Full wwPDB EM Validation Report ⓘ

Nov 20, 2021 – 05:09 am GMT

PDB ID	:	7P1G
EMDB ID	:	EMD-13158
Title	:	Structure of the P. aeruginosa ExoY-F-actin complex
Authors	:	Belyy, A.; Merino, F.; Raunser, S.
Deposited on	:	2021-07-01
Resolution	:	3.20 Å(reported)
Based on initial models	:	5XNW, 7AD9

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

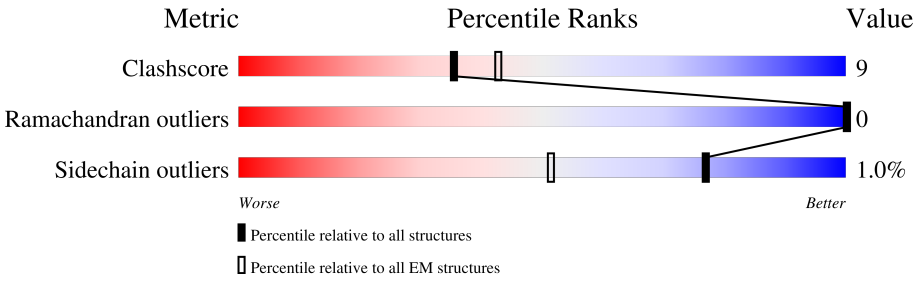
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4 (270009), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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	K	773	10% 35% 10% 55%
1	L	773	10% 36% 9% 55%
1	M	773	7% 35% 10% 55%
1	N	773	9% 35% 9% 55%
1	O	773	14% 35% 10% 55%
2	A	377	82% 16%
2	B	377	82% 16%
2	C	377	82% 16%

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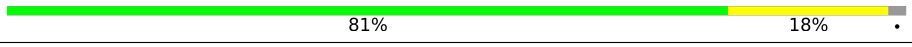
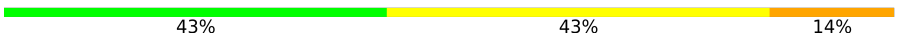
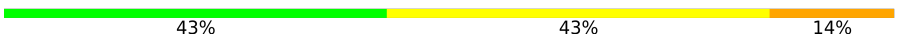
Mol	Chain	Length	Quality of chain
2	D	377	
2	E	377	
3	F	7	
3	G	7	
3	H	7	
3	I	7	
3	J	7	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 28580 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 Maltose/maltodextrin-binding periplasmic protein,Adenylate cyclase ExoY.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	347	Total	C	N	O	S	0	0
			2697	1680	500	504	13		
1	K	347	Total	C	N	O	S	0	0
			2697	1680	500	504	13		
1	L	347	Total	C	N	O	S	0	0
			2697	1680	500	504	13		
1	N	347	Total	C	N	O	S	0	0
			2697	1680	500	504	13		
1	O	347	Total	C	N	O	S	0	0
			2697	1680	500	504	13		

There are 155 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-394	MET	-	initiating methionine	UNP P0AEX9
M	-393	GLY	-	expression tag	UNP P0AEX9
M	-392	SER	-	expression tag	UNP P0AEX9
M	-391	SER	-	expression tag	UNP P0AEX9
M	-390	HIS	-	expression tag	UNP P0AEX9
M	-389	HIS	-	expression tag	UNP P0AEX9
M	-388	HIS	-	expression tag	UNP P0AEX9
M	-387	HIS	-	expression tag	UNP P0AEX9
M	-386	HIS	-	expression tag	UNP P0AEX9
M	-385	HIS	-	expression tag	UNP P0AEX9
M	-384	SER	-	expression tag	UNP P0AEX9
M	-383	SER	-	expression tag	UNP P0AEX9
M	-382	GLY	-	expression tag	UNP P0AEX9
M	-381	LEU	-	expression tag	UNP P0AEX9
M	-380	VAL	-	expression tag	UNP P0AEX9
M	-379	PRO	-	expression tag	UNP P0AEX9
M	-378	ARG	-	expression tag	UNP P0AEX9
M	-377	GLY	-	expression tag	UNP P0AEX9
M	-376	SER	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-375	HIS	-	expression tag	UNP P0AEX9
M	-374	MET	-	expression tag	UNP P0AEX9
M	-62	VAL	ALA	conflict	UNP P0AEX9
M	-7	ASN	-	linker	UNP P0AEX9
M	-6	SER	-	linker	UNP P0AEX9
M	-5	GLY	-	linker	UNP P0AEX9
M	-4	SER	-	linker	UNP P0AEX9
M	-3	SER	-	linker	UNP P0AEX9
M	-2	GLY	-	linker	UNP P0AEX9
M	-1	SER	-	linker	UNP P0AEX9
M	0	SER	-	linker	UNP P0AEX9
M	1	GLY	-	linker	UNP P0AEX9
K	-394	MET	-	initiating methionine	UNP P0AEX9
K	-393	GLY	-	expression tag	UNP P0AEX9
K	-392	SER	-	expression tag	UNP P0AEX9
K	-391	SER	-	expression tag	UNP P0AEX9
K	-390	HIS	-	expression tag	UNP P0AEX9
K	-389	HIS	-	expression tag	UNP P0AEX9
K	-388	HIS	-	expression tag	UNP P0AEX9
K	-387	HIS	-	expression tag	UNP P0AEX9
K	-386	HIS	-	expression tag	UNP P0AEX9
K	-385	HIS	-	expression tag	UNP P0AEX9
K	-384	SER	-	expression tag	UNP P0AEX9
K	-383	SER	-	expression tag	UNP P0AEX9
K	-382	GLY	-	expression tag	UNP P0AEX9
K	-381	LEU	-	expression tag	UNP P0AEX9
K	-380	VAL	-	expression tag	UNP P0AEX9
K	-379	PRO	-	expression tag	UNP P0AEX9
K	-378	ARG	-	expression tag	UNP P0AEX9
K	-377	GLY	-	expression tag	UNP P0AEX9
K	-376	SER	-	expression tag	UNP P0AEX9
K	-375	HIS	-	expression tag	UNP P0AEX9
K	-374	MET	-	expression tag	UNP P0AEX9
K	-62	VAL	ALA	conflict	UNP P0AEX9
K	-7	ASN	-	linker	UNP P0AEX9
K	-6	SER	-	linker	UNP P0AEX9
K	-5	GLY	-	linker	UNP P0AEX9
K	-4	SER	-	linker	UNP P0AEX9
K	-3	SER	-	linker	UNP P0AEX9
K	-2	GLY	-	linker	UNP P0AEX9
K	-1	SER	-	linker	UNP P0AEX9
K	0	SER	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1	GLY	-	linker	UNP P0AEX9
L	-394	MET	-	initiating methionine	UNP P0AEX9
L	-393	GLY	-	expression tag	UNP P0AEX9
L	-392	SER	-	expression tag	UNP P0AEX9
L	-391	SER	-	expression tag	UNP P0AEX9
L	-390	HIS	-	expression tag	UNP P0AEX9
L	-389	HIS	-	expression tag	UNP P0AEX9
L	-388	HIS	-	expression tag	UNP P0AEX9
L	-387	HIS	-	expression tag	UNP P0AEX9
L	-386	HIS	-	expression tag	UNP P0AEX9
L	-385	HIS	-	expression tag	UNP P0AEX9
L	-384	SER	-	expression tag	UNP P0AEX9
L	-383	SER	-	expression tag	UNP P0AEX9
L	-382	GLY	-	expression tag	UNP P0AEX9
L	-381	LEU	-	expression tag	UNP P0AEX9
L	-380	VAL	-	expression tag	UNP P0AEX9
L	-379	PRO	-	expression tag	UNP P0AEX9
L	-378	ARG	-	expression tag	UNP P0AEX9
L	-377	GLY	-	expression tag	UNP P0AEX9
L	-376	SER	-	expression tag	UNP P0AEX9
L	-375	HIS	-	expression tag	UNP P0AEX9
L	-374	MET	-	expression tag	UNP P0AEX9
L	-62	VAL	ALA	conflict	UNP P0AEX9
L	-7	ASN	-	linker	UNP P0AEX9
L	-6	SER	-	linker	UNP P0AEX9
L	-5	GLY	-	linker	UNP P0AEX9
L	-4	SER	-	linker	UNP P0AEX9
L	-3	SER	-	linker	UNP P0AEX9
L	-2	GLY	-	linker	UNP P0AEX9
L	-1	SER	-	linker	UNP P0AEX9
L	0	SER	-	linker	UNP P0AEX9
L	1	GLY	-	linker	UNP P0AEX9
N	-394	MET	-	initiating methionine	UNP P0AEX9
N	-393	GLY	-	expression tag	UNP P0AEX9
N	-392	SER	-	expression tag	UNP P0AEX9
N	-391	SER	-	expression tag	UNP P0AEX9
N	-390	HIS	-	expression tag	UNP P0AEX9
N	-389	HIS	-	expression tag	UNP P0AEX9
N	-388	HIS	-	expression tag	UNP P0AEX9
N	-387	HIS	-	expression tag	UNP P0AEX9
N	-386	HIS	-	expression tag	UNP P0AEX9
N	-385	HIS	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-384	SER	-	expression tag	UNP P0AEX9
N	-383	SER	-	expression tag	UNP P0AEX9
N	-382	GLY	-	expression tag	UNP P0AEX9
N	-381	LEU	-	expression tag	UNP P0AEX9
N	-380	VAL	-	expression tag	UNP P0AEX9
N	-379	PRO	-	expression tag	UNP P0AEX9
N	-378	ARG	-	expression tag	UNP P0AEX9
N	-377	GLY	-	expression tag	UNP P0AEX9
N	-376	SER	-	expression tag	UNP P0AEX9
N	-375	HIS	-	expression tag	UNP P0AEX9
N	-374	MET	-	expression tag	UNP P0AEX9
N	-62	VAL	ALA	conflict	UNP P0AEX9
N	-7	ASN	-	linker	UNP P0AEX9
N	-6	SER	-	linker	UNP P0AEX9
N	-5	GLY	-	linker	UNP P0AEX9
N	-4	SER	-	linker	UNP P0AEX9
N	-3	SER	-	linker	UNP P0AEX9
N	-2	GLY	-	linker	UNP P0AEX9
N	-1	SER	-	linker	UNP P0AEX9
N	0	SER	-	linker	UNP P0AEX9
N	1	GLY	-	linker	UNP P0AEX9
O	-394	MET	-	initiating methionine	UNP P0AEX9
O	-393	GLY	-	expression tag	UNP P0AEX9
O	-392	SER	-	expression tag	UNP P0AEX9
O	-391	SER	-	expression tag	UNP P0AEX9
O	-390	HIS	-	expression tag	UNP P0AEX9
O	-389	HIS	-	expression tag	UNP P0AEX9
O	-388	HIS	-	expression tag	UNP P0AEX9
O	-387	HIS	-	expression tag	UNP P0AEX9
O	-386	HIS	-	expression tag	UNP P0AEX9
O	-385	HIS	-	expression tag	UNP P0AEX9
O	-384	SER	-	expression tag	UNP P0AEX9
O	-383	SER	-	expression tag	UNP P0AEX9
O	-382	GLY	-	expression tag	UNP P0AEX9
O	-381	LEU	-	expression tag	UNP P0AEX9
O	-380	VAL	-	expression tag	UNP P0AEX9
O	-379	PRO	-	expression tag	UNP P0AEX9
O	-378	ARG	-	expression tag	UNP P0AEX9
O	-377	GLY	-	expression tag	UNP P0AEX9
O	-376	SER	-	expression tag	UNP P0AEX9
O	-375	HIS	-	expression tag	UNP P0AEX9
O	-374	MET	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-62	VAL	ALA	conflict	UNP P0AEX9
O	-7	ASN	-	linker	UNP P0AEX9
O	-6	SER	-	linker	UNP P0AEX9
O	-5	GLY	-	linker	UNP P0AEX9
O	-4	SER	-	linker	UNP P0AEX9
O	-3	SER	-	linker	UNP P0AEX9
O	-2	GLY	-	linker	UNP P0AEX9
O	-1	SER	-	linker	UNP P0AEX9
O	0	SER	-	linker	UNP P0AEX9
O	1	GLY	-	linker	UNP P0AEX9

- Molecule 2 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	371	Total	C	N	O	S	0	0
			2899	1836	489	553	21		
2	A	371	Total	C	N	O	S	0	0
			2899	1836	489	553	21		
2	B	371	Total	C	N	O	S	0	0
			2899	1836	489	553	21		
2	D	371	Total	C	N	O	S	0	0
			2899	1836	489	553	21		
2	E	371	Total	C	N	O	S	0	0
			2899	1836	489	553	21		

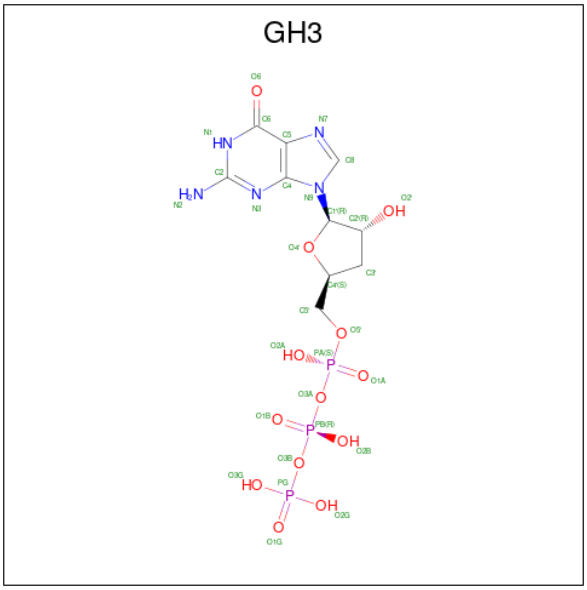
- Molecule 3 is a protein called Phalloidin.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	7	Total	C	N	O	S	0	0
			55	35	8	11	1		
3	F	7	Total	C	N	O	S	0	0
			55	35	8	11	1		
3	G	7	Total	C	N	O	S	0	0
			55	35	8	11	1		
3	I	7	Total	C	N	O	S	0	0
			55	35	8	11	1		
3	J	7	Total	C	N	O	S	0	0
			55	35	8	11	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
4	M	1	Total Mg 1 1	0
4	C	1	Total Mg 1 1	0
4	K	1	Total Mg 1 1	0
4	A	1	Total Mg 1 1	0
4	L	1	Total Mg 1 1	0
4	B	1	Total Mg 1 1	0
4	N	1	Total Mg 1 1	0
4	D	1	Total Mg 1 1	0
4	O	1	Total Mg 1 1	0
4	E	1	Total Mg 1 1	0

