.8378	0.4890
M	0.8086	0.4750
N	0.8413	0.4900