Full wwPDB EM Validation Report (i)

Feb 25, 2024 – 07:42 AM EST

PDB ID	:	7JLX
EMDB ID	:	EMD-22383
Title	:	Structure of the activated Roq1 resistosome directly recognizing the pathogen effector XopQ (TIR domains)
Authors	:	Martin, R.; Qi, T.; Zhang, H.; Lui, F.; King, M.; Toth, C.; Nogales, E.; Staskawicz, B.J.
Deposited on	:	2020-07-30
Resolution	:	4.60 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

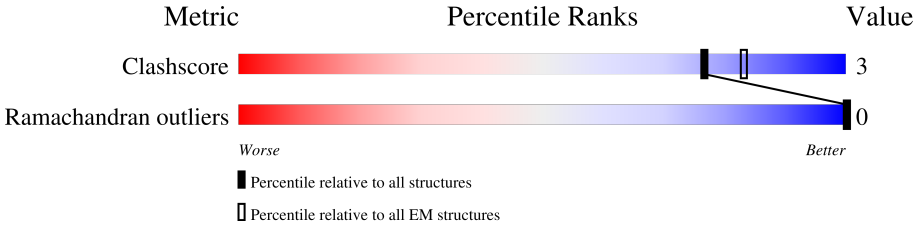
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.60 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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1328	12% • 88%
1	B	1328	12% • 88%
1	C	1328	12% 88%
1	D	1328	12% 88%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3288 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 Disease resistance protein Roq1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	B	166	822	490	166	166	0	0
1	C	166	822	490	166	166	0	0
1	A	166	822	490	166	166	0	0
1	D	166	822	490	166	166	0	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1307	ASP	-	expression tag	UNP A0A290U7C4
B	1308	TYR	-	expression tag	UNP A0A290U7C4
B	1309	LYS	-	expression tag	UNP A0A290U7C4
B	1310	ASP	-	expression tag	UNP A0A290U7C4
B	1311	HIS	-	expression tag	UNP A0A290U7C4
B	1312	ASP	-	expression tag	UNP A0A290U7C4
B	1313	GLY	-	expression tag	UNP A0A290U7C4
B	1314	ASP	-	expression tag	UNP A0A290U7C4
B	1315	TYR	-	expression tag	UNP A0A290U7C4
B	1316	LYS	-	expression tag	UNP A0A290U7C4
B	1317	ASP	-	expression tag	UNP A0A290U7C4
B	1318	HIS	-	expression tag	UNP A0A290U7C4
B	1319	ASP	-	expression tag	UNP A0A290U7C4
B	1320	ILE	-	expression tag	UNP A0A290U7C4
B	1321	ASP	-	expression tag	UNP A0A290U7C4
B	1322	TYR	-	expression tag	UNP A0A290U7C4
B	1323	LYS	-	expression tag	UNP A0A290U7C4
B	1324	ASP	-	expression tag	UNP A0A290U7C4
B	1325	ASP	-	expression tag	UNP A0A290U7C4
B	1326	ASP	-	expression tag	UNP A0A290U7C4
B	1327	ASP	-	expression tag	UNP A0A290U7C4
B	1328	LYS	-	expression tag	UNP A0A290U7C4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1307	ASP	-	expression tag	UNP A0A290U7C4
C	1308	TYR	-	expression tag	UNP A0A290U7C4
C	1309	LYS	-	expression tag	UNP A0A290U7C4
C	1310	ASP	-	expression tag	UNP A0A290U7C4
C	1311	HIS	-	expression tag	UNP A0A290U7C4
C	1312	ASP	-	expression tag	UNP A0A290U7C4
C	1313	GLY	-	expression tag	UNP A0A290U7C4
C	1314	ASP	-	expression tag	UNP A0A290U7C4
C	1315	TYR	-	expression tag	UNP A0A290U7C4
C	1316	LYS	-	expression tag	UNP A0A290U7C4
C	1317	ASP	-	expression tag	UNP A0A290U7C4
C	1318	HIS	-	expression tag	UNP A0A290U7C4
C	1319	ASP	-	expression tag	UNP A0A290U7C4
C	1320	ILE	-	expression tag	UNP A0A290U7C4
C	1321	ASP	-	expression tag	UNP A0A290U7C4
C	1322	TYR	-	expression tag	UNP A0A290U7C4
C	1323	LYS	-	expression tag	UNP A0A290U7C4
C	1324	ASP	-	expression tag	UNP A0A290U7C4
C	1325	ASP	-	expression tag	UNP A0A290U7C4
C	1326	ASP	-	expression tag	UNP A0A290U7C4
C	1327	ASP	-	expression tag	UNP A0A290U7C4
C	1328	LYS	-	expression tag	UNP A0A290U7C4
A	1307	ASP	-	expression tag	UNP A0A290U7C4
A	1308	TYR	-	expression tag	UNP A0A290U7C4
A	1309	LYS	-	expression tag	UNP A0A290U7C4
A	1310	ASP	-	expression tag	UNP A0A290U7C4
A	1311	HIS	-	expression tag	UNP A0A290U7C4
A	1312	ASP	-	expression tag	UNP A0A290U7C4
A	1313	GLY	-	expression tag	UNP A0A290U7C4
A	1314	ASP	-	expression tag	UNP A0A290U7C4
A	1315	TYR	-	expression tag	UNP A0A290U7C4
A	1316	LYS	-	expression tag	UNP A0A290U7C4
A	1317	ASP	-	expression tag	UNP A0A290U7C4
A	1318	HIS	-	expression tag	UNP A0A290U7C4
A	1319	ASP	-	expression tag	UNP A0A290U7C4
A	1320	ILE	-	expression tag	UNP A0A290U7C4
A	1321	ASP	-	expression tag	UNP A0A290U7C4
A	1322	TYR	-	expression tag	UNP A0A290U7C4
A	1323	LYS	-	expression tag	UNP A0A290U7C4
A	1324	ASP	-	expression tag	UNP A0A290U7C4
A	1325	ASP	-	expression tag	UNP A0A290U7C4
A	1326	ASP	-	expression tag	UNP A0A290U7C4

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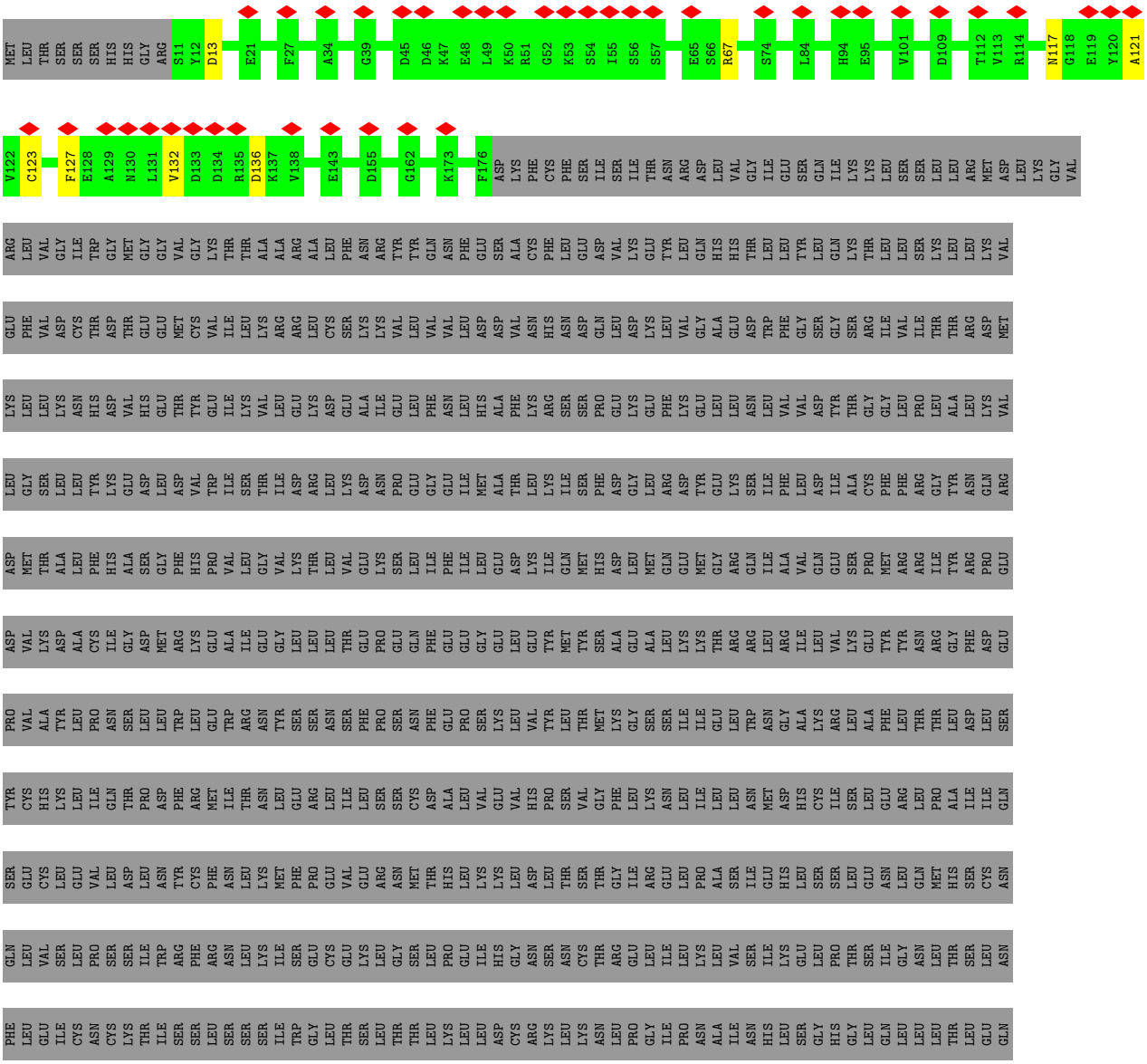
Chain	Residue	Modelled	Actual	Comment	Reference
A	1327	ASP	-	expression tag	UNP A0A290U7C4
A	1328	LYS	-	expression tag	UNP A0A290U7C4
D	1307	ASP	-	expression tag	UNP A0A290U7C4
D	1308	TYR	-	expression tag	UNP A0A290U7C4
D	1309	LYS	-	expression tag	UNP A0A290U7C4
D	1310	ASP	-	expression tag	UNP A0A290U7C4
D	1311	HIS	-	expression tag	UNP A0A290U7C4
D	1312	ASP	-	expression tag	UNP A0A290U7C4
D	1313	GLY	-	expression tag	UNP A0A290U7C4
D	1314	ASP	-	expression tag	UNP A0A290U7C4
D	1315	TYR	-	expression tag	UNP A0A290U7C4
D	1316	LYS	-	expression tag	UNP A0A290U7C4
D	1317	ASP	-	expression tag	UNP A0A290U7C4
D	1318	HIS	-	expression tag	UNP A0A290U7C4
D	1319	ASP	-	expression tag	UNP A0A290U7C4
D	1320	ILE	-	expression tag	UNP A0A290U7C4
D	1321	ASP	-	expression tag	UNP A0A290U7C4
D	1322	TYR	-	expression tag	UNP A0A290U7C4
D	1323	LYS	-	expression tag	UNP A0A290U7C4
D	1324	ASP	-	expression tag	UNP A0A290U7C4
D	1325	ASP	-	expression tag	UNP A0A290U7C4
D	1326	ASP	-	expression tag	UNP A0A290U7C4
D	1327	ASP	-	expression tag	UNP A0A290U7C4
D	1328	LYS	-	expression tag	UNP A0A290U7C4