- Molecule 5 is 3'-DEOXY-GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GH3) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms	AltConf
5	M	1	Total C N O P 31 10 5 13 3	0

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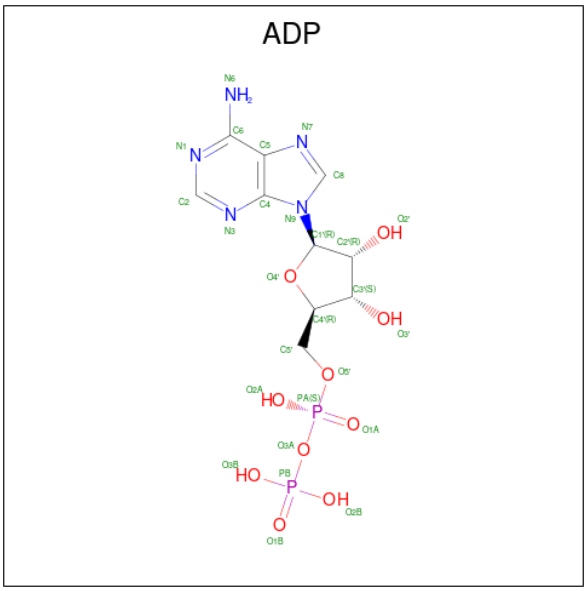
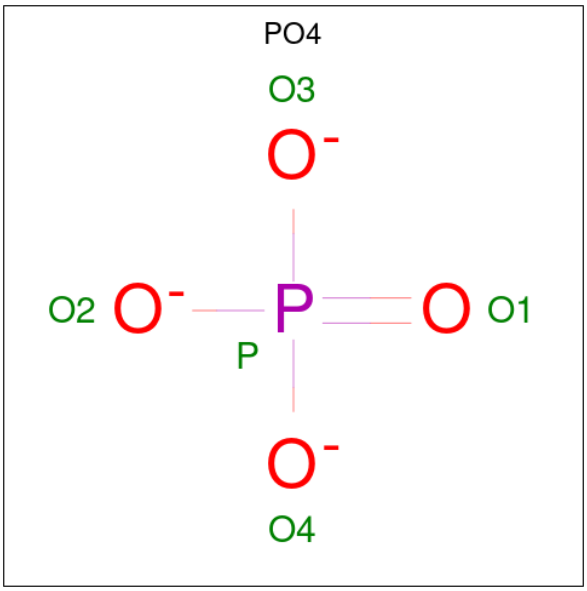
Mol	Chain	Residues	Atoms					AltConf
5	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	N	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	O	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
6	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

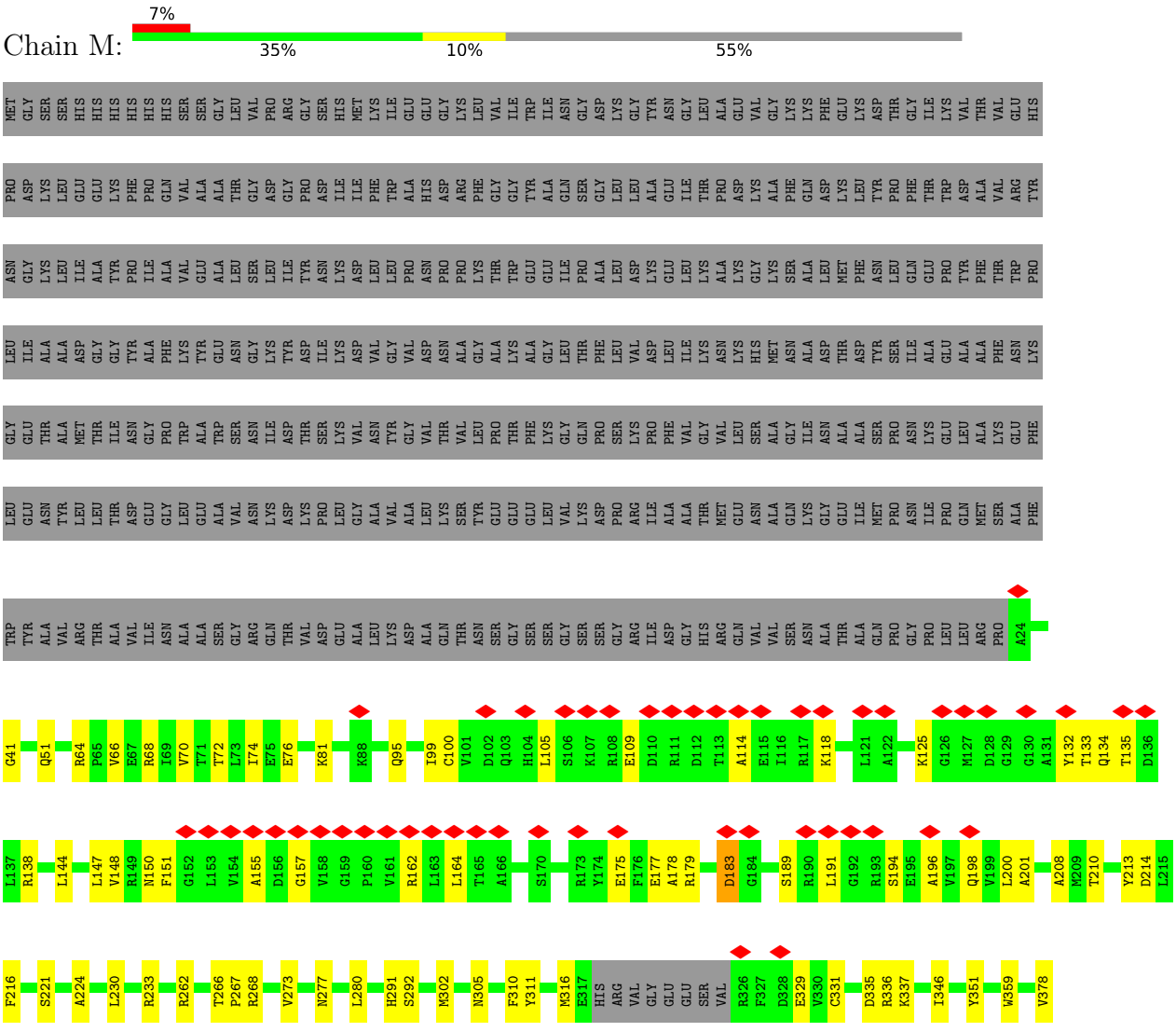


Mol	Chain	Residues	Atoms			AltConf
7	C	1	Total	O	P	0
			5	4	1	
7	A	1	Total	O	P	0
			5	4	1	
7	B	1	Total	O	P	0
			5	4	1	
7	D	1	Total	O	P	0
			5	4	1	
7	E	1	Total	O	P	0
			5	4	1	

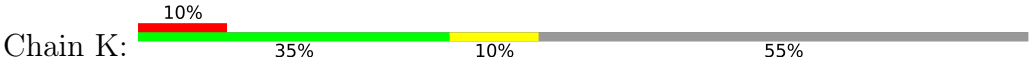
3 Residue-property plots (i)

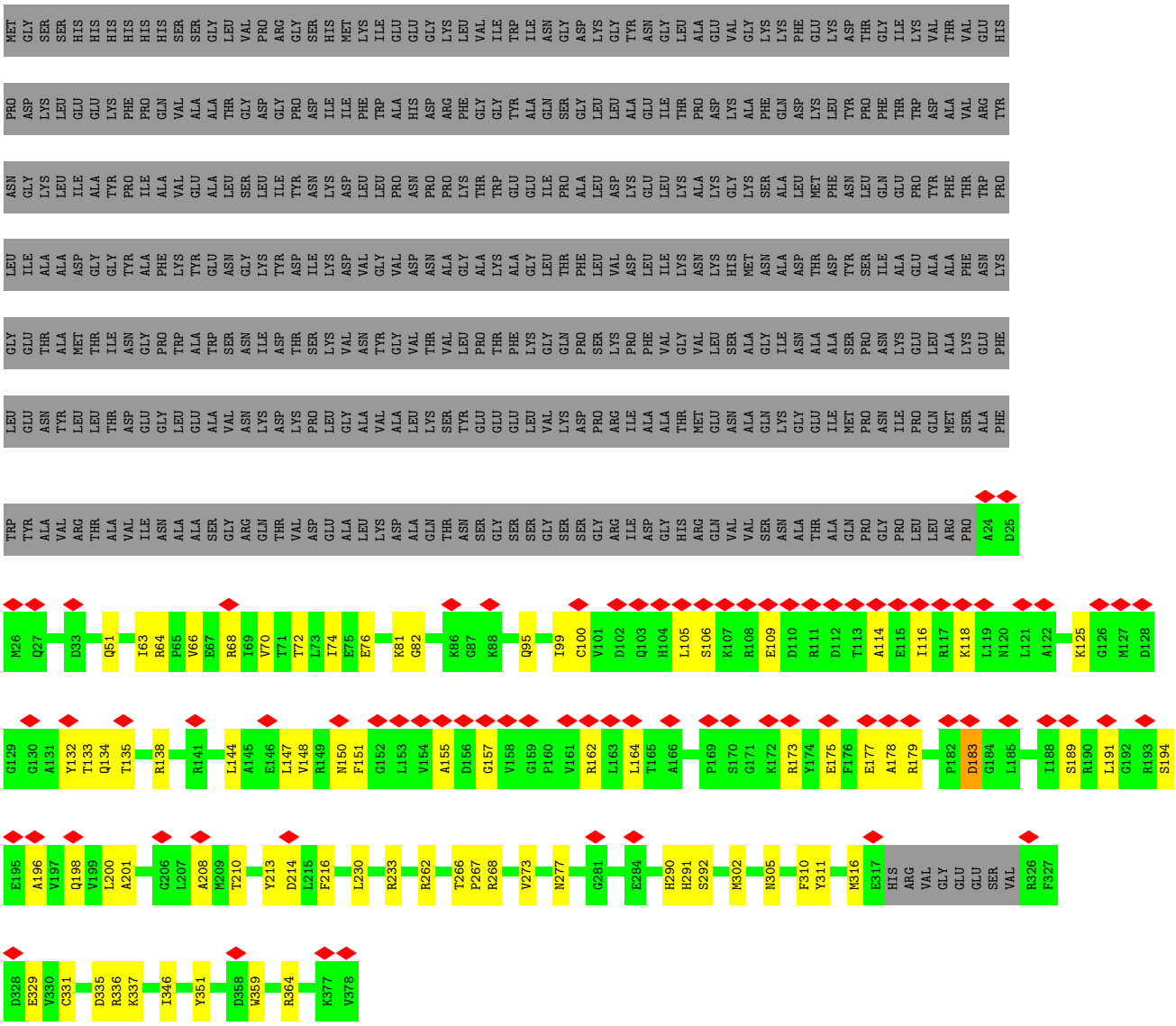
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Maltose/maltodextrin-binding periplasmic protein,Adenylate cyclase ExoY



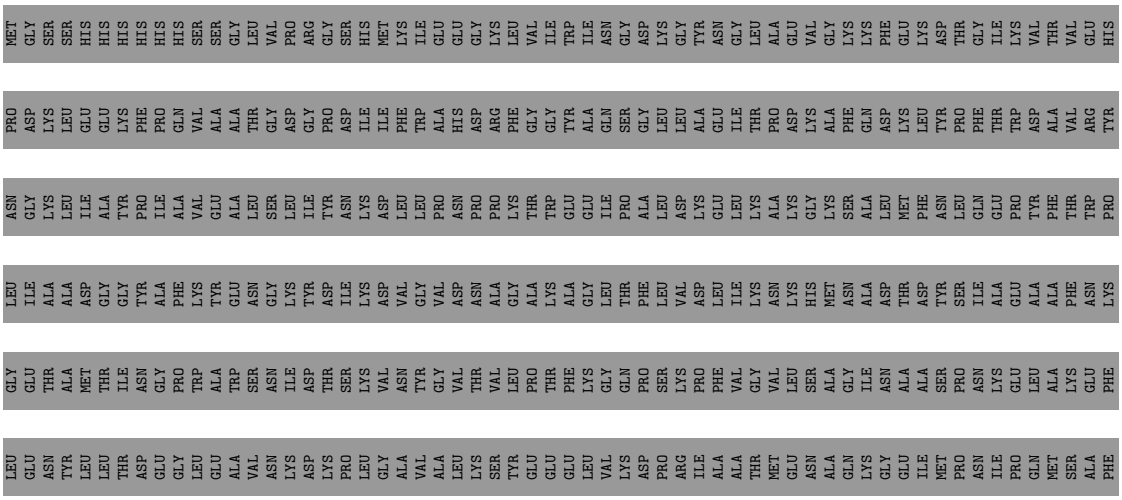
• Molecule 1: Maltose/maltodextrin-binding periplasmic protein,Adenylate cyclase ExoY

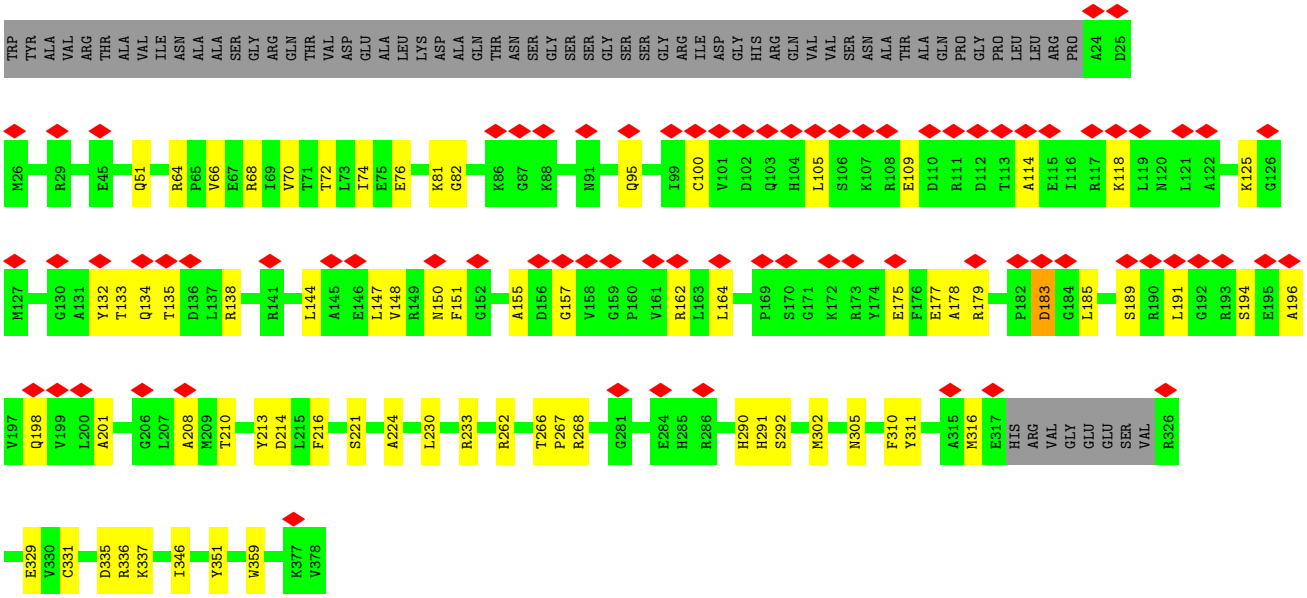




• Molecule 1: Maltose/maltodextrin-binding periplasmic protein,Adenylate cyclase ExoY

