wwPDB EM Validation Summary Report (i)

Sep 24, 2026 – 08:29 am BST

PDB ID	:	9S29 / pdb_00009s29
EMDB ID	:	EMD-54482
Title	:	MVV CSC intasome in complex with LEDGF
Authors	:	Punch, E.K.; Hope, J.; Cherepanov, P.
Deposited on	:	2025-07-21
Resolution	:	2.80 Å(reported)
Based on initial models	:	7U32, 3HPH

This is a wwPDB EM Validation Summary 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:

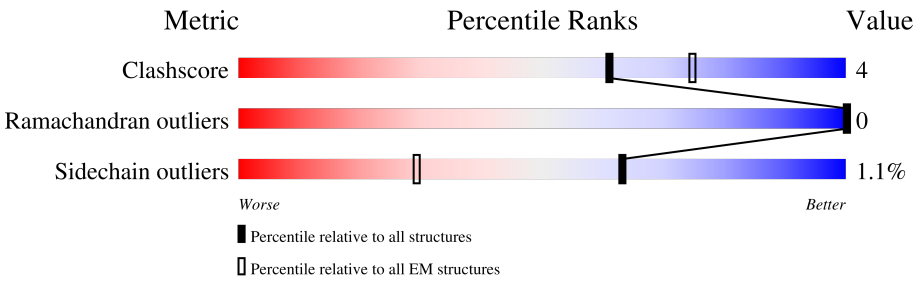
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

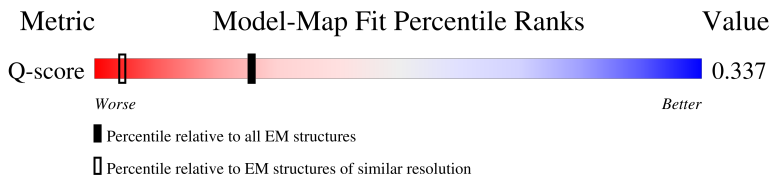
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	281	89% 9%
1	B	281	10% 80% 10% 10%
1	C	281	12% 83% 12% 6%
1	D	281	15% 84% 9% 6%

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Mol	Chain	Length	Quality of chain
1	E	281	83% 12%
1	F	281	84% 11% 5%
1	G	281	5% 76% 12% 12%
1	H	281	77% 17% 6%
1	I	281	90% 8%
1	J	281	10% 79% 10% 10%
1	K	281	12% 83% 12% 6%
1	L	281	11% 84% 9% 6%
1	M	281	83% 12%
1	N	281	84% 11% 5%
1	O	281	6% 76% 12% 12%
1	P	281	76% 17% 6%
2	W	21	14% 52% 48%
2	Y	21	10% 52% 48%
3	X	19	16% 47% 53%
3	Z	19	16% 47% 53%
4	a	530	14% 85%
4	b	530	14% 85%
4	c	530	13% 85%
4	d	530	14% 85%
4	e	530	14% 85%
4	f	530	8% 14% 85%
4	g	530	14% 85%
4	h	530	14% 85%
4	i	530	13% 85%

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Mol	Chain	Length	Quality