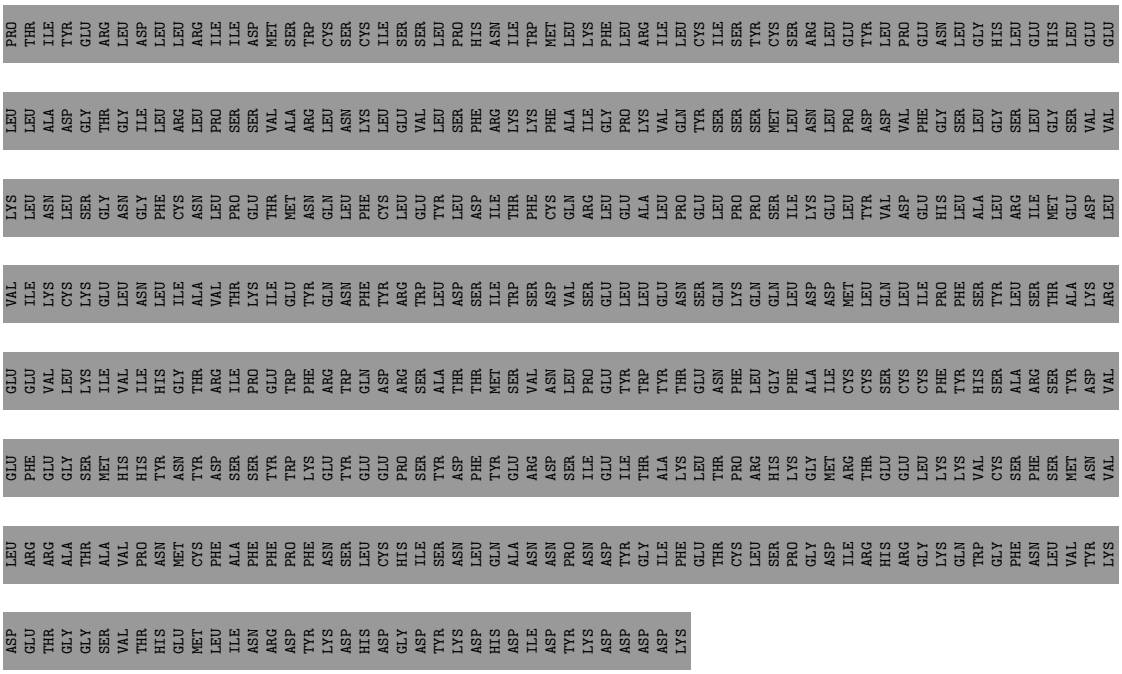
3 Residue-property plots (i)

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: Disease resistance protein Roq1

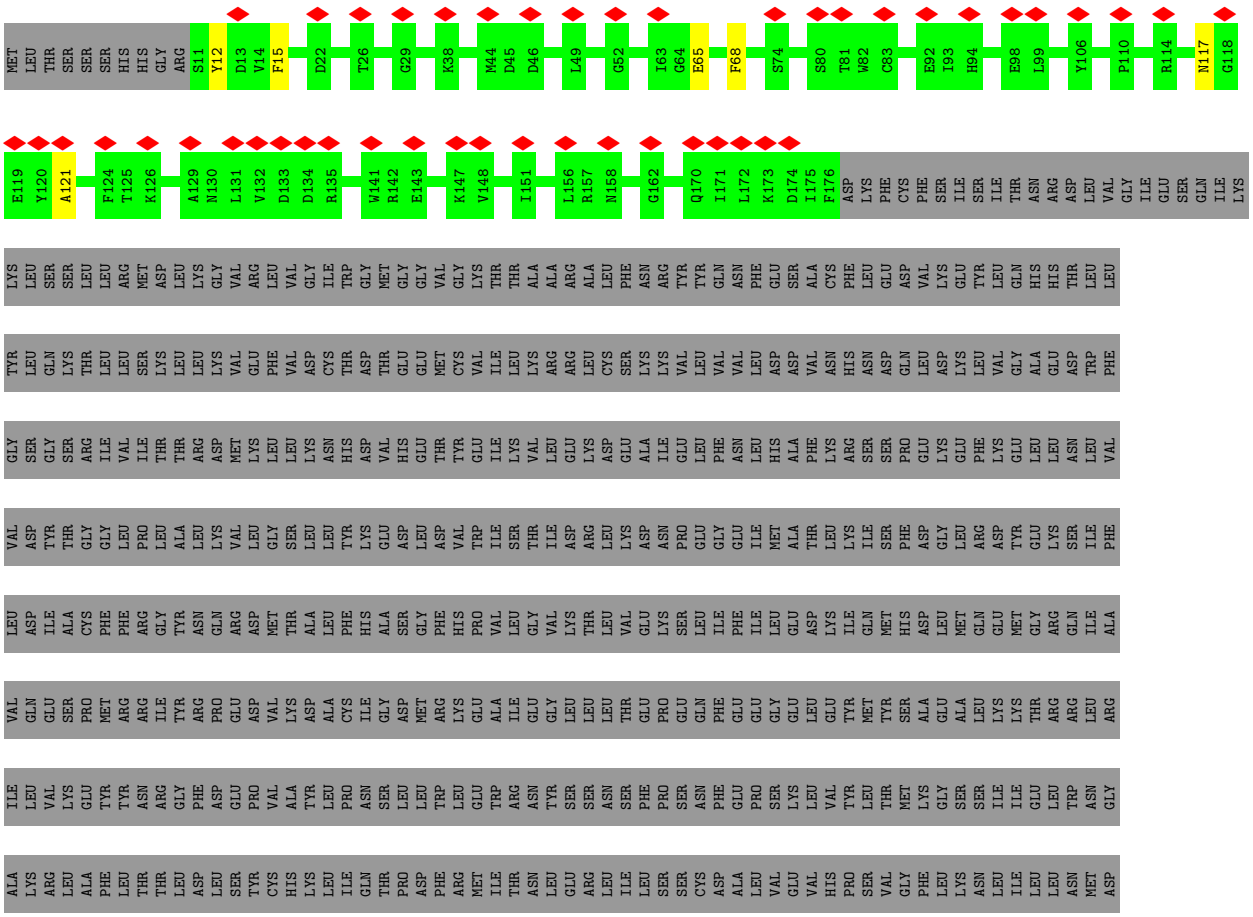
Chain B:





• Molecule 1: Disease resistance protein Roq1

Chain C: 12% 88%



HIS CYS ILE SER LEU GLU ARG LEU PRO ALA ILE ILE GLN SER GLU CYS LEU GLU VAL LEU ASP LEU ASN TYR CYS PHE ASN LEU LYS MET PHE PRO GLU VAL GLU ARG ASN MET THR HIS LEU LYS LYS LEU ASP LEU THR SER THR GLY ILE ARG GLU LEU PRO ALA SER ILE GLU HIS

LEU SER SER LEU GLU ASN LEU GLN MET HIS SER CYS ASN GLN LEU VAL SER LEU PRO SER SER ILE TRP ARG PHE ARG ASN LEU LYS ILE SER GLU CYS GLU LYS LEU GLY SER LEU PRO GLU ILE HIS GLY ASN SER ASN CYS THR ARG GLU LEU ILE LEU LYS LEU VAL SER ILE LYS

GLU LEU PRO THR SER ILE GLY ASN LEU THR SER LEU ASN PHE LEU GLU ILE CYS ASN CYS LYS THR ILE SER SER LEU SER SER ILE TRP GLY LEU THR SER LEU THR THR LEU LYS LEU LEU ASP CYS ARG LYS LEU LYS ASN LEU PRO GLY ILE PRO ASN ALA ILE ASN HIS LEU

SER GLY HIS GLY LEU GLN LEU LEU LEU THR LEU GLU GLN PRO THR ILE TYR GLU ARG LEU ASP LEU LEU ARG ILE ILE ASP MET SER TRP CYS SER CYS ILE SER SER LEU THR THR LEU LYS PHE LEU ARG ILE LEU CYS ILE SER SER TYR CYS SER ARG LEU GLU TYR

LEU PRO GLU ASN LEU GLY HIS LEU LEU GLU HIS LEU GLU GLU LEU LEU ALA ASP GLY THR GLY ILE LEU ARG LEU PRO SER SER VAL ALA ARG LEU ASN LYS LEU GLU VAL LEU SER PHE ARG LYS LYS PHE ALA ILE GLY PRO LYS VAL GLN TYR SER SER SER MET LEU ASN LEU PRO ASP

ASP VAL PHE GLY SER LEU GLY SER LEU GLY SER VAL VAL LYS LEU ASN LEU SER GLY ASN GLY PHE CYS ASN LEU PRO GLU THR MET ASN GLN LEU PHE CYS LEU LEU GLU TYR LEU ASP ILE THR PHE CYS GLN ARG LEU GLU ALA LEU PRO GLU LEU PRO PRO SER ILE LYS GLU LEU TYR

VAL ASP GLU HIS LEU ALA LEU ARG ILE MET GLU ASP LEU VAL ILE LYS CYS LYS GLU LEU ASN LEU ILE ALA VAL THR LYS ILE GLU TYR GLN ASN PHE TYR ARG TRP LEU ASP SER ILE TRP SER ASP VAL SER GLU LEU GLU ASN SER GLN LYS GLN GLN LEU ASP ASP MET LEU

GLN LEU ILE PRO PHE SER TYR LEU SER THR ALA LYS ARG GLU GLU VAL LEU LYS ILE VAL ILE HIS GLY THR ARG ILE PRO GLU TRP PHE ARG TRP GLN ASP ARG SER ALA THR THR MET SER VAL ASN LEU PRO GLU TYR TRP TYR THR GLU ASN PHE LEU GLY PHE ALA ILE CYS CYS

SER CYS CYS PHE TYR HIS SER ALA ARG SER TYR ASP VAL GLU PHE GLU GLY SER MET HIS HIS TYR ASN TYR ASP SER SER TYR TRP LYS GLU TYR GLU GLU PRO SER TYR ASP PHE TYR GLU ARG ASP SER ILE GLU ILE THR ALA LYS LEU THR PRO ARG HIS LYS GLY MET ARG THR

GLU GLU LEU LYS LYS VAL CYS SER PHE SER MET ASN VAL LEU ARG ARG ALA THR ALA VAL PRO ASN MET CYS PHE ALA PHE PHE PRO PHE ASN SER LEU CYS HIS ILE SER ASN LEU GLN ALA ASN ASN PRO ASN ASP TYR GLY ILE PHE GLU THR CYS LEU SER PRO GLY ASP ILE ARG

HIS ARG GLY LYS GLN TRP GLY PHE ASN LEU VAL TYR LYS ASP GLU THR GLY GLY SER VAL THR HIS GLU MET LEU ILE ILE ASN ARG ASP TYR LYS HIS ASP GLY ASP TYR LYS ASP HIS ASP ILE ASP TYR LYS ASP ASP ASP ASP LYS

- Molecule 1: Disease resistance protein Roq1

Chain A: 12% 88%

MET LEU THR SER SER SER HIS HIS GLY ARG S11 Y12 D13 F27 H30 K38 G39 D45 D46 K47 E48 L49 K50 R51 G52 K53 S54 I55 S56 S57 E58 E65 S66 R67 W82 E92 I93 H94 E95 K96 V101 F105 R114 N117 G118 E119 Y120 A121 V122

C123 F127 N130 L131 V132 D133 D134 R135 D136 K137 V138 L139 R140 D155 N161 F176 ASP LYS PHE CYS PHE SER ILE SER ILE THR ASN ARG ASP LEU VAL GLY ILE GLU SER GLN ILE LYS LYS LEU SER SER LEU LEU ARG MET ASP LEU LYS GLY VAL ARG LEU VAL GLY

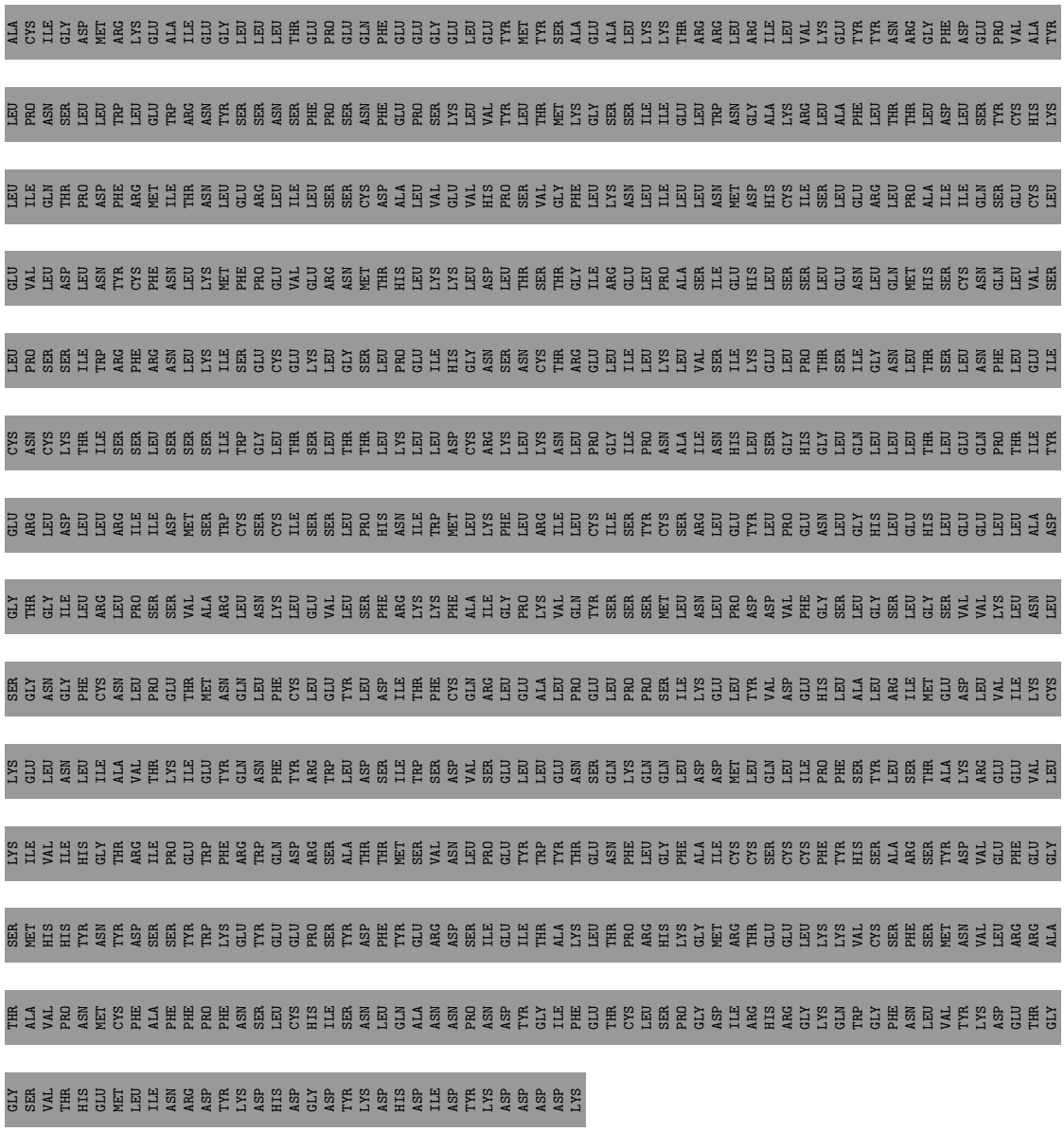
ILE TRP GLY MET GLY GLY VAL GLY LYS THR THR ALA ALA ARG ALA LEU PHE ASN ARG TYR TYR GLN ASN PHE GLU SER ALA CYS PHE LEU GLU ASP VAL LYS GLU TYR LEU GLN HIS HIS THR LEU LEU TYR LEU GLN LYS THR LEU LEU SER LYS LEU LEU LYS VAL GLU PHE VAL ASP