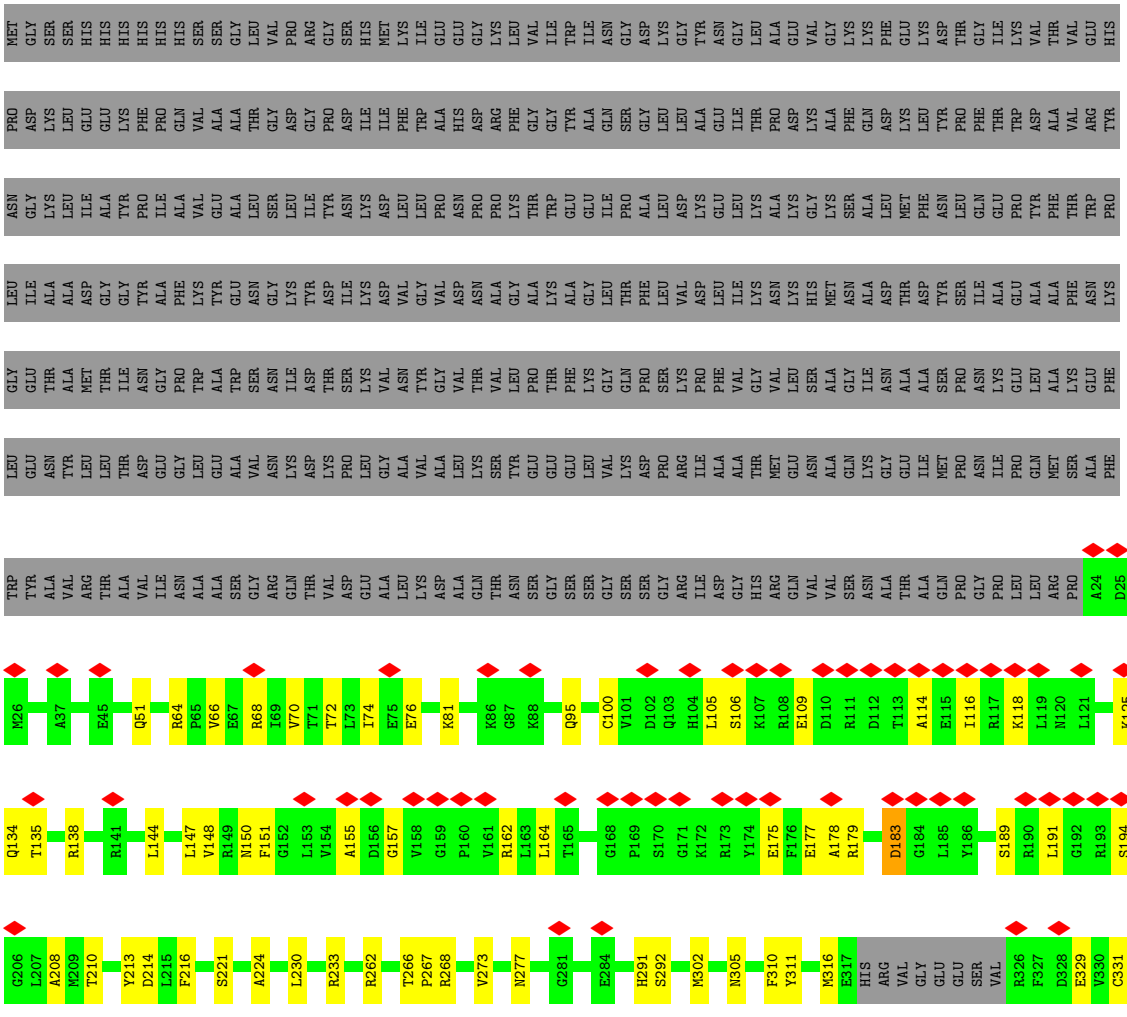
Chain L:

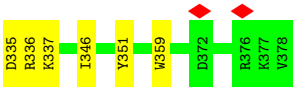




• Molecule 1: Maltose/maltodextrin-binding periplasmic protein,Adenylate cyclase ExoY

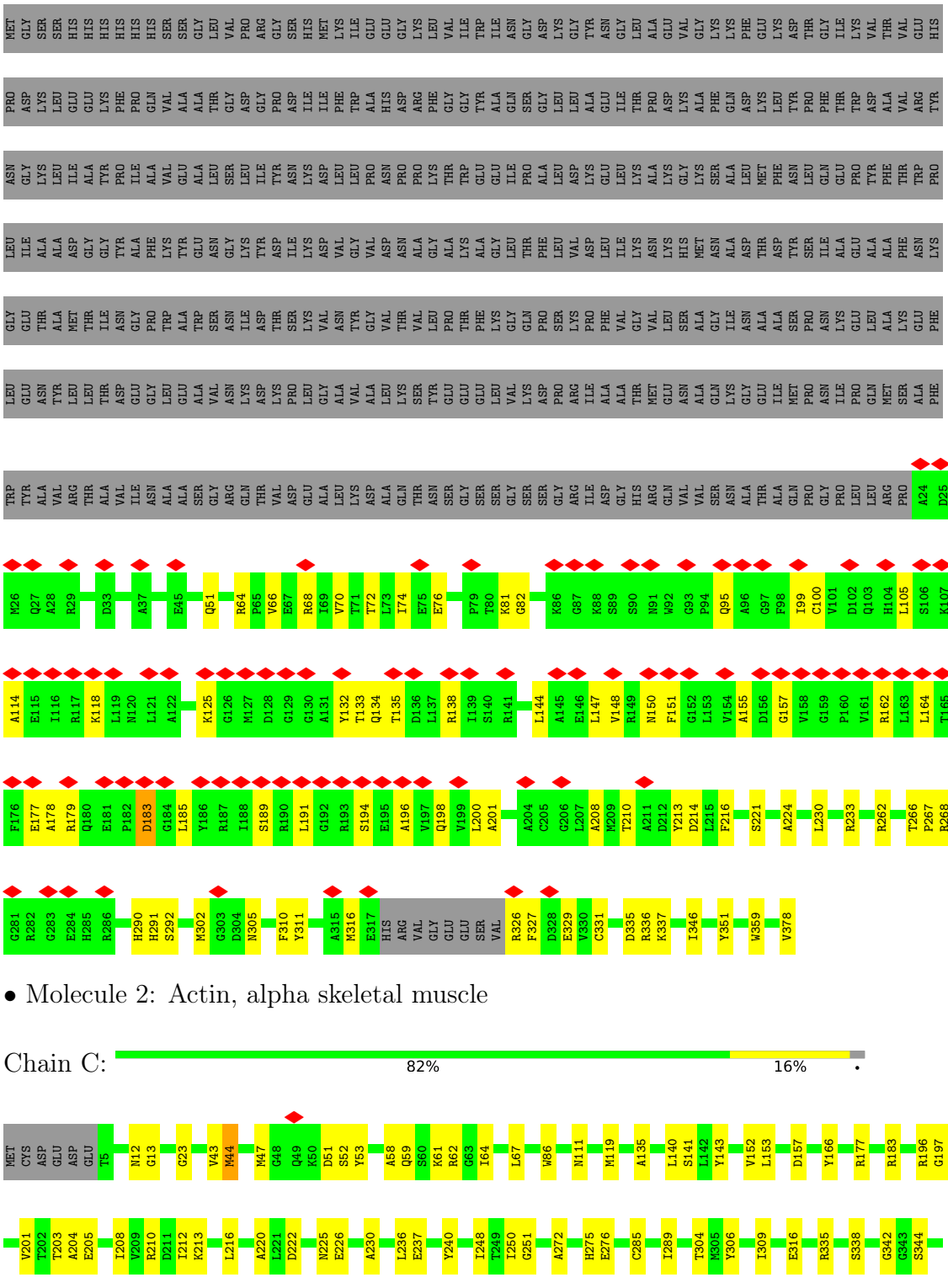
Chain N:





• Molecule 1: Maltose/maltodextrin-binding periplasmic protein,Adenylate cyclase ExoY

Chain O:

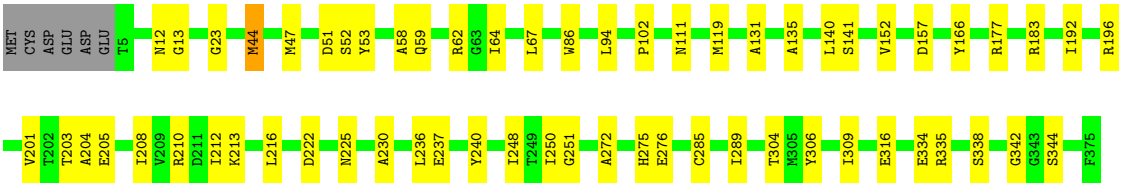


• Molecule 2: Actin, alpha skeletal muscle

Chain C:

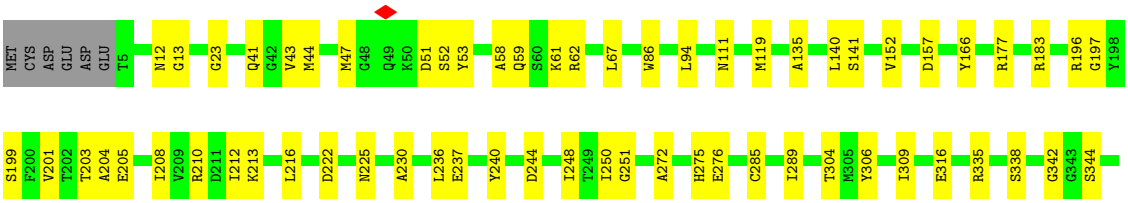
• Molecule 2: Actin, alpha skeletal muscle

Chain A:



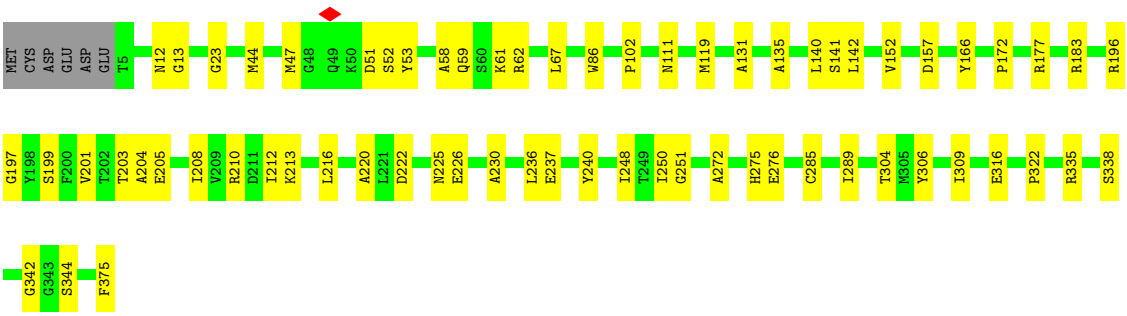
• Molecule 2: Actin, alpha skeletal muscle

Chain B:



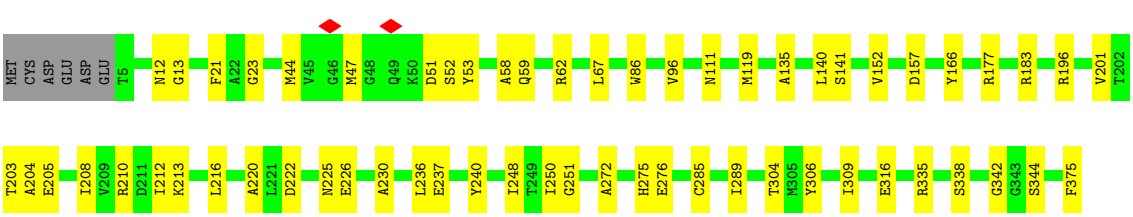
• Molecule 2: Actin, alpha skeletal muscle

Chain D:



• Molecule 2: Actin, alpha skeletal muscle

Chain E:

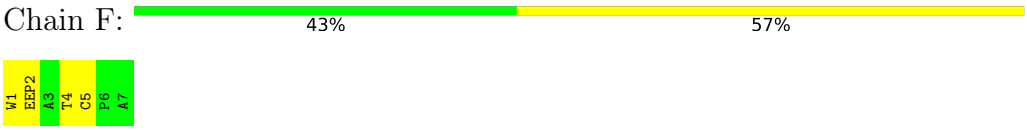


• Molecule 3: Phalloidin

Chain H:

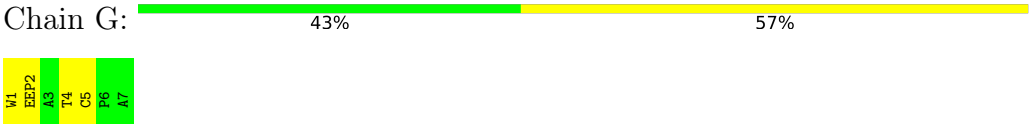
• Molecule 3: Phalloidin

Chain F:



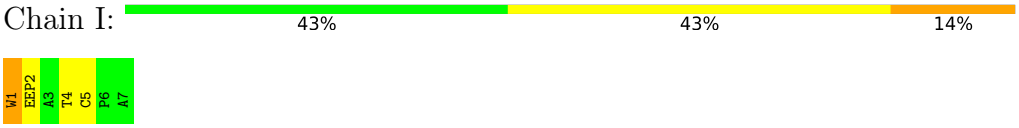
• Molecule 3: Phalloidin

Chain G:



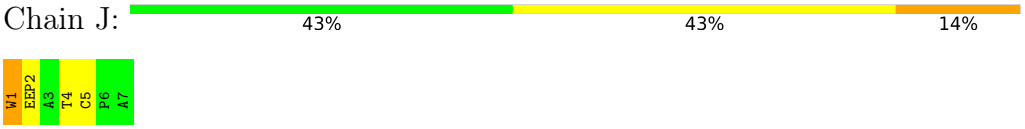
• Molecule 3: Phalloidin

Chain I:



• Molecule 3: Phalloidin

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1535755	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 ($e^-/Å^2$)	93	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.263	Depositor
Minimum map value	-0.148	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.023	Depositor
Map size (Å)	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DTH, MG, PO4, HYP, ADP, GH3, EEP

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	K	0.64	0/2752	0.64	0/3717
1	L	0.64	0/2752	0.64	0/3717
1	M	0.64	0/2752	0.64	0/3717
1	N	0.64	0/2752	0.64	0/3717
1	O	0.64	0/2752	0.64	0/3717
2	A	1.01	0/2962	0.74	0/4012
2	B	1.01	0/2962	0.74	0/4012
2	C	1.01	0/2962	0.74	0/4012
2	D	1.01	0/2962	0.74	0/4012
2	E	1.01	0/2962	0.74	0/4012
3	F	2.51	1/28 (3.6%)	2.56	2/33 (6.1%)
3	G	2.51	1/28 (3.6%)	2.54	2/33 (6.1%)
3	H	2.51	1/28 (3.6%)	2.55	2/33 (6.1%)
3	I	2.50	1/28 (3.6%)	2.55	2/33 (6.1%)
3	J	2.50	1/28 (3.6%)	2.54	2/33 (6.1%)
All	All	0.87	5/28710 (0.0%)	0.71	10/38810 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	TRP	CD2-CE2	-5.27	1.35	1.41
3	H	1	TRP	CD2-CE2	-5.22	1.35	1.41
3	G	1	TRP	CD2-CE2	-5.22	1.35	1.41
3	I	1	TRP	CD2-CE2	-5.21	1.35	1.41
3	J	1	TRP	CD2-CE2	-5.20	1.35	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	1	TRP	CB-CA-C	-5.82	98.76	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1	TRP	CB-CA-C	-5.81	98.78	110.40
3	F	1	TRP	CB-CA-C	-5.81	98.79	110.40
3	J	1	TRP	CB-CA-C	-5.80	98.80	110.40
3	G	1	TRP	CB-CA-C	-5.79	98.81	110.40
3	F	1	TRP	N-CA-CB	-5.05	101.51	110.60
3	H	1	TRP	N-CA-CB	-5.04	101.53	110.60
3	I	1	TRP	N-CA-CB	-5.03	101.54	110.60
3	G	1	TRP	N-CA-CB	-5.02	101.56	110.60
3	J	1	TRP	N-CA-CB	-5.02	101.57	110.60

There are no chirality outliers.

There are no planarity outliers.

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	K	2697	0	2634	49	0
1	L	2697	0	2634	45	0
1	M	2697	0	2634	48	0
1	N	2697	0	2634	45	0
1	O	2697	0	2634	49	0
2	A	2899	0	2871	46	0
2	B	2899	0	2871	48	0
2	C	2899	0	2871	50	0
2	D	2899	0	2871	50	0
2	E	2899	0	2871	42	0
3	F	55	0	38	2	0
3	G	55	0	38	2	0
3	H	55	0	38	4	0
3	I	55	0	38	4	0
3	J	55	0	38	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
5	K	31	0	12	5	0
5	L	31	0	12	5	0
5	M	31	0	12	5	0
5	N	31	0	12	5	0
5	O	31	0	12	5	0
6	A	27	0	12	4	0
6	B	27	0	12	4	0
6	C	27	0	12	4	0
6	D	27	0	12	4	0
6	E	27	0	12	4	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
7	C	5	0	0	0	0
7	D	5	0	0	0	0
7	E	5	0	0	0	0
All	All	28580	0	27835	487	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 9.