CYS THR ASP THR GLU GLU MET CYS VAL ILE LEU LYS ARG ARG LEU CYS SER LYS LYS VAL LEU VAL VAL LEU ASP ASP VAL ASN HIS ASN ASP GLN LEU ASP LYS LEU VAL GLY ALA GLU ASP TRP PHE GLY SER GLY SER ARG ILE VAL ILE THR THR ARG ASP MET LYS LEU LEU LYS

ASN HIS ASP VAL HIS GLU THR TYR GLU ILE LYS VAL LEU GLU LYS ASP GLU ALA ILE GLU GLU LEU PHE ASN LEU HIS ALA PHE LYS ARG SER SER PRO GLU LYS GLU PHE LYS GLU GLU LEU LEU ASN LEU VAL VAL ASP TYR THR GLY GLY LEU PRO LEU ALA LEU LYS VAL LEU GLY SER LEU

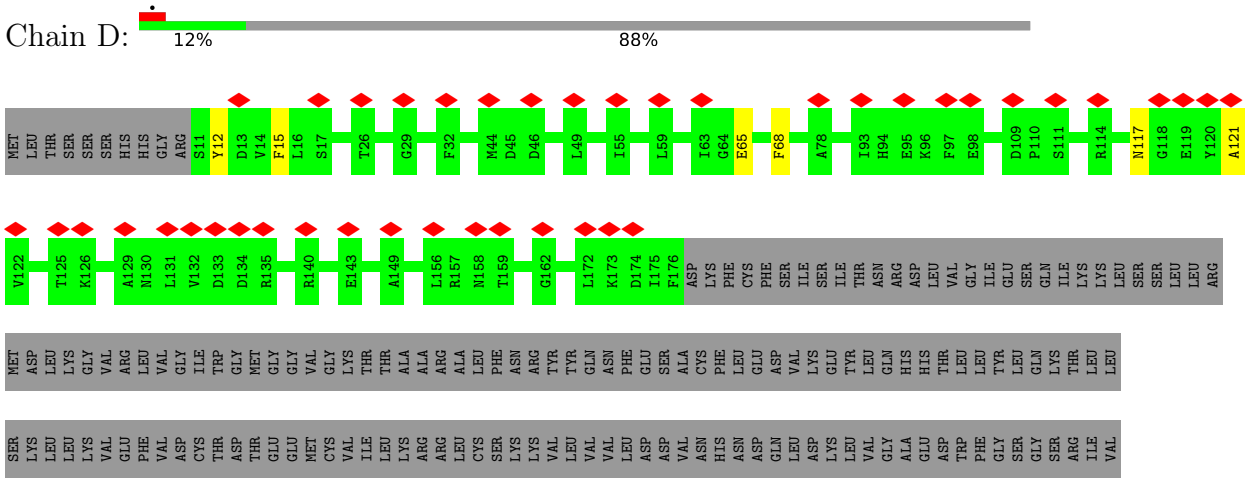
LEU TYR LYS GLU ASP LEU ASP VAL TRP ILE SER THR ILE ASP ARG LEU LYS ASP ASN PRO GLU GLY GLU ILE MET ALA THR LEU LYS ILE SER PHE ASP GLY LEU ARG ASP TYR GLU LYS SER ILE PHE LEU ASP ILE ALA CYS PHE PHE ARG GLY TYR ASN GLN ARG ASP MET THR ALA

LEU PHE HIS ALA SER GLY PHE HIS PRO VAL LEU GLY VAL LYS THR LEU VAL GLU LYS SER LEU ILE PHE ILE LEU GLU ASP LYS ILE GLN MET HIS ASP LEU MET GLN GLU MET GLY ARG GLN ILE ALA VAL GLN GLU SER PRO MET ARG ARG ILE TYR ARG PRO GLU ASP VAL LYS ASP



- Molecule 1: Disease resistance protein Roq1

Chain D:



ILE THR THR ARG ASP MET LYS LEU LEU LYS ASN HIS ASP VAL HIS GLU THR TYR GLU ILE LYS VAL LEU GLU LYS ASP GLU ALA ILE GLU LEU PHE ASN LEU HIS ALA PHE LYS ARG SER SER PRO GLU LYS GLU PHE LYS GLU LEU LEU ASN LEU VAL VAL ASP TYR THR GLY GLY LEU

PRO LEU ALA LEU LYS VAL LEU GLY SER LEU LEU TYR LYS GLU ASP LEU ASP VAL TRP ILE SER THR ILE ASP ARG LEU LYS ASP ASN PRO GLU GLY GLU ILE MET ALA THR LEU LYS ILE SER PHE ASP GLY LEU ARG ASP TYR GLU LYS SER ILE PHE LEU ASP ILE ALA CYS PHE PHE

ARG GLY TYR ASN GLN ARG ASP MET THR ALA LEU PHE HIS ALA SER GLY PHE HIS PRO VAL LEU GLY VAL LYS THR LEU VAL GLU LYS SER LEU ILE PHE ILE LEU GLU ASP LYS ILE GLN MET HIS ASP LEU MET GLN GLU MET GLY ARG GLN ILE ALA VAL GLN GLU SER PRO MET ARG

ARG ILE TYR ARG PRO GLU ASP VAL LYS ASP ALA CYS ILE GLY ASP MET ARG LYS GLU ALA ILE GLU GLY LEU LEU LEU THR GLU PRO GLU GLN PHE GLU GLU GLY GLU LEU GLU TYR MET TYR SER ALA GLU ALA LEU LYS LYS THR ARG ARG LEU ARG ILE LEU VAL LYS GLU TYR TYR

ASN ARG GLY PHE ASP GLU PRO VAL ALA TYR LEU PRO ASN SER LEU LEU TRP LEU GLU TRP ARG ASN TYR SER SER ASN SER PHE PRO SER ASN PHE GLU PRO SER LYS LEU VAL TYR LEU THR MET LYS GLY SER SER ILE ILE GLU LEU TRP ASN GLY ALA LYS ARG LEU ALA PHE LEU

THR THR LEU ASP LEU SER TYR CYS HIS LYS LEU ILE GLN THR PRO ASP PHE ARG MET ILE THR ASN LEU GLU ARG LEU ILE LEU SER SER CYS ASP ALA LEU VAL GLU VAL HIS PRO SER VAL GLY PHE LEU LYS ASN LEU ILE LEU LEU ASN MET ASP HIS CYS ILE SER LEU GLU ARG

LEU PRO ALA ILE ILE GLN SER GLU CYS LEU GLU VAL LEU ASP LEU ASN TYR CYS PHE ASN LEU LYS MET PHE PRO GLU VAL GLU ARG ASN MET THR HIS LEU LYS LYS LEU ASP LEU THR SER THR GLY ILE ARG GLU LEU PRO ALA SER ILE GLU HIS LEU SER SER LEU GLU ASN LEU

GLN MET HIS SER CYS ASN GLN LEU VAL SER LEU PRO SER SER ILE TRP ARG PHE ARG ASN LEU LYS ILE SER GLU CYS GLU LYS LEU GLY SER LEU PRO GLU ILE HIS GLY ASN SER ASN CYS THR ARG GLU LEU ILE LEU LYS LEU VAL SER ILE LYS GLU LEU PRO THR SER ILE GLY

ASN LEU THR SER LEU ASN PHE LEU GLU ILE CYS ASN CYS LYS THR ILE SER SER LEU SER SER ILE TRP GLY LEU THR SER LEU THR THR LEU LYS LEU LEU ASP CYS ARG LYS LEU LYS ASN LEU PRO GLY ILE PRO ASN ALA ILE ASN HIS LEU SER GLY HIS GLY LEU GLN LEU

LEU LEU THR LEU GLU GLN PRO THR ILE TYR GLU ARG LEU ASP LEU LEU ARG ILE ILE ASP MET SER TRP CYS SER CYS ILE SER SER LEU PRO HIS ASN ILE TRP MET LEU LYS PHE LEU ARG ILE LEU CYS ILE SER TYR CYS SER ARG LEU GLU TYR LEU PRO GLU ASN LEU GLY HIS

LEU GLU HIS LEU GLU GLU LEU LEU ALA ASP GLY THR GLY ILE LEU ARG LEU PRO SER SER VAL ALA ARG LEU ASN LYS LEU GLU VAL LEU SER PHE ARG LYS LYS PHE ALA ILE GLY PRO LYS VAL GLN TYR SER SER SER MET LEU ASN LEU PRO ASP ASP VAL PHE GLY SER LEU GLY