All (487) 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)
5:K:402:GH3:O4'	5:K:402:GH3:C1'	1.69	1.32
5:L:402:GH3:O4'	5:L:402:GH3:C1'	1.69	1.25
5:N:402:GH3:O4'	5:N:402:GH3:C1'	1.69	1.24
5:O:402:GH3:O4'	5:O:402:GH3:C1'	1.69	1.20
5:M:402:GH3:O4'	5:M:402:GH3:C1'	1.69	1.20
2:B:43:VAL:HG11	2:D:375:PHE:HZ	1.42	0.85
2:D:197:GLY:O	3:J:1:TRP:HE3	1.60	0.83
2:B:59:GLN:OE1	2:B:210:ARG:NH2	2.12	0.83
2:C:59:GLN:OE1	2:C:210:ARG:NH2	2.12	0.83
2:E:59:GLN:OE1	2:E:210:ARG:NH2	2.12	0.83
2:D:59:GLN:OE1	2:D:210:ARG:NH2	2.12	0.82
2:A:59:GLN:OE1	2:A:210:ARG:NH2	2.12	0.82
1:K:292:SER:OG	5:K:402:GH3:N2	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:292:SER:OG	5:N:402:GH3:N2	2.15	0.80
1:O:292:SER:OG	5:O:402:GH3:N2	2.15	0.80
1:L:292:SER:OG	5:L:402:GH3:N2	2.15	0.80
1:M:292:SER:OG	5:M:402:GH3:N2	2.15	0.79
1:M:68:ARG:NH2	1:M:150:ASN:OD1	2.17	0.78
1:O:68:ARG:NH2	1:O:150:ASN:OD1	2.17	0.78
1:K:68:ARG:NH2	1:K:150:ASN:OD1	2.17	0.77
1:N:68:ARG:NH2	1:N:150:ASN:OD1	2.17	0.76
1:L:68:ARG:NH2	1:L:150:ASN:OD1	2.17	0.75
2:E:304:THR:O	2:E:335:ARG:NH1	2.23	0.72
2:A:304:THR:O	2:A:335:ARG:NH1	2.23	0.72
2:D:304:THR:O	2:D:335:ARG:NH1	2.23	0.72
2:B:304:THR:O	2:B:335:ARG:NH1	2.23	0.71
2:C:304:THR:O	2:C:335:ARG:NH1	2.23	0.71
2:B:43:VAL:HG11	2:D:375:PHE:CZ	2.25	0.70
1:L:346:ILE:HG23	1:L:351:TYR:HB2	1.76	0.68
1:N:346:ILE:HG23	1:N:351:TYR:HB2	1.76	0.68
1:K:346:ILE:HG23	1:K:351:TYR:HB2	1.76	0.67
1:M:346:ILE:HG23	1:M:351:TYR:HB2	1.76	0.67
3:H:1:TRP:HE3	2:B:197:GLY:O	1.78	0.66
1:O:346:ILE:HG23	1:O:351:TYR:HB2	1.76	0.66
1:L:105:LEU:O	1:L:109:GLU:N	2.28	0.65
1:M:336:ARG:NH2	1:M:359:TRP:O	2.30	0.65
1:K:336:ARG:NH2	1:K:359:TRP:O	2.30	0.65
1:N:105:LEU:O	1:N:109:GLU:N	2.28	0.65
1:O:336:ARG:NH2	1:O:359:TRP:O	2.30	0.65
1:L:336:ARG:NH2	1:L:359:TRP:O	2.30	0.65
2:A:285:CYS:HB3	2:A:289:ILE:HD11	1.80	0.64
2:B:285:CYS:HB3	2:B:289:ILE:HD11	1.80	0.64
2:D:197:GLY:O	3:J:1:TRP:CE3	2.46	0.64
1:N:336:ARG:NH2	1:N:359:TRP:O	2.30	0.64
2:C:285:CYS:HB3	2:C:289:ILE:HD11	1.80	0.64
1:O:105:LEU:O	1:O:109:GLU:N	2.28	0.64
2:D:285:CYS:HB3	2:D:289:ILE:HD11	1.80	0.64
1:M:105:LEU:O	1:M:109:GLU:N	2.28	0.63
1:M:144:LEU:HD21	1:M:164:LEU:HD21	1.81	0.63
3:I:2:EEP:N	3:I:2:EEP:O1	2.31	0.63
1:O:144:LEU:HD21	1:O:164:LEU:HD21	1.81	0.63
2:E:285:CYS:HB3	2:E:289:ILE:HD11	1.80	0.63
1:K:144:LEU:HD21	1:K:164:LEU:HD21	1.81	0.63
3:J:2:EEP:N	3:J:2:EEP:O1	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:111:ASN:HB3	2:D:177:ARG:NH1	2.15	0.62
2:B:111:ASN:HB3	2:B:177:ARG:NH1	2.15	0.62
3:G:2:EEP:N	3:G:2:EEP:O1	2.31	0.62
1:K:105:LEU:O	1:K:109:GLU:N	2.28	0.62
2:D:59:GLN:O	2:D:62:ARG:HB2	2.00	0.62
2:E:59:GLN:O	2:E:62:ARG:HB2	2.00	0.62
2:A:157:ASP:OD2	2:A:183:ARG:NH2	2.30	0.62
2:B:157:ASP:OD2	2:B:183:ARG:NH2	2.30	0.62
1:N:144:LEU:HD21	1:N:164:LEU:HD21	1.81	0.62
2:A:111:ASN:HB3	2:A:177:ARG:NH1	2.15	0.62
2:B:59:GLN:O	2:B:62:ARG:HB2	2.00	0.62
2:E:111:ASN:HB3	2:E:177:ARG:NH1	2.15	0.62
2:C:59:GLN:O	2:C:62:ARG:HB2	1.99	0.61
2:C:157:ASP:OD2	2:C:183:ARG:NH2	2.30	0.61
3:H:2:EEP:N	3:H:2:EEP:O1	2.30	0.61
1:L:144:LEU:HD21	1:L:164:LEU:HD21	1.81	0.61
2:A:59:GLN:O	2:A:62:ARG:HB2	1.99	0.61
2:C:111:ASN:HB3	2:C:177:ARG:NH1	2.15	0.61
1:O:138:ARG:NH2	1:O:183:ASP:OD2	2.26	0.61
1:O:302:MET:HG2	1:O:336:ARG:HE	1.67	0.60
1:N:302:MET:HG2	1:N:336:ARG:HE	1.67	0.60
1:L:302:MET:HG2	1:L:336:ARG:HE	1.67	0.60
2:D:111:ASN:HB3	2:D:177:ARG:HH12	1.67	0.60
2:A:213:LYS:NZ	6:A:402:ADP:O2'	2.35	0.60
1:M:302:MET:HG2	1:M:336:ARG:HE	1.67	0.59
2:C:213:LYS:NZ	6:C:402:ADP:O2'	2.35	0.59
2:B:213:LYS:NZ	6:B:402:ADP:O2'	2.35	0.59
1:M:138:ARG:NH2	1:M:183:ASP:OD2	2.26	0.59
2:B:111:ASN:HB3	2:B:177:ARG:HH12	1.67	0.59
1:N:138:ARG:NH2	1:N:183:ASP:OD2	2.26	0.59
2:A:111:ASN:HB3	2:A:177:ARG:HH12	1.67	0.59
3:F:2:EEP:N	3:F:2:EEP:O1	2.30	0.59
1:K:302:MET:HG2	1:K:336:ARG:HE	1.67	0.58
2:C:111:ASN:HB3	2:C:177:ARG:HH12	1.67	0.58
1:L:138:ARG:NH2	1:L:183:ASP:OD2	2.26	0.58
2:E:213:LYS:NZ	6:E:402:ADP:O2'	2.35	0.58
2:E:201:VAL:N	2:E:205:GLU:OE2	2.33	0.57
2:C:201:VAL:N	2:C:205:GLU:OE2	2.34	0.57
2:D:213:LYS:NZ	6:D:402:ADP:O2'	2.35	0.57
2:A:201:VAL:N	2:A:205:GLU:OE2	2.34	0.57
2:E:111:ASN:HB3	2:E:177:ARG:HH12	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:222:ASP:OD2	2:A:225:ASN:ND2	2.34	0.57
2:C:197:GLY:O	3:I:1:TRP:HE3	1.88	0.56
1:K:138:ARG:NH2	1:K:183:ASP:OD2	2.26	0.56
1:O:316:MET:N	1:O:329:GLU:OE1	2.38	0.56
2:E:157:ASP:OD2	2:E:183:ARG:NH2	2.30	0.56
2:B:201:VAL:N	2:B:205:GLU:OE2	2.33	0.56
1:M:316:MET:N	1:M:329:GLU:OE1	2.38	0.56
2:D:157:ASP:OD2	2:D:183:ARG:NH2	2.30	0.56
1:K:316:MET:N	1:K:329:GLU:OE1	2.38	0.56
1:N:316:MET:N	1:N:329:GLU:OE1	2.38	0.56
1:L:316:MET:N	1:L:329:GLU:OE1	2.38	0.55
2:B:222:ASP:OD2	2:B:225:ASN:ND2	2.34	0.55
1:M:135:THR:O	1:M:196:ALA:HB1	2.06	0.55
1:L:329:GLU:N	1:L:329:GLU:OE2	2.40	0.55
1:N:135:THR:O	1:N:196:ALA:HB1	2.06	0.55
1:N:329:GLU:OE2	1:N:329:GLU:N	2.40	0.55
1:O:329:GLU:N	1:O:329:GLU:OE2	2.40	0.55
1:O:177:GLU:OE1	1:O:179:ARG:NE	2.37	0.55
1:M:329:GLU:N	1:M:329:GLU:OE2	2.40	0.55
1:K:329:GLU:OE2	1:K:329:GLU:N	2.40	0.55
1:O:175:GLU:HB2	1:O:191:LEU:HD13	1.89	0.55
1:L:135:THR:O	1:L:196:ALA:HB1	2.06	0.54
2:B:141:SER:HB2	2:B:152:VAL:HG11	1.90	0.54
2:D:222:ASP:OD2	2:D:225:ASN:ND2	2.34	0.54
2:D:201:VAL:N	2:D:205:GLU:OE2	2.33	0.54
1:M:175:GLU:HB2	1:M:191:LEU:HD13	1.89	0.54
2:C:196:ARG:NH1	2:C:250:ILE:O	2.41	0.54
2:A:196:ARG:NH1	2:A:250:ILE:O	2.41	0.54
2:D:141:SER:HB2	2:D:152:VAL:HG11	1.90	0.54
1:O:64:ARG:NH2	1:O:305:ASN:OD1	2.38	0.54
1:K:135:THR:O	1:K:196:ALA:HB1	2.06	0.54
1:N:175:GLU:HB2	1:N:191:LEU:HD13	1.89	0.54
1:L:175:GLU:HB2	1:L:191:LEU:HD13	1.89	0.54
1:N:335:ASP:OD2	1:N:337:LYS:NZ	2.35	0.54
1:O:135:THR:O	1:O:196:ALA:HB1	2.06	0.54
2:B:196:ARG:NH1	2:B:250:ILE:O	2.41	0.54
2:D:196:ARG:NH1	2:D:250:ILE:O	2.41	0.54
2:E:222:ASP:OD2	2:E:225:ASN:ND2	2.34	0.54
1:L:177:GLU:OE1	1:L:179:ARG:NE	2.37	0.54
1:K:175:GLU:HB2	1:K:191:LEU:HD13	1.89	0.53
2:E:47:MET:N	2:E:47:MET:SD	2.80	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:196:ARG:NH1	2:E:250:ILE:O	2.41	0.53
1:O:335:ASP:OD2	1:O:337:LYS:NZ	2.35	0.53
2:C:141:SER:HB2	2:C:152:VAL:HG11	1.90	0.53
2:B:304:THR:HA	2:B:309:ILE:HD13	1.91	0.53
2:C:222:ASP:OD2	2:C:225:ASN:ND2	2.34	0.53
1:K:106:SER:OG	1:K:116:ILE:O	2.24	0.53
2:A:141:SER:HB2	2:A:152:VAL:HG11	1.90	0.52
2:E:141:SER:HB2	2:E:152:VAL:HG11	1.90	0.52
1:M:64:ARG:NH2	1:M:305:ASN:OD1	2.39	0.52
2:D:304:THR:HA	2:D:309:ILE:HD13	1.91	0.52
2:B:41:GLN:NE2	2:D:172:PRO:HG3	2.25	0.52
1:M:135:THR:HA	1:M:198:GLN:HG2	1.92	0.52
1:L:135:THR:HA	1:L:198:GLN:HG2	1.92	0.52
1:K:135:THR:HA	1:K:198:GLN:HG2	1.92	0.52
1:M:51:GLN:NE2	1:M:329:GLU:HB3	2.25	0.52
2:C:157:ASP:N	6:C:402:ADP:O3B	2.41	0.52
2:A:304:THR:HA	2:A:309:ILE:HD13	1.91	0.52
1:K:64:ARG:NH2	1:K:305:ASN:OD1	2.38	0.52
1:O:51:GLN:NE2	1:O:329:GLU:HB3	2.25	0.52
1:O:135:THR:HA	1:O:198:GLN:HG2	1.92	0.52
1:N:51:GLN:NE2	1:N:329:GLU:HB3	2.25	0.51
1:N:135:THR:HA	1:N:198:GLN:HG2	1.92	0.51
2:E:304:THR:HA	2:E:309:ILE:HD13	1.91	0.51
2:C:304:THR:HA	2:C:309:ILE:HD13	1.91	0.51
1:K:177:GLU:OE1	1:K:179:ARG:NE	2.38	0.51
2:E:216:LEU:HD22	2:E:250:ILE:HD12	1.93	0.51
1:K:51:GLN:NE2	1:K:329:GLU:HB3	2.25	0.51
1:L:51:GLN:NE2	1:L:329:GLU:HB3	2.25	0.51
2:A:216:LEU:HD22	2:A:250:ILE:HD12	1.93	0.51
2:D:157:ASP:N	6:D:402:ADP:O3B	2.41	0.51
2:E:140:LEU:O	2:E:342:GLY:HA3	2.11	0.51
2:C:216:LEU:HD22	2:C:250:ILE:HD12	1.93	0.51
2:B:140:LEU:O	2:B:342:GLY:HA3	2.10	0.50
2:C:140:LEU:O	2:C:342:GLY:HA3	2.11	0.50
2:A:140:LEU:O	2:A:342:GLY:HA3	2.10	0.50
2:D:208:ILE:O	2:D:212:ILE:HG13	2.12	0.50
1:N:177:GLU:OE1	1:N:179:ARG:NE	2.38	0.50
2:A:208:ILE:O	2:A:212:ILE:HG13	2.12	0.50
1:L:64:ARG:NH2	1:L:305:ASN:OD1	2.39	0.50
1:L:310:PHE:HB2	1:L:331:CYS:SG	2.52	0.50
1:K:189:SER:OG	1:K:194:SER:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:335:ASP:OD2	1:L:337:LYS:NZ	2.35	0.50
2:B:230:ALA:HB2	2:B:236:LEU:HD22	1.93	0.50
1:K:310:PHE:HB2	1:K:331:CYS:SG	2.52	0.50
2:A:86:TRP:HH2	2:A:119:MET:HG2	1.77	0.50
2:B:86:TRP:HH2	2:B:119:MET:HG2	1.77	0.50
2:E:208:ILE:O	2:E:212:ILE:HG13	2.12	0.50
1:L:189:SER:OG	1:L:194:SER:HA	2.12	0.50
2:D:140:LEU:O	2:D:342:GLY:HA3	2.11	0.50
2:D:216:LEU:HD22	2:D:250:ILE:HD12	1.93	0.50
2:D:237:GLU:HA	2:D:251:GLY:HA2	1.94	0.50
2:B:208:ILE:O	2:B:212:ILE:HG13	2.12	0.49
1:N:189:SER:OG	1:N:194:SER:HA	2.12	0.49
2:D:230:ALA:HB2	2:D:236:LEU:HD22	1.93	0.49
2:C:230:ALA:HB2	2:C:236:LEU:HD22	1.93	0.49
2:A:230:ALA:HB2	2:A:236:LEU:HD22	1.93	0.49
1:O:189:SER:OG	1:O:194:SER:HA	2.12	0.49
2:B:216:LEU:HD22	2:B:250:ILE:HD12	1.93	0.49
2:C:237:GLU:HA	2:C:251:GLY:HA2	1.94	0.49
2:A:237:GLU:HA	2:A:251:GLY:HA2	1.94	0.49
2:E:237:GLU:HA	2:E:251:GLY:HA2	1.95	0.49
1:M:310:PHE:HB2	1:M:331:CYS:SG	2.52	0.49
2:C:208:ILE:O	2:C:212:ILE:HG13	2.12	0.49
1:N:310:PHE:HB2	1:N:331:CYS:SG	2.52	0.49
2:E:230:ALA:HB2	2:E:236:LEU:HD22	1.93	0.49
1:O:114:ALA:O	1:O:118:LYS:HB2	2.13	0.49
1:O:310:PHE:HB2	1:O:331:CYS:SG	2.52	0.49
1:K:157:GLY:HA3	1:K:162:ARG:HH11	1.78	0.49
2:E:86:TRP:HH2	2:E:119:MET:HG2	1.77	0.49
1:M:189:SER:OG	1:M:194:SER:HA	2.12	0.49
1:K:201:ALA:HA	1:K:208:ALA:HA	1.95	0.49
1:L:114:ALA:O	1:L:118:LYS:HB2	2.13	0.49
1:M:114:ALA:O	1:M:118:LYS:HB2	2.13	0.49
1:N:114:ALA:O	1:N:118:LYS:HB2	2.13	0.49
1:O:157:GLY:HA3	1:O:162:ARG:HH11	1.78	0.49
2:D:86:TRP:HH2	2:D:119:MET:HG2	1.77	0.48
5:K:402:GH3:H4'	5:K:402:GH3:O2A	2.13	0.48
2:B:157:ASP:N	6:B:402:ADP:O3B	2.41	0.48
2:B:237:GLU:HA	2:B:251:GLY:HA2	1.94	0.48
1:L:157:GLY:HA3	1:L:162:ARG:HH11	1.78	0.48
2:E:157:ASP:N	6:E:402:ADP:O3B	2.41	0.48
1:M:157:GLY:HA3	1:M:162:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:402:GH3:O2A	5:M:402:GH3:H4'	2.13	0.48
1:N:64:ARG:NH2	1:N:305:ASN:OD1	2.38	0.48
1:M:201:ALA:HA	1:M:208:ALA:HA	1.95	0.48
1:K:81:LYS:NZ	5:K:402:GH3:O2A	2.41	0.48
5:K:402:GH3:N3	5:K:402:GH3:H2'	2.29	0.48
1:N:72:THR:O	1:N:76:GLU:HG2	2.14	0.48
5:O:402:GH3:N3	5:O:402:GH3:H2'	2.28	0.48
5:O:402:GH3:O2A	5:O:402:GH3:H4'	2.13	0.48
1:L:201:ALA:HA	1:L:208:ALA:HA	1.95	0.48
1:K:114:ALA:O	1:K:118:LYS:HB2	2.13	0.48
1:N:157:GLY:HA3	1:N:162:ARG:HH11	1.78	0.48
1:L:233:ARG:HA	1:L:266:THR:HG22	1.96	0.48
1:O:201:ALA:HA	1:O:208:ALA:HA	1.95	0.48
5:L:402:GH3:H2'	5:L:402:GH3:N3	2.29	0.48
1:N:233:ARG:HA	1:N:266:THR:HG22	1.96	0.48
2:C:86:TRP:HH2	2:C:119:MET:HG2	1.77	0.47
2:E:53:TYR:HB2	2:E:58:ALA:HB2	1.96	0.47
5:L:402:GH3:O2A	5:L:402:GH3:H4'	2.13	0.47
1:N:201:ALA:HA	1:N:208:ALA:HA	1.95	0.47
5:N:402:GH3:H4'	5:N:402:GH3:O2A	2.13	0.47
1:O:72:THR:O	1:O:76:GLU:HG2	2.14	0.47
1:O:233:ARG:HA	1:O:266:THR:HG22	1.96	0.47
2:E:166:TYR:CD1	2:E:289:ILE:HB	2.49	0.47
1:M:72:THR:O	1:M:76:GLU:HG2	2.14	0.47
2:C:166:TYR:CD1	2:C:289:ILE:HB	2.49	0.47
2:A:157:ASP:N	6:A:402:ADP:O3B	2.41	0.47
1:L:72:THR:O	1:L:76:GLU:HG2	2.14	0.47
2:C:53:TYR:HB2	2:C:58:ALA:HB2	1.96	0.47
2:E:51:ASP:OD1	2:E:52:SER:N	2.48	0.47
1:M:177:GLU:OE1	1:M:179:ARG:NE	2.37	0.47
2:A:53:TYR:HB2	2:A:58:ALA:HB2	1.96	0.47
2:A:166:TYR:CD1	2:A:289:ILE:HB	2.49	0.47
2:B:306:TYR:CE1	6:B:402:ADP:H2	2.33	0.47
1:M:233:ARG:HA	1:M:266:THR:HG22	1.96	0.47
5:M:402:GH3:H2'	5:M:402:GH3:N3	2.28	0.47
1:K:72:THR:O	1:K:76:GLU:HG2	2.14	0.47
2:D:51:ASP:OD1	2:D:52:SER:N	2.48	0.47
1:K:81:LYS:N	1:K:210:THR:O	2.48	0.47
1:K:233:ARG:HA	1:K:266:THR:HG22	1.96	0.46
2:B:51:ASP:OD1	2:B:52:SER:N	2.48	0.46
1:O:147:LEU:HA	1:O:151:PHE:HD1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:51:ASP:OD1	2:A:52:SER:N	2.48	0.46
2:D:53:TYR:HB2	2:D:58:ALA:HB2	1.96	0.46
2:D:199:SER:HB2	3:J:1:TRP:CE2	2.50	0.46
1:K:147:LEU:HA	1:K:151:PHE:HD1	1.80	0.46
5:N:402:GH3:H2'	5:N:402:GH3:N3	2.29	0.46
2:C:306:TYR:CE1	6:C:402:ADP:H2	2.33	0.46
2:A:306:TYR:CE1	6:A:402:ADP:H2	2.33	0.46
2:B:166:TYR:CD1	2:B:289:ILE:HB	2.49	0.46
2:D:166:TYR:CD1	2:D:289:ILE:HB	2.49	0.46
2:D:306:TYR:CE1	6:D:402:ADP:H2	2.33	0.46
2:E:306:TYR:CE1	6:E:402:ADP:H2	2.33	0.46
2:A:275:HIS:CD2	2:A:316:GLU:HB3	2.50	0.46
1:L:51:GLN:HE22	1:L:329:GLU:HB3	1.81	0.46
1:O:81:LYS:N	1:O:210:THR:O	2.48	0.46
1:M:147:LEU:HA	1:M:151:PHE:HD1	1.80	0.46
2:C:51:ASP:OD1	2:C:52:SER:N	2.48	0.46
2:B:53:TYR:HB2	2:B:58:ALA:HB2	1.96	0.46
1:N:147:LEU:HA	1:N:151:PHE:HD1	1.80	0.46
2:D:275:HIS:CD2	2:D:316:GLU:HB3	2.50	0.46
2:C:47:MET:HE2	1:O:378:VAL:HB	1.97	0.45
2:D:203:THR:O	2:D:204:ALA:HB3	2.16	0.45
1:L:157:GLY:HA3	1:L:162:ARG:NH1	2.31	0.45
1:M:81:LYS:N	1:M:210:THR:O	2.48	0.45
2:C:275:HIS:CD2	2:C:316:GLU:HB3	2.50	0.45
2:B:275:HIS:CD2	2:B:316:GLU:HB3	2.50	0.45
1:N:81:LYS:N	1:N:210:THR:O	2.48	0.45
2:E:203:THR:O	2:E:204:ALA:HB3	2.16	0.45
2:E:275:HIS:CD2	2:E:316:GLU:HB3	2.50	0.45
1:M:81:LYS:NZ	5:M:402:GH3:O2A	2.41	0.45
1:N:230:LEU:HA	1:N:267:PRO:HB2	1.98	0.45
2:C:47:MET:N	2:C:47:MET:SD	2.81	0.45
1:L:81:LYS:N	1:L:210:THR:O	2.48	0.45
2:B:203:THR:O	2:B:204:ALA:HB3	2.16	0.45
1:M:51:GLN:HE22	1:M:329:GLU:HB3	1.81	0.45
1:K:335:ASP:OD2	1:K:337:LYS:NZ	2.35	0.45
1:O:51:GLN:HE22	1:O:329:GLU:HB3	1.81	0.45
1:M:378:VAL:HB	2:A:47:MET:HE2	1.98	0.45
1:K:157:GLY:HA3	1:K:162:ARG:NH1	2.32	0.45
1:L:147:LEU:HA	1:L:151:PHE:HD1	1.80	0.45
2:C:203:THR:O	2:C:204:ALA:HB3	2.16	0.45
1:M:157:GLY:HA3	1:M:162:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:51:GLN:HE22	1:K:329:GLU:HB3	1.81	0.45
1:O:70:VAL:HG12	1:O:74:ILE:HG13	1.99	0.45
2:B:272:ALA:HB1	2:B:276:GLU:HB2	1.99	0.44
2:A:203:THR:O	2:A:204:ALA:HB3	2.16	0.44
1:N:162:ARG:O	1:N:178:ALA:HB3	2.17	0.44
1:M:230:LEU:HA	1:M:267:PRO:HB2	1.99	0.44
2:C:143:TYR:OH	2:A:44:MET:HA	2.16	0.44
1:L:162:ARG:O	1:L:178:ALA:HB3	2.17	0.44
2:B:12:ASN:CG	2:B:86:TRP:HE1	2.21	0.44
1:N:51:GLN:HE22	1:N:329:GLU:HB3	1.81	0.44
1:N:70:VAL:HG12	1:N:74:ILE:HG13	1.99	0.44
1:N:157:GLY:HA3	1:N:162:ARG:NH1	2.31	0.44
2:A:94:LEU:HD23	2:A:94:LEU:HA	1.78	0.44
1:L:230:LEU:HA	1:L:267:PRO:HB2	1.99	0.44
1:K:162:ARG:O	1:K:178:ALA:HB3	2.17	0.44
2:A:44:MET:HB3	2:A:47:MET:HE1	1.98	0.44
2:D:47:MET:SD	2:D:47:MET:N	2.81	0.44
1:O:134:GLN:O	1:O:198:GLN:HA	2.18	0.44
1:M:70:VAL:HG12	1:M:74:ILE:HG13	1.99	0.44
1:K:230:LEU:HA	1:K:267:PRO:HB2	1.98	0.44
2:D:216:LEU:CD2	2:D:250:ILE:HD12	2.48	0.44
2:D:272:ALA:HB1	2:D:276:GLU:HB2	2.00	0.44
2:E:12:ASN:CG	2:E:86:TRP:HE1	2.21	0.44
2:A:272:ALA:HB1	2:A:276:GLU:HB2	1.99	0.44
2:B:47:MET:SD	2:B:47:MET:N	2.81	0.44
2:D:12:ASN:CG	2:D:86:TRP:HE1	2.21	0.44
1:O:162:ARG:O	1:O:178:ALA:HB3	2.17	0.44
1:L:70:VAL:HG12	1:L:74:ILE:HG13	2.00	0.44
2:B:216:LEU:CD2	2:B:250:ILE:HD12	2.48	0.44
1:O:157:GLY:HA3	1:O:162:ARG:NH1	2.31	0.44
1:K:70:VAL:HG12	1:K:74:ILE:HG13	2.00	0.44
3:I:4:DTH:H	3:I:4:DTH:HG23	1.48	0.44
2:A:62:ARG:HG3	2:A:67:LEU:HD11	2.00	0.43
2:B:61:LYS:HE2	2:B:61:LYS:HB2	1.78	0.43
2:D:135:ALA:HB3	2:D:140:LEU:HD11	2.00	0.43
1:M:221:SER:O	1:M:224:ALA:N	2.50	0.43
2:B:62:ARG:HG3	2:B:67:LEU:HD11	2.00	0.43
2:D:62:ARG:HG3	2:D:67:LEU:HD11	2.00	0.43
2:E:216:LEU:CD2	2:E:250:ILE:HD12	2.48	0.43
1:M:162:ARG:O	1:M:178:ALA:HB3	2.17	0.43
1:M:311:TYR:CD1	1:M:311:TYR:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:ASN:CG	2:C:86:TRP:HE1	2.21	0.43
2:C:23:GLY:N	2:C:344:SER:OG	2.51	0.43
1:L:221:SER:O	1:L:224:ALA:N	2.50	0.43
1:L:311:TYR:CD1	1:L:311:TYR:N	2.87	0.43
2:B:244:ASP:O	2:D:322:PRO:HG3	2.18	0.43
1:K:311:TYR:N	1:K:311:TYR:CD1	2.86	0.43
2:A:12:ASN:CG	2:A:86:TRP:HE1	2.21	0.43
2:B:135:ALA:HB3	2:B:140:LEU:HD11	2.01	0.43
1:N:346:ILE:CG2	1:N:351:TYR:HB2	2.46	0.43
1:M:134:GLN:O	1:M:198:GLN:HA	2.18	0.43
2:C:216:LEU:CD2	2:C:250:ILE:HD12	2.48	0.43
1:O:214:ASP:OD2	1:O:291:HIS:HE1	2.02	0.43
1:O:230:LEU:HA	1:O:267:PRO:HB2	1.98	0.43
1:N:134:GLN:O	1:N:198:GLN:HA	2.18	0.43
1:N:311:TYR:CD1	1:N:311:TYR:N	2.86	0.43
2:D:142:LEU:HD23	2:D:142:LEU:HA	1.81	0.43
1:O:135:THR:HA	1:O:198:GLN:HA	2.01	0.43
2:E:23:GLY:N	2:E:344:SER:OG	2.51	0.43
2:E:135:ALA:HB3	2:E:140:LEU:HD11	2.00	0.43
1:M:214:ASP:OD2	1:M:291:HIS:HE1	2.02	0.43
1:M:280:LEU:HD23	1:M:280:LEU:HA	1.85	0.43
2:A:64:ILE:HD13	2:A:64:ILE:HA	1.79	0.43
2:C:62:ARG:HG3	2:C:67:LEU:HD11	2.00	0.43
3:H:1:TRP:CE3	2:B:197:GLY:O	2.64	0.43
1:L:135:THR:HA	1:L:198:GLN:HA	2.01	0.43
2:B:248:ILE:HD13	2:B:248:ILE:HG21	1.73	0.43
2:E:240:TYR:O	2:E:248:ILE:HG22	2.19	0.43
2:E:272:ALA:HB1	2:E:276:GLU:HB2	2.00	0.43
3:J:4:DTH:H	3:J:4:DTH:HG23	1.48	0.43
2:C:272:ALA:HB1	2:C:276:GLU:HB2	2.00	0.43
2:B:23:GLY:N	2:B:344:SER:OG	2.51	0.43
2:D:240:TYR:O	2:D:248:ILE:HG22	2.19	0.43
1:K:134:GLN:O	1:K:198:GLN:HA	2.18	0.43
1:K:214:ASP:OD2	1:K:291:HIS:HE1	2.02	0.43
2:A:216:LEU:CD2	2:A:250:ILE:HD12	2.48	0.43
1:O:346:ILE:CG2	1:O:351:TYR:HB2	2.46	0.43
1:M:135:THR:HA	1:M:198:GLN:HA	2.01	0.42
2:C:135:ALA:HB3	2:C:140:LEU:HD11	2.01	0.42
2:C:197:GLY:O	3:I:1:TRP:CE3	2.70	0.42
2:B:240:TYR:O	2:B:248:ILE:HG22	2.19	0.42
1:N:132:TYR:CG	1:N:133:THR:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:135:THR:HA	1:N:198:GLN:HA	2.01	0.42
2:A:240:TYR:O	2:A:248:ILE:HG22	2.19	0.42
2:C:240:TYR:O	2:C:248:ILE:HG22	2.19	0.42
1:L:134:GLN:O	1:L:198:GLN:HA	2.18	0.42
1:O:230:LEU:HB3	1:O:268:ARG:HB2	2.01	0.42
2:E:13:GLY:HA3	6:E:402:ADP:O2B	2.19	0.42
2:C:248:ILE:HD13	2:C:248:ILE:HG21	1.73	0.42
1:K:230:LEU:HB3	1:K:268:ARG:HB2	2.01	0.42
1:N:214:ASP:OD2	1:N:291:HIS:HE1	2.01	0.42
1:O:81:LYS:NZ	5:O:402:GH3:O2A	2.41	0.42
1:L:132:TYR:CG	1:L:133:THR:N	2.88	0.42
1:L:214:ASP:OD2	1:L:291:HIS:HE1	2.01	0.42
1:N:148:VAL:HG21	1:N:155:ALA:HB2	2.02	0.42
2:D:61:LYS:HE2	2:D:61:LYS:HB2	1.78	0.42
2:E:62:ARG:HG3	2:E:67:LEU:HD11	2.00	0.42
1:M:335:ASP:OD2	1:M:337:LYS:NZ	2.35	0.42
2:A:135:ALA:HB3	2:A:140:LEU:HD11	2.00	0.42
2:B:12:ASN:ND2	2:B:86:TRP:HE1	2.18	0.42
1:M:230:LEU:HB3	1:M:268:ARG:HB2	2.01	0.42
1:L:81:LYS:NZ	5:L:402:GH3:O2A	2.41	0.42
2:D:23:GLY:N	2:D:344:SER:OG	2.51	0.42
2:D:199:SER:HB2	3:J:1:TRP:CD2	2.55	0.42
2:E:12:ASN:ND2	2:E:86:TRP:HE1	2.18	0.42
2:A:192:ILE:HD12	2:A:192:ILE:HG23	1.90	0.42
1:L:346:ILE:CG2	1:L:351:TYR:HB2	2.46	0.42
1:N:81:LYS:NZ	5:N:402:GH3:O2A	2.41	0.42
1:O:132:TYR:CG	1:O:133:THR:N	2.87	0.42
1:O:311:TYR:CD1	1:O:311:TYR:N	2.87	0.42
2:C:44:MET:HB3	2:C:47:MET:HE1	2.01	0.42
3:F:4:DTH:H	3:F:4:DTH:HG23	1.48	0.42
1:O:95:GLN:HG3	1:O:100:CYS:SG	2.60	0.42
1:K:135:THR:HA	1:K:198:GLN:HA	2.01	0.41
2:D:248:ILE:HD13	2:D:248:ILE:HG21	1.73	0.41
1:O:148:VAL:HG21	1:O:155:ALA:HB2	2.02	0.41
1:M:95:GLN:HG3	1:M:100:CYS:SG	2.60	0.41
1:M:132:TYR:CG	1:M:133:THR:N	2.87	0.41
2:E:248:ILE:HD13	2:E:248:ILE:HG21	1.73	0.41
1:M:148:VAL:HG21	1:M:155:ALA:HB2	2.02	0.41
1:M:346:ILE:CG2	1:M:351:TYR:HB2	2.46	0.41
2:C:12:ASN:ND2	2:C:86:TRP:HE1	2.18	0.41
3:H:1:TRP:CD2	2:B:199:SER:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:148:VAL:HG21	1:K:155:ALA:HB2	2.02	0.41
2:C:13:GLY:HA3	6:C:402:ADP:O2B	2.19	0.41
2:A:13:GLY:HA3	6:A:402:ADP:O2B	2.19	0.41
1:N:221:SER:O	1:N:224:ALA:N	2.50	0.41
1:N:273:VAL:O	1:N:277:ASN:ND2	2.50	0.41
2:E:220:ALA:HB1	2:E:226:GLU:HG3	2.03	0.41
2:C:335:ARG:HA	2:C:338:SER:OG	2.21	0.41
1:K:132:TYR:CG	1:K:133:THR:N	2.87	0.41
2:B:94:LEU:HA	2:B:94:LEU:HD23	1.78	0.41
1:O:273:VAL:O	1:O:277:ASN:ND2	2.50	0.41
2:C:61:LYS:HB2	2:C:61:LYS:HE2	1.78	0.41
2:C:220:ALA:HB1	2:C:226:GLU:HG3	2.03	0.41
1:K:95:GLN:HG3	1:K:100:CYS:SG	2.60	0.41
2:B:13:GLY:HA3	6:B:402:ADP:O2B	2.19	0.41
2:D:13:GLY:HA3	6:D:402:ADP:O2B	2.20	0.41
2:E:237:GLU:HA	2:E:251:GLY:CA	2.51	0.41
1:K:273:VAL:O	1:K:277:ASN:ND2	2.50	0.41
1:L:230:LEU:HB3	1:L:268:ARG:HB2	2.01	0.41
2:B:335:ARG:HA	2:B:338:SER:OG	2.21	0.41
1:N:66:VAL:HG21	1:N:213:TYR:CD2	2.56	0.41
2:D:12:ASN:ND2	2:D:86:TRP:HE1	2.18	0.41
2:C:43:VAL:HG11	2:E:375:PHE:HZ	1.86	0.41
2:C:53:TYR:CB	2:C:58:ALA:HB2	2.51	0.41
2:C:64:ILE:HA	2:C:64:ILE:HD13	1.79	0.41
2:C:237:GLU:HA	2:C:251:GLY:CA	2.51	0.41
2:A:47:MET:N	2:A:47:MET:SD	2.80	0.41
1:L:95:GLN:HG3	1:L:100:CYS:SG	2.60	0.41
1:N:230:LEU:HB3	1:N:268:ARG:HB2	2.01	0.41
1:N:106:SER:OG	1:N:116:ILE:O	2.24	0.41
1:M:41:GLY:N	1:M:66:VAL:O	2.53	0.40
1:K:173:ARG:HH11	1:K:173:ARG:HD3	1.78	0.40
1:K:346:ILE:CG2	1:K:351:TYR:HB2	2.46	0.40
2:D:102:PRO:HA	2:D:131:ALA:O	2.22	0.40
1:O:221:SER:O	1:O:224:ALA:N	2.50	0.40
2:E:335:ARG:HA	2:E:338:SER:OG	2.21	0.40
1:M:66:VAL:HG21	1:M:213:TYR:CD2	2.56	0.40
2:A:23:GLY:N	2:A:344:SER:OG	2.51	0.40
1:L:66:VAL:HG21	1:L:213:TYR:CD2	2.56	0.40
2:B:53:TYR:CB	2:B:58:ALA:HB2	2.51	0.40
1:N:95:GLN:HG3	1:N:100:CYS:SG	2.60	0.40
1:M:99:ILE:HG21	1:M:200:LEU:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:63:ILE:HG22	1:K:64:ARG:O	2.22	0.40
1:K:66:VAL:HG21	1:K:213:TYR:CD2	2.56	0.40
1:K:364:ARG:NH2	2:A:334:GLU:OE2	2.54	0.40
2:A:12:ASN:ND2	2:A:86:TRP:HE1	2.18	0.40
2:A:237:GLU:HA	2:A:251:GLY:CA	2.51	0.40
1:L:148:VAL:HG21	1:L:155:ALA:HB2	2.02	0.40
3:G:4:DTH:H	3:G:4:DTH:HG23	1.48	0.40
2:D:335:ARG:HA	2:D:338:SER:OG	2.21	0.40
1:O:66:VAL:HG21	1:O:213:TYR:CD2	2.56	0.40
1:O:138:ARG:HB3	1:O:185:LEU:HD13	2.03	0.40
2:C:153:LEU:O	2:C:153:LEU:HG	2.22	0.40
1:K:99:ILE:HG21	1:K:200:LEU:HD12	2.04	0.40
2:A:102:PRO:HA	2:A:131:ALA:O	2.22	0.40
1:L:82:GLY:HA2	1:L:290:HIS:ND1	2.36	0.40
1:M:273:VAL:O	1:M:277:ASN:ND2	2.50	0.40
1:K:82:GLY:HA2	1:K:290:HIS:ND1	2.36	0.40
2:A:335:ARG:HA	2:A:338:SER:OG	2.21	0.40
1:L:138:ARG:HB3	1:L:185:LEU:HD13	2.03	0.40
2:D:220:ALA:HB1	2:D:226:GLU:HG3	2.03	0.40
1:O:82:GLY:HA2	1:O:290:HIS:ND1	2.36	0.40
1:O:99:ILE:HG21	1:O:200:LEU:HD12	2.04	0.40
1:O:326:ARG:HG3	1:O:327:PHE:CD1	2.57	0.40
2:E:21:PHE:CE1	2:E:96:VAL:HG11	2.57	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	K	343/773 (44%)	325 (95%)	18 (5%)	0	100	100
1	L	343/773 (44%)	325 (95%)	18 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	343/773 (44%)	325 (95%)	18 (5%)	0	100	100
1	N	343/773 (44%)	324 (94%)	19 (6%)	0	100	100
1	O	343/773 (44%)	324 (94%)	19 (6%)	0	100	100
2	A	369/377 (98%)	345 (94%)	24 (6%)	0	100	100
2	B	369/377 (98%)	344 (93%)	25 (7%)	0	100	100
2	C	369/377 (98%)	345 (94%)	24 (6%)	0	100	100
2	D	369/377 (98%)	344 (93%)	25 (7%)	0	100	100
2	E	369/377 (98%)	345 (94%)	24 (6%)	0	100	100
3	F	2/7 (29%)	2 (100%)	0	0	100	100
3	G	2/7 (29%)	2 (100%)	0	0	100	100
3	H	2/7 (29%)	2 (100%)	0	0	100	100
3	I	2/7 (29%)	2 (100%)	0	0	100	100
3	J	2/7 (29%)	2 (100%)	0	0	100	100
All	All	3570/5785 (62%)	3356 (94%)	214 (6%)	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	K	280/623 (45%)	276 (99%)	4 (1%)	67	86
1	L	280/623 (45%)	276 (99%)	4 (1%)	67	86
1	M	280/623 (45%)	276 (99%)	4 (1%)	67	86
1	N	280/623 (45%)	276 (99%)	4 (1%)	67	86
1	O	280/623 (45%)	276 (99%)	4 (1%)	67	86
2	A	314/320 (98%)	313 (100%)	1 (0%)	92	96
2	B	314/320 (98%)	313 (100%)	1 (0%)	92	96
2	C	314/320 (98%)	313 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	314/320 (98%)	313 (100%)	1 (0%)	92 96
2	E	314/320 (98%)	313 (100%)	1 (0%)	92 96
3	F	2/2 (100%)	1 (50%)	1 (50%)	0 0
3	G	2/2 (100%)	1 (50%)	1 (50%)	0 0
3	H	2/2 (100%)	1 (50%)	1 (50%)	0 0
3	I	2/2 (100%)	1 (50%)	1 (50%)	0 0
3	J	2/2 (100%)	1 (50%)	1 (50%)	0 0
All	All	2980/4725 (63%)	2950 (99%)	30 (1%)	77 90