SER LEU GLY SER VAL VAL LYS LEU ASN LEU SER GLY ASN GLY PHE CYS ASN LEU PRO GLU THR MET ASN GLN LEU PHE CYS LEU GLU TYR LEU ASP ILE THR PHE CYS GLN ARG LEU GLU ALA LEU PRO GLU LEU PRO PRO SER ILE LYS GLU LEU TYR VAL ASP GLU HIS LEU ALA LEU

ARG ILE MET GLU ASP LEU VAL ILE LYS CYS LYS GLU LEU ASN LEU ILE ALA VAL THR LYS ILE GLU TYR GLN ASN PHE TYR ARG TRP LEU ASP SER ILE TRP SER ASP VAL SER GLU LEU LEU GLU ASN SER GLN LYS GLN GLN LEU ASP ASP MET LEU GLN LEU ILE PRO PHE SER TYR

LEU SER THR ALA LYS ARG GLU GLU VAL LEU LYS ILE VAL ILE HIS GLY THR ARG ILE PRO GLU TRP PHE ARG TRP GLN ASP ARG SER ALA THR THR MET SER VAL ASN LEU PRO GLU TYR TRP TYR THR GLU ASN PHE LEU GLY PHE ALA ILE CYS CYS SER CYS CYS PHE TYR HIS SER

ALA ARG SER TYR ASP VAL GLU PHE GLU GLY SER MET HIS HIS TYR ASN TYR ASP SER SER TYR TRP LYS GLU TYR GLU GLU PRO SER TYR ASP PHE TYR GLU ARG ASP SER ILE GLU ILE THR ALA LYS LEU THR PRO ARG HIS LYS GLY MET ARG THR GLU GLU LEU LYS LYS VAL CYS

SER PHE SER MET ASN VAL LEU ARG ARG ALA THR ALA VAL PRO ASN MET CYS PHE ALA PHE PHE PRO PHE ASN SER LEU CYS HIS ILE SER ASN LEU GLN ALA ASN ASN PRO ASN ASP TYR GLY ILE PHE GLU THR CYS LEU SER PRO GLY ASP ILE ARG HIS ARG GLY LYS GLN TRP GLY

PHE ASN LEU VAL TYR LYS ASP GLU THR GLY GLY SER VAL THR HIS GLU MET LEU ILE ASN ARG ASP TYR LYS ASP HIS ASP GLY ASP TYR LYS ASP HIS ASP ILE ASP TYR LYS ASP ASP ASP ASP LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	5466	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	-900	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	80879	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.059	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0125	Depositor
Map size (Å)	450.528, 450.528, 450.528	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9386, 0.9386, 0.9386	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	A	0.24	0/821	0.40	0/1143
1	B	0.24	0/821	0.40	0/1143
1	C	0.23	0/821	0.40	0/1143
1	D	0.23	0/821	0.40	0/1143
All	All	0.23	0/3284	0.40	0/4572

There are no bond length outliers.

There are no bond angle outliers.

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	A	822	0	361	4	0
1	B	822	0	361	4	0
1	C	822	0	361	3	0
1	D	822	0	361	3	0
All	All	3288	0	1444	14	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 3.

All (14) 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:D:117:ASN:HA	1:D:121:ALA:HB2	1.77	0.65
1:C:117:ASN:HA	1:C:121:ALA:HB2	1.78	0.65
1:B:117:ASN:HA	1:B:121:ALA:HB2	1.80	0.63
1:A:117:ASN:HA	1:A:121:ALA:HB2	1.80	0.62
1:B:132:VAL:O	1:B:136:ASP:N	2.24	0.58
1:A:132:VAL:O	1:A:136:ASP:N	2.24	0.54
1:B:13:ASP:O	1:B:67:ARG:N	2.42	0.53
1:D:12:TYR:N	1:D:65:GLU:O	2.42	0.52
1:A:13:ASP:O	1:A:67:ARG:N	2.42	0.52
1:C:12:TYR:N	1:C:65:GLU:O	2.42	0.51
1:D:15:PHE:N	1:D:68:PHE:O	2.44	0.51
1:B:123:CYS:O	1:B:127:PHE:N	2.43	0.50
1:C:15:PHE:N	1:C:68:PHE:O	2.44	0.49
1:A:123:CYS:O	1:A:127:PHE:N	2.43	0.46

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	164/1328 (12%)	154 (94%)	10 (6%)	0	100	100
1	B	164/1328 (12%)	154 (94%)	10 (6%)	0	100	100
1	C	164/1328 (12%)	152 (93%)	12 (7%)	0	100	100
1	D	164/1328 (12%)	152 (93%)	12 (7%)	0	100	100
All	All	656/5312 (12%)	612 (93%)	44 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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.

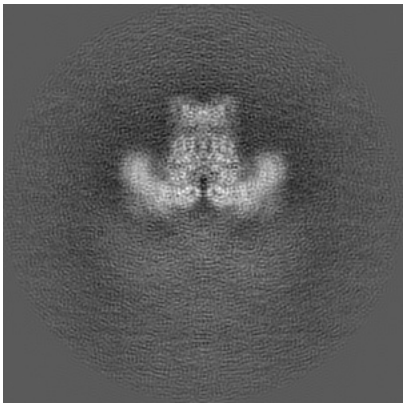
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22383. These allow visual inspection of the internal detail of the map and identification of artifacts.

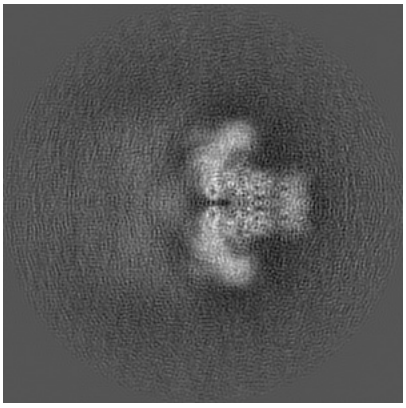
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

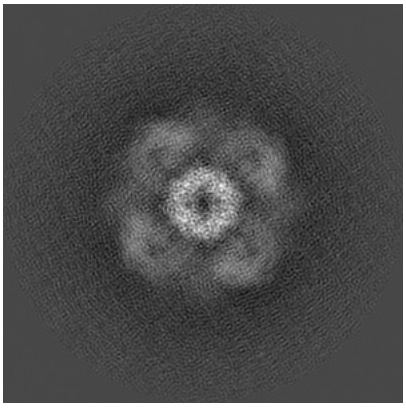
6.1.1 Primary map



X



Y

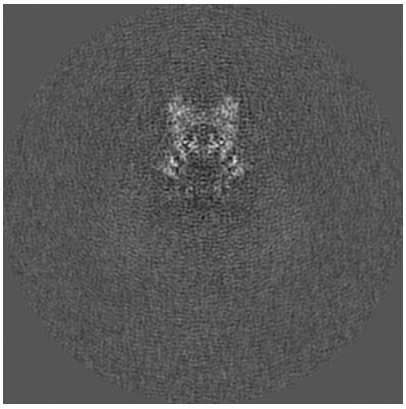


Z

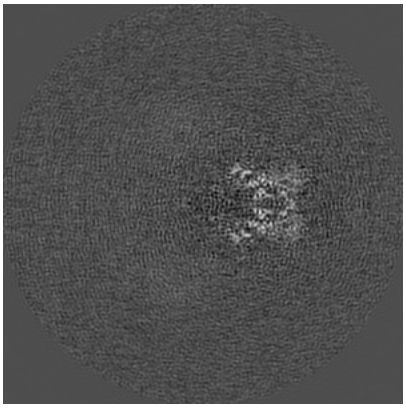
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

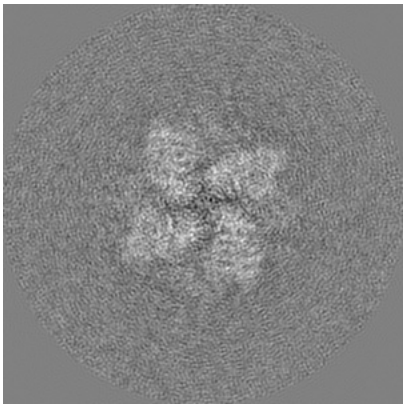
6.2.1 Primary map



X Index: 240



Y Index: 240

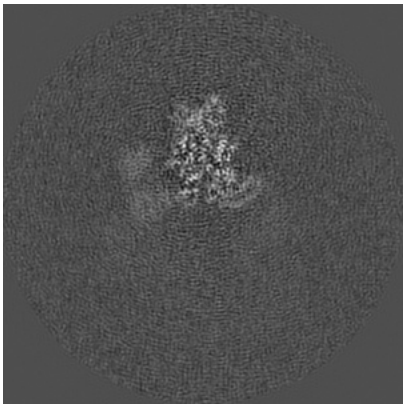


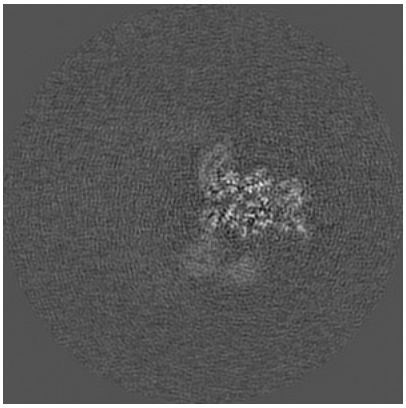
Z Index: 240

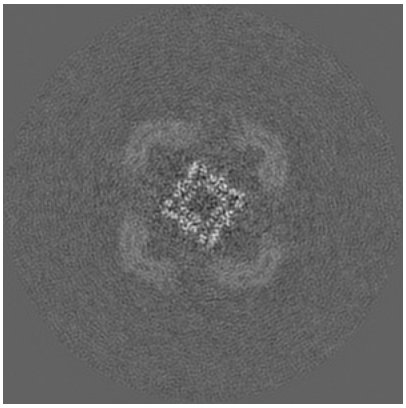
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 263