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	125	LYS
1	M	183	ASP
1	M	216	PHE
1	M	262	ARG
2	C	44	MET
3	H	5	CYS
1	K	125	LYS
1	K	183	ASP
1	K	216	PHE
1	K	262	ARG
2	A	44	MET
3	F	5	CYS
1	L	125	LYS
1	L	183	ASP
1	L	216	PHE
1	L	262	ARG
2	B	44	MET
3	G	5	CYS
1	N	125	LYS
1	N	183	ASP
1	N	216	PHE
1	N	262	ARG
2	D	44	MET
3	I	5	CYS
1	O	125	LYS
1	O	183	ASP
1	O	216	PHE
1	O	262	ARG

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Mol	Chain	Res	Type
2	E	44	MET
3	J	5	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	51	GLN
1	M	103	GLN
2	C	246	GLN
1	K	51	GLN
1	K	103	GLN
2	A	246	GLN
1	L	51	GLN
1	L	103	GLN
2	B	41	GLN
2	B	246	GLN
1	N	51	GLN
1	N	103	GLN
2	D	246	GLN
1	O	51	GLN
1	O	103	GLN
2	E	246	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 10 are monoatomic - leaving 15 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

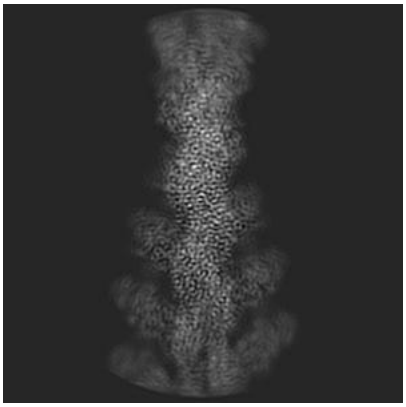
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13158. These allow visual inspection of the internal detail of the map and identification of artifacts.

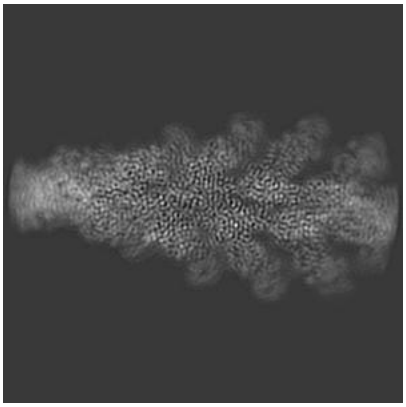
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

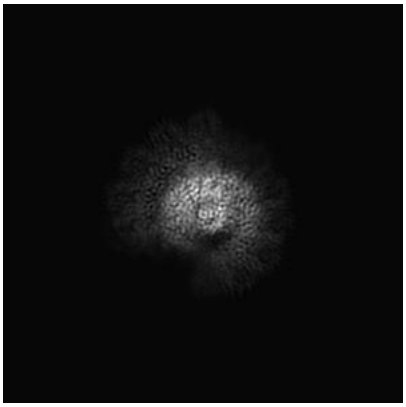
6.1.1 Primary map



X



Y

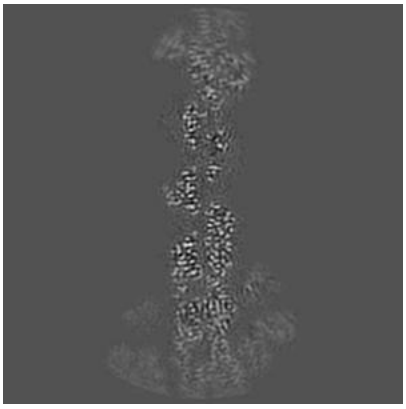


Z

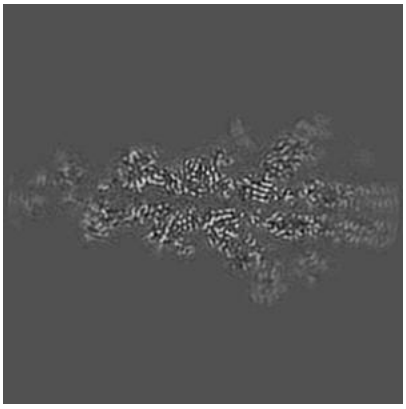
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 150



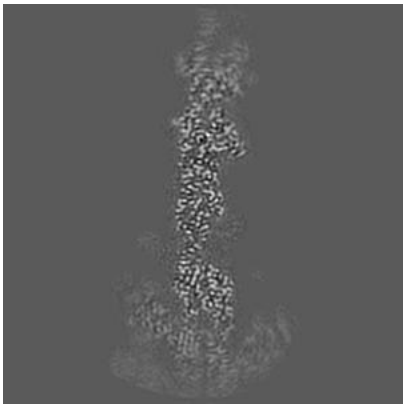
Y Index: 150

Z Index: 150

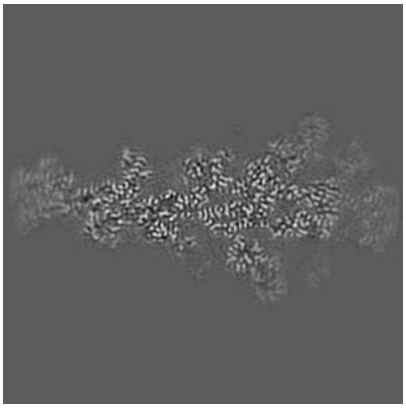
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 162



Y Index: 157

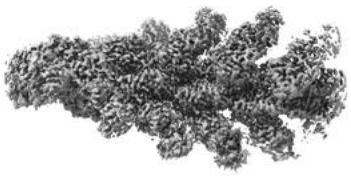
Z Index: 168

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

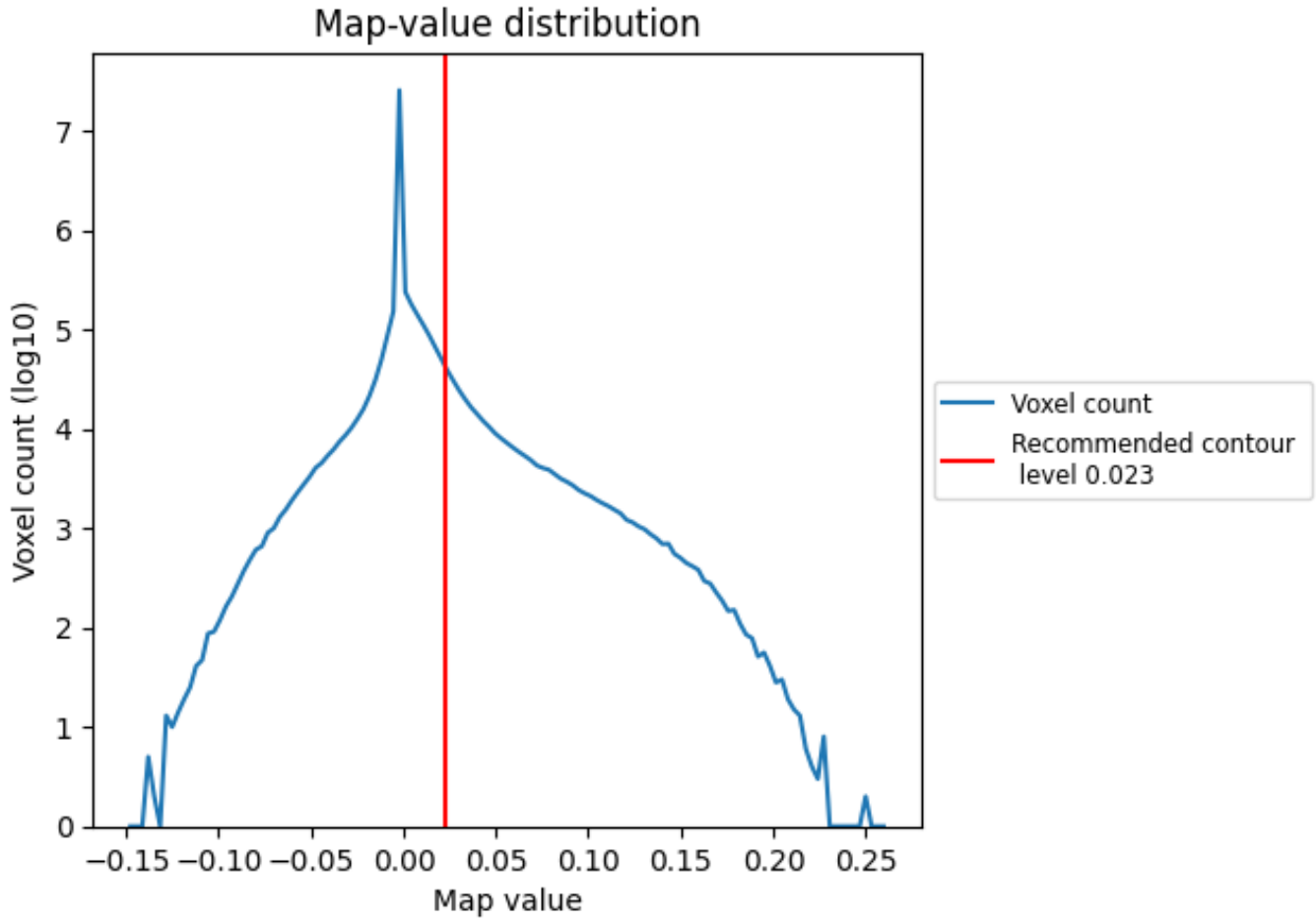
6.5 Mask visualisation (i)

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

7 Map analysis

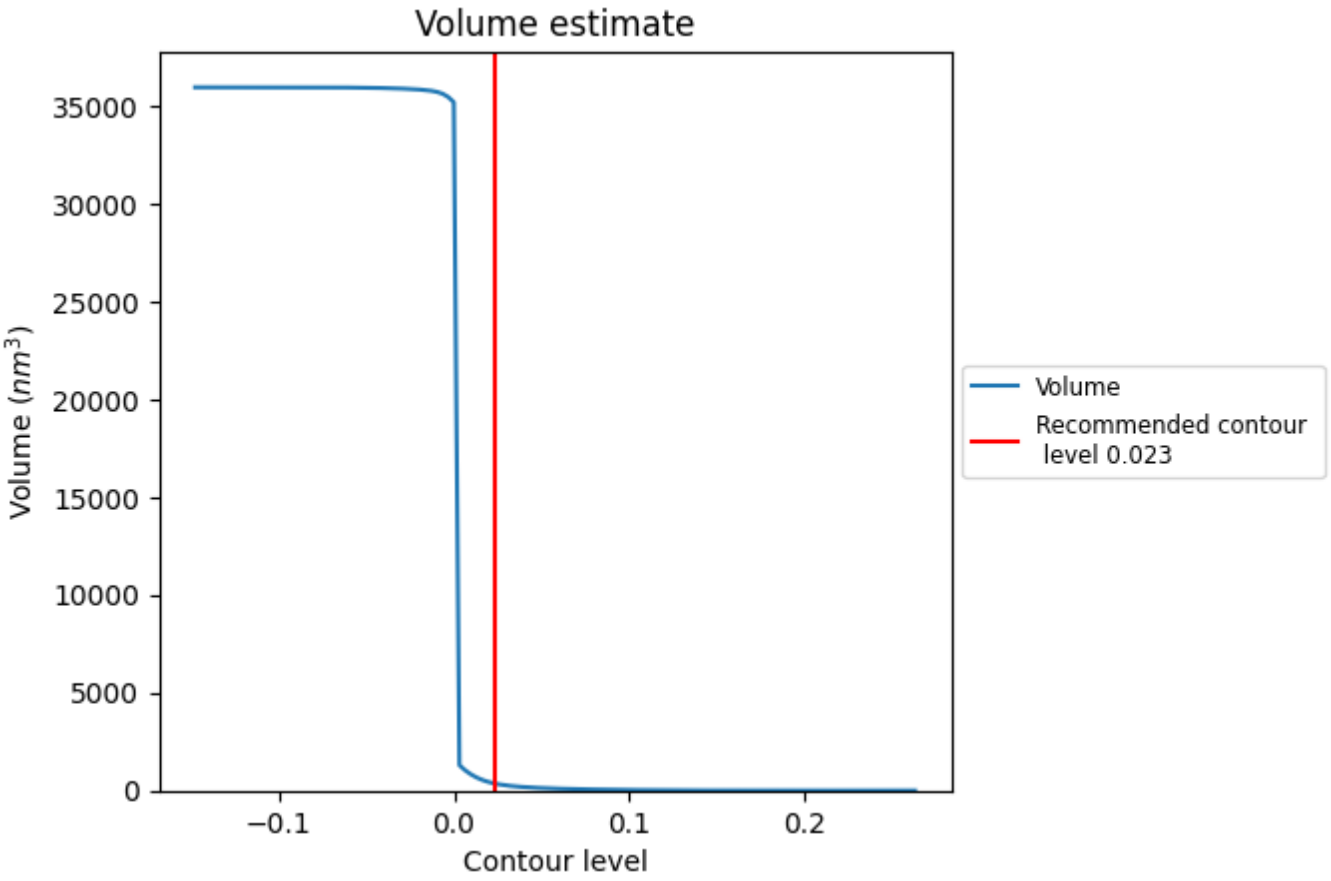
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

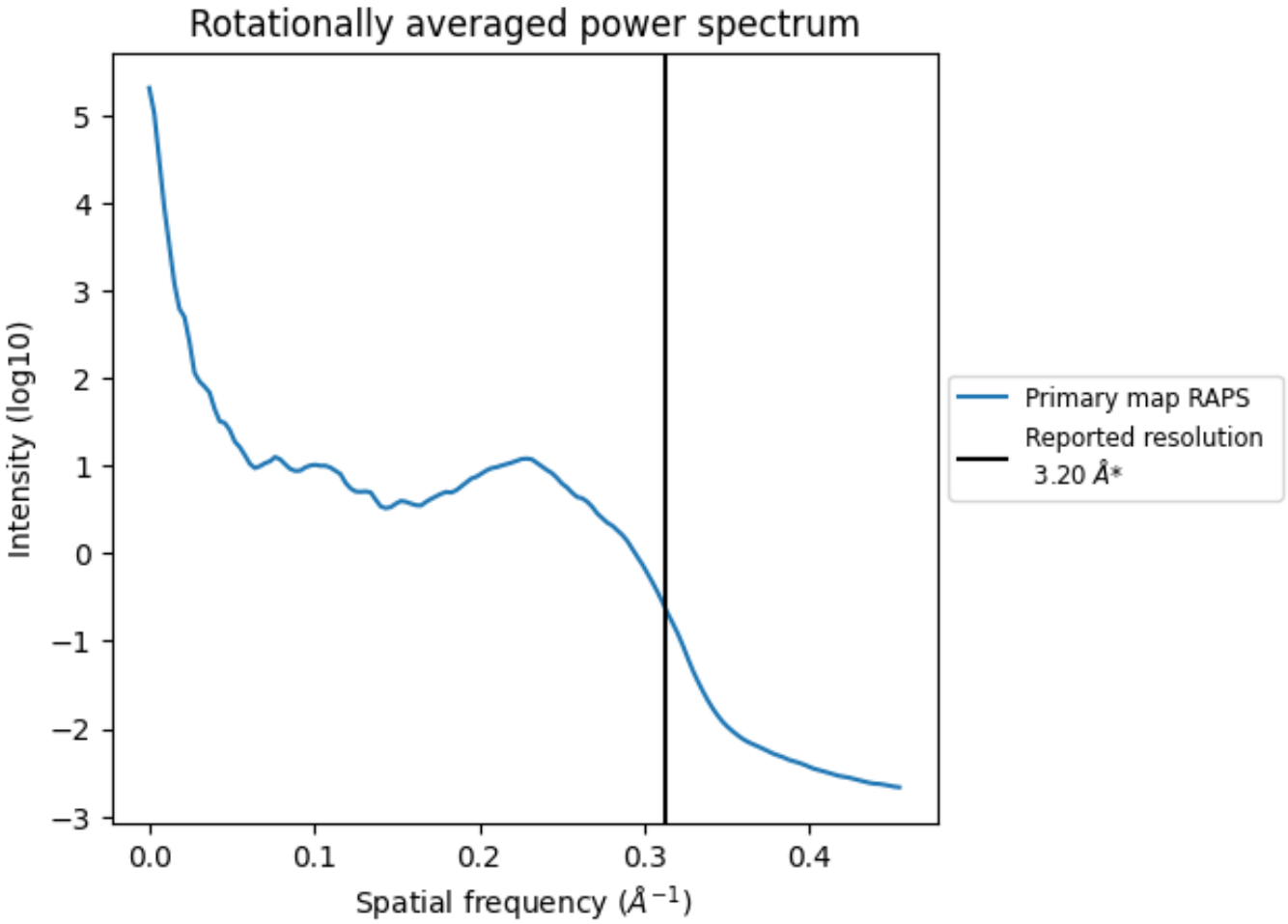
7.2 Volume estimate



The volume at the recommended contour level is 366 nm^3; this corresponds to an approximate mass of 330 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)

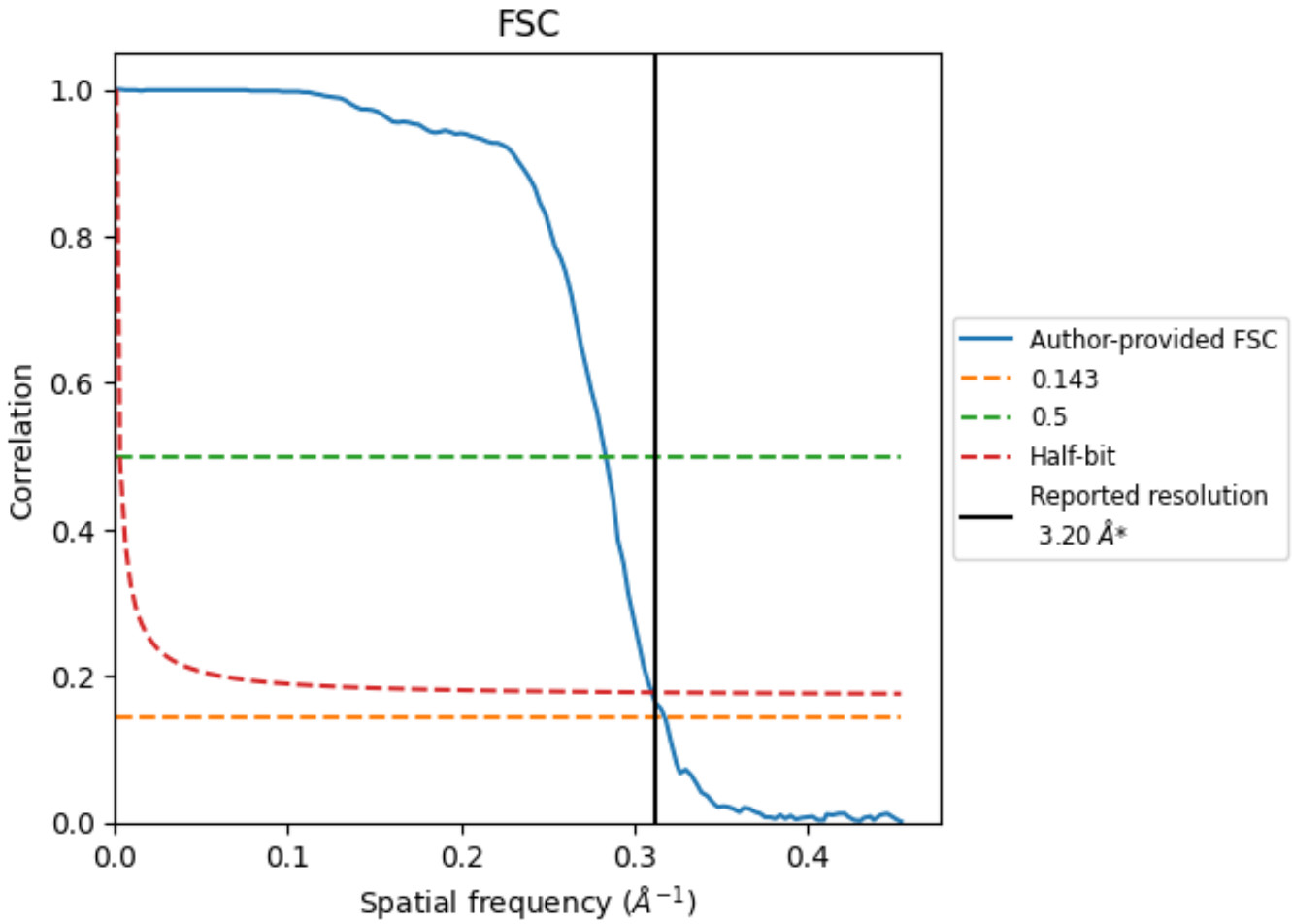


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

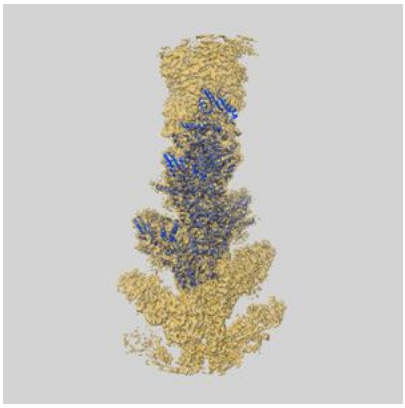
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.53	3.22
Unmasked-calculated*	-	-	-

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

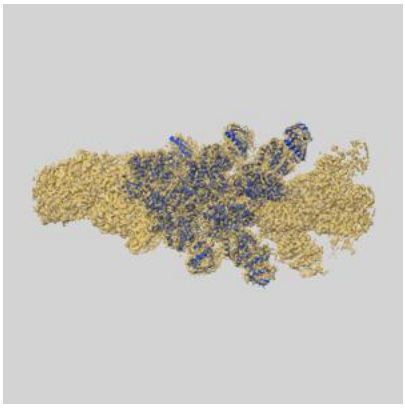
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13158 and PDB model 7P1G. Per-residue inclusion information can be found in section 3 on page 12.

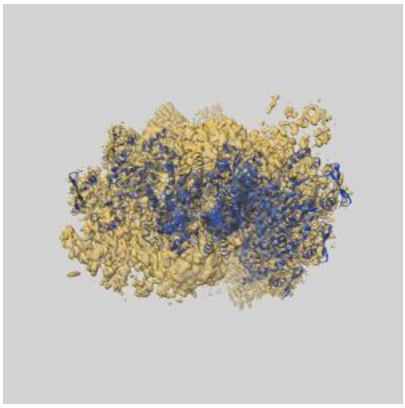
9.1 Map-model overlay



X



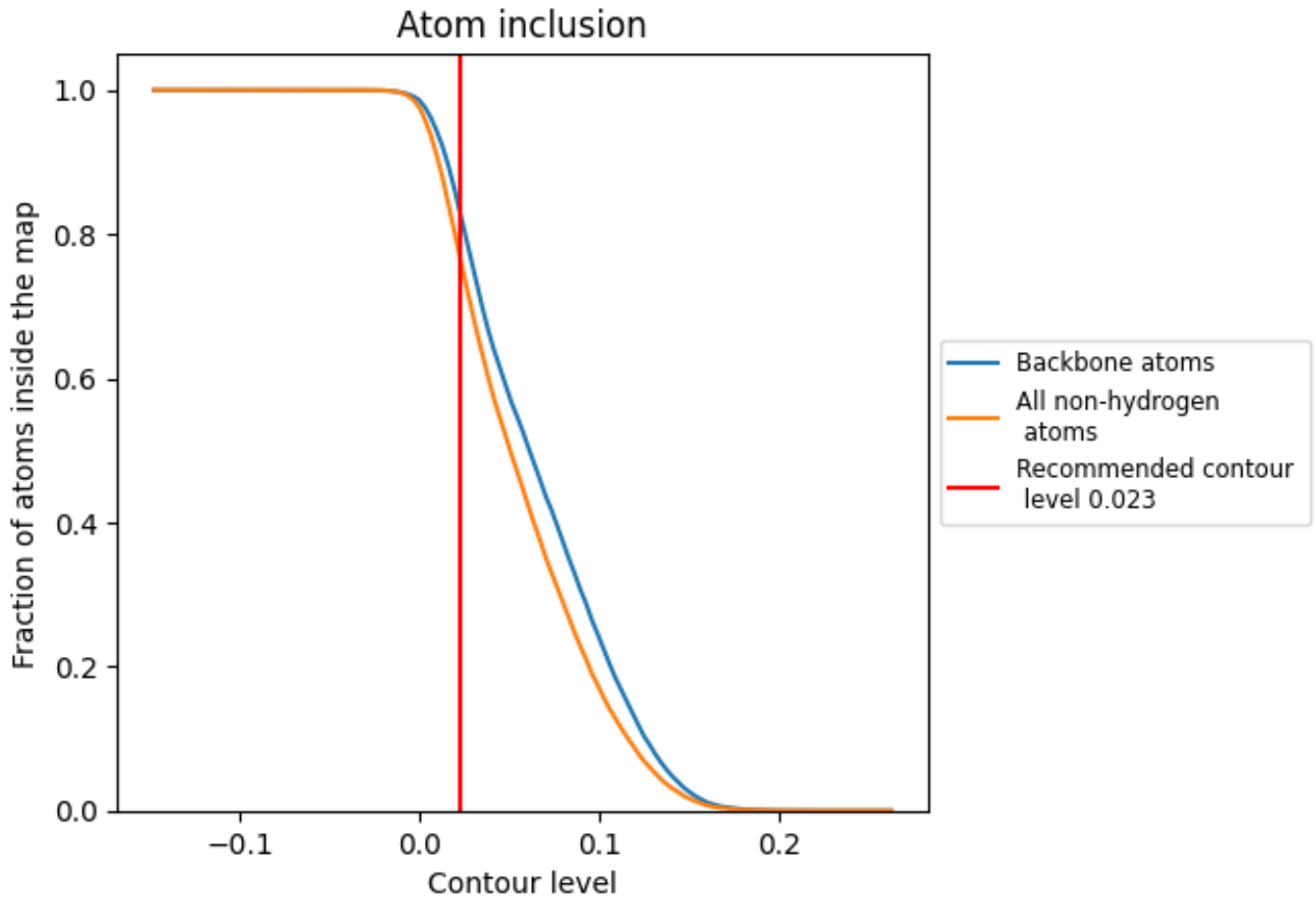
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.023 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 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.