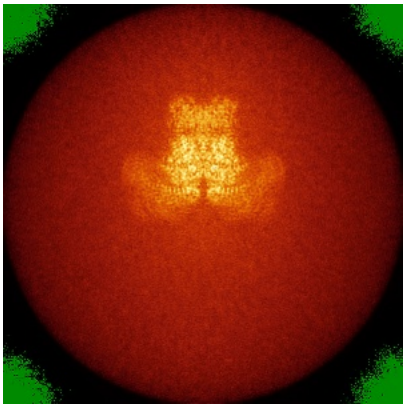

Y Index: 217

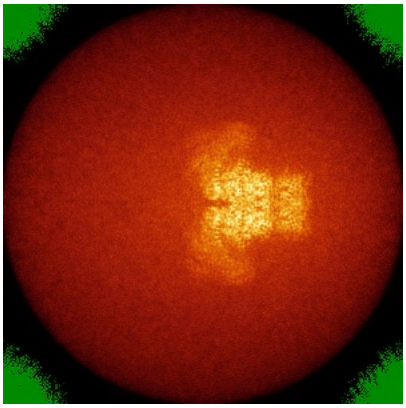

Z Index: 281

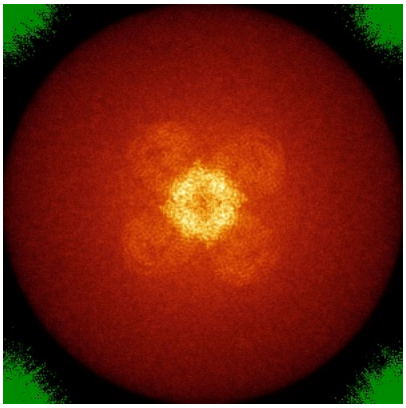
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

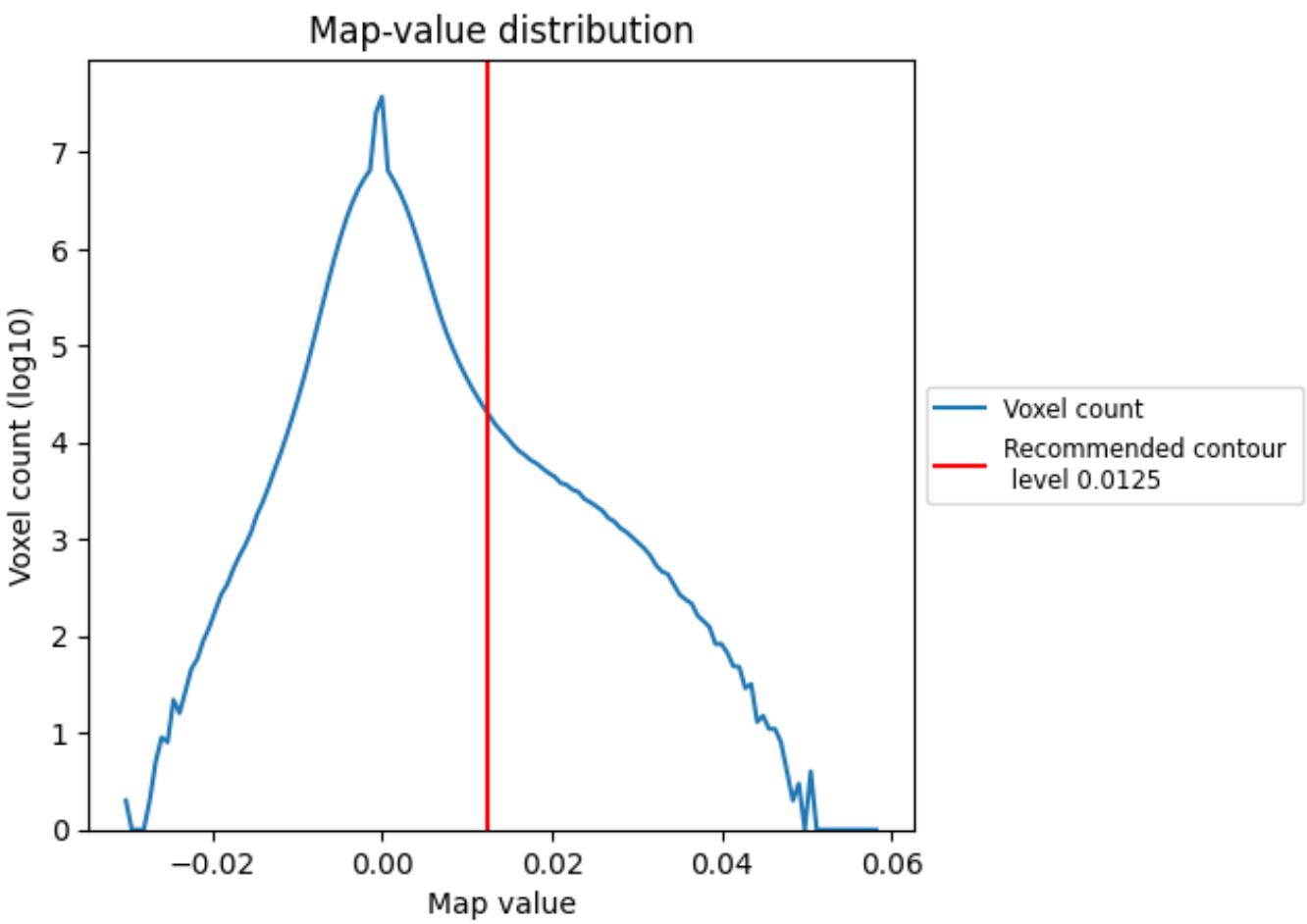
6.6 Mask visualisation (i)

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

7 Map analysis (i)

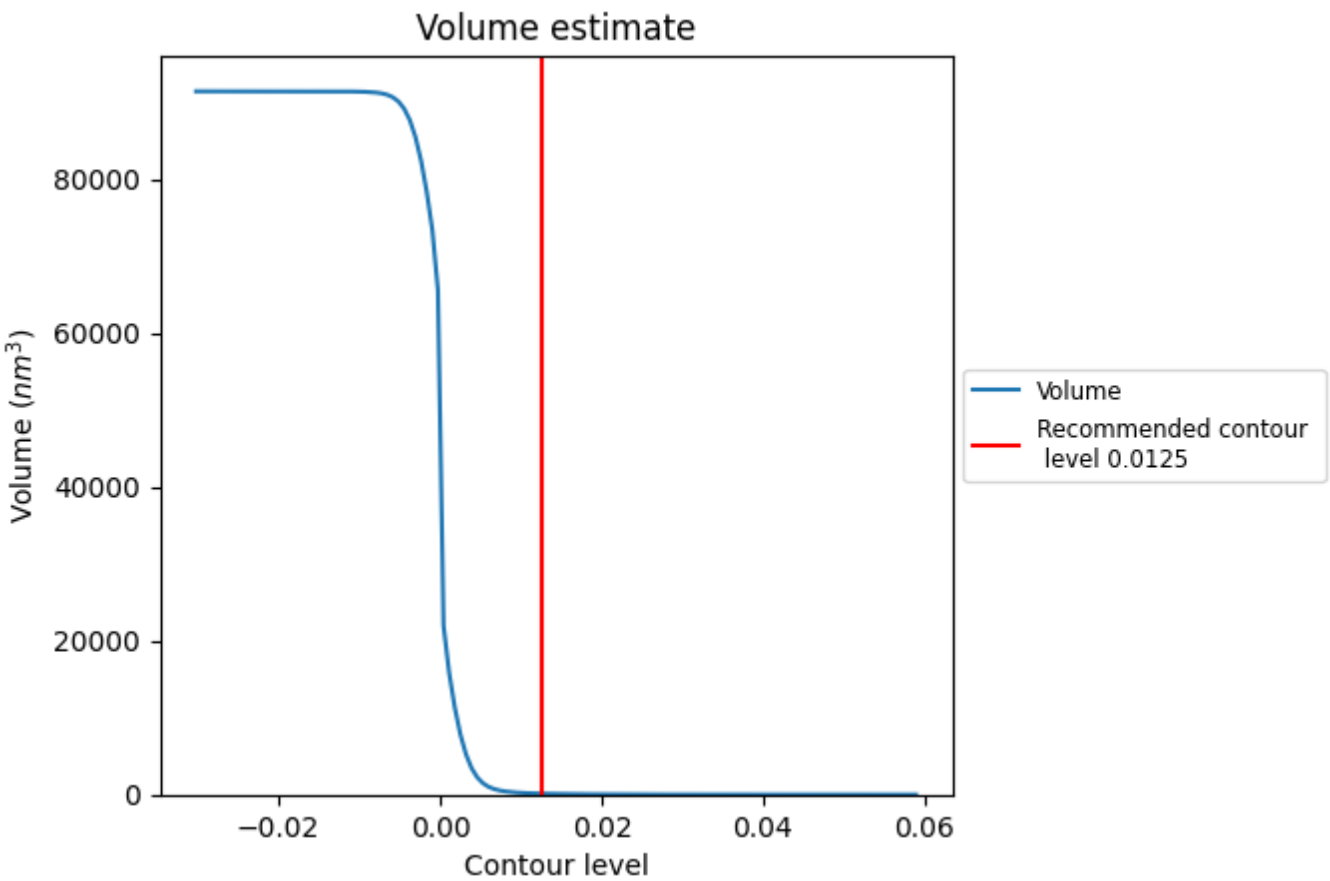
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

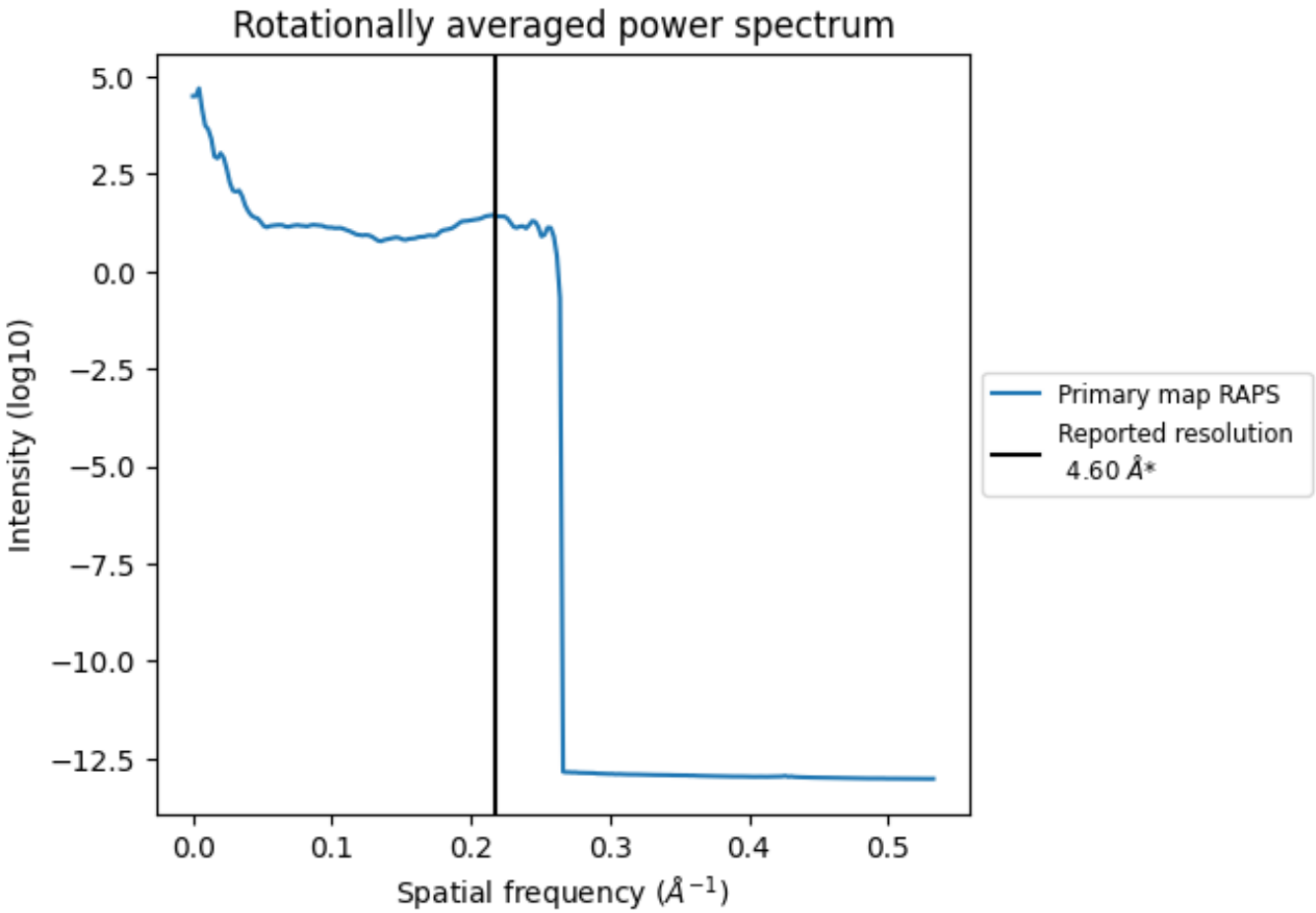
7.2 Volume estimate (i)



The volume at the recommended contour level is 124 nm^3; this corresponds to an approximate mass of 112 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)

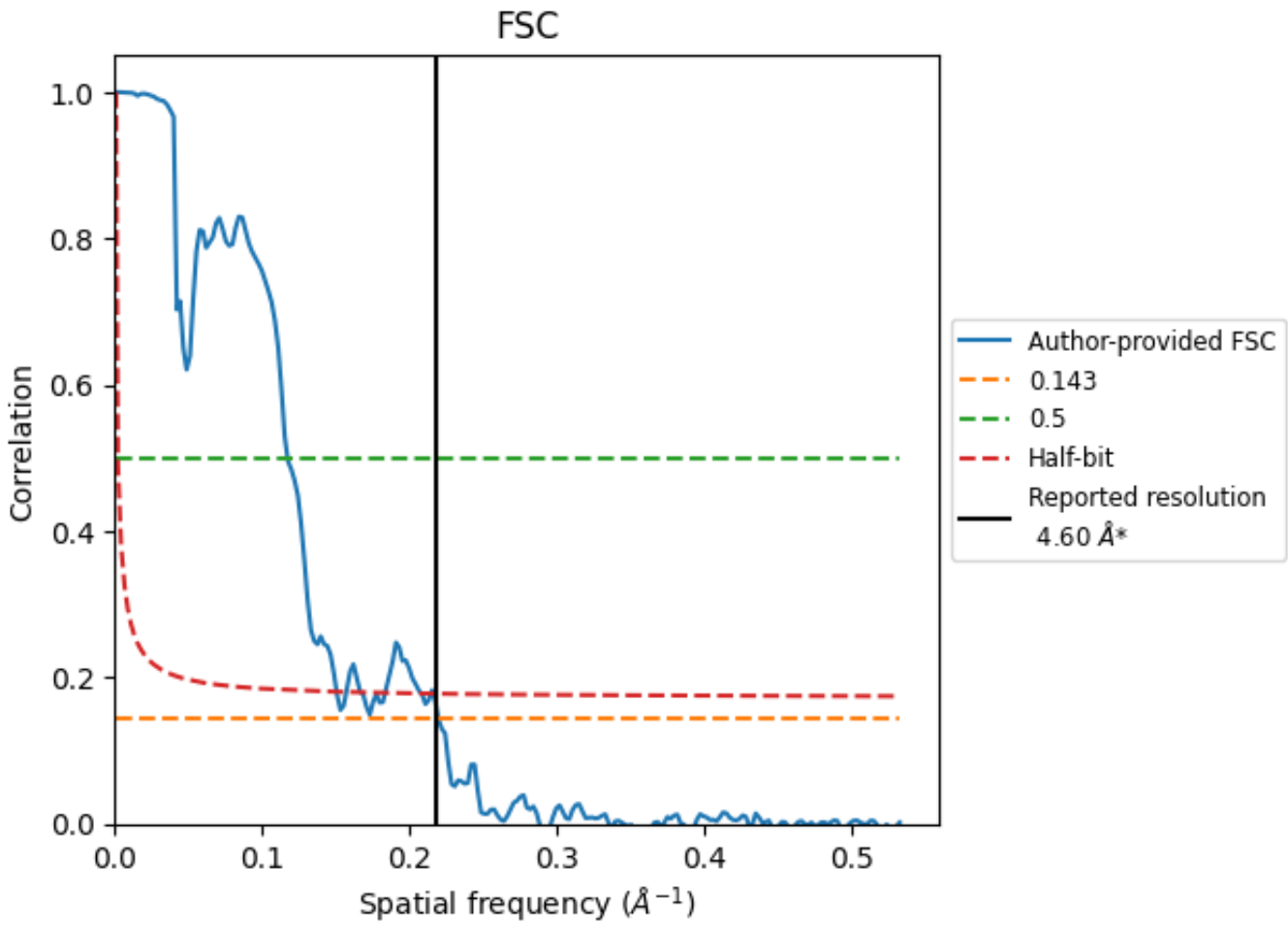


*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

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 0.217 Å^{-1}

8.2 Resolution estimates (i)

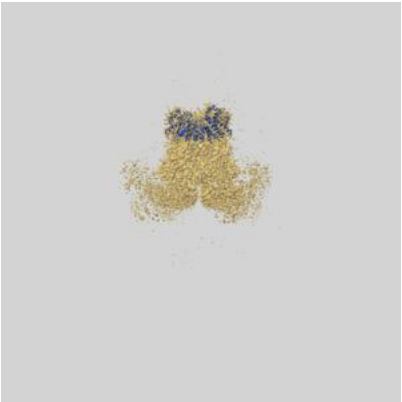
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.55	8.53	6.64
Unmasked-calculated*	-	-	-

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

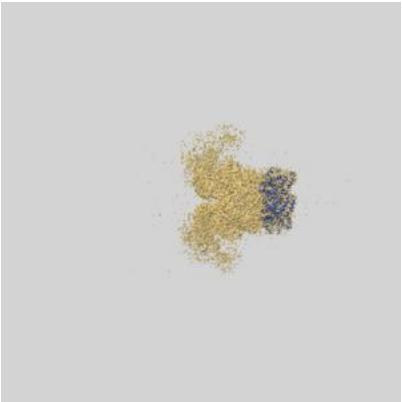
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22383 and PDB model 7JLX. Per-residue inclusion information can be found in section 3 on page 6.

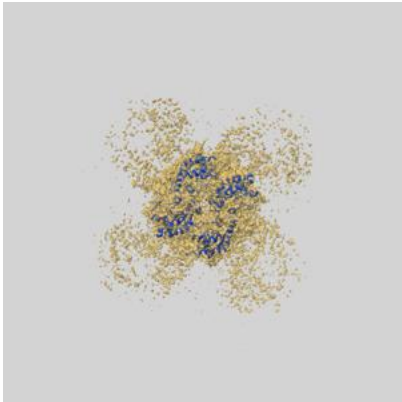
9.1 Map-model overlay (i)



X



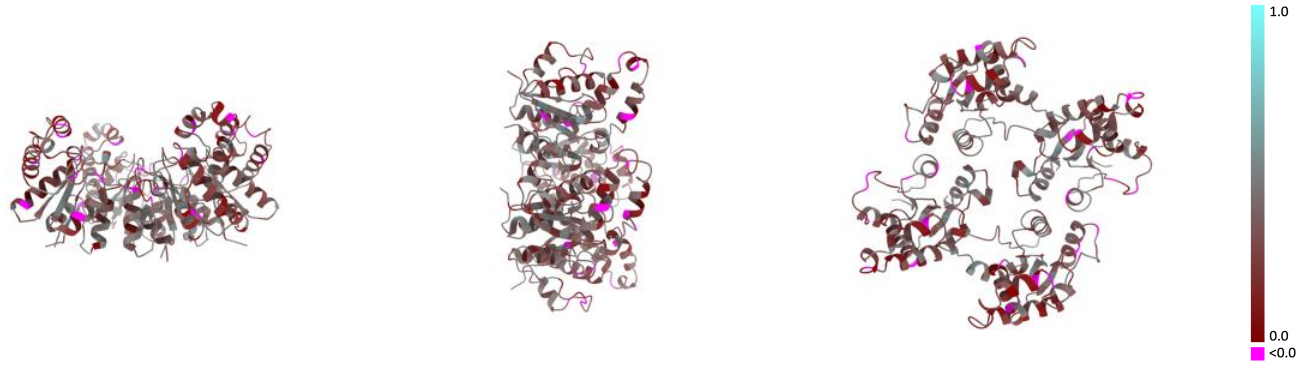
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

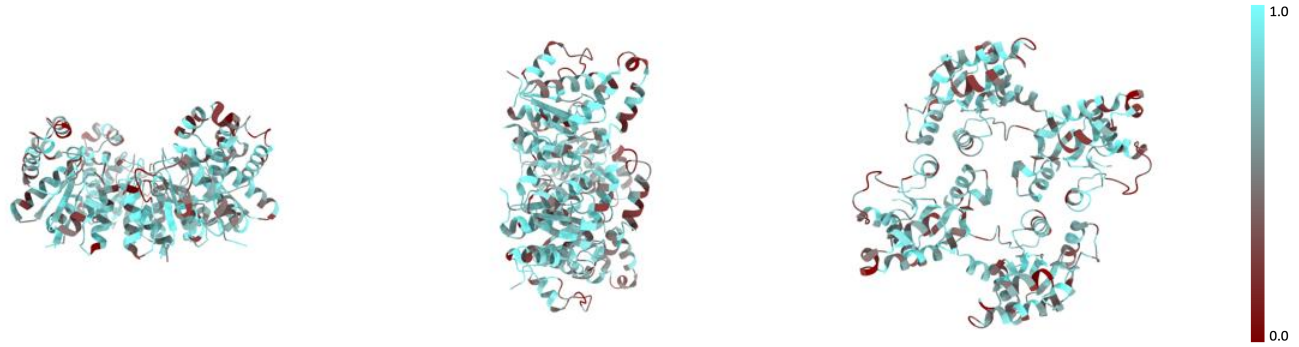
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

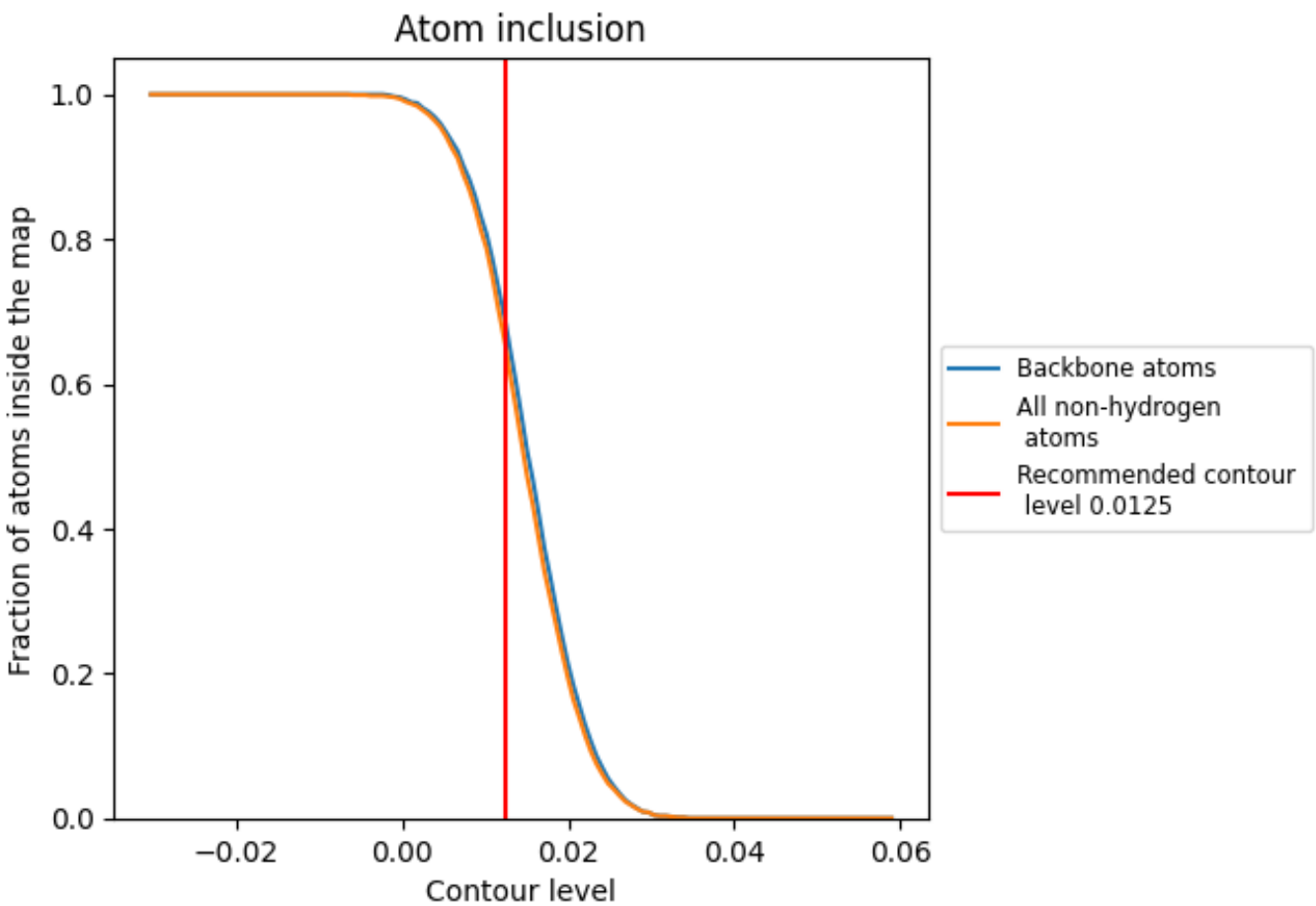
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0125).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6510	0.3120
A	0.6670	0.3200
B	0.6570	0.3090
C	0.6290	0.3010
D	0.6500	0.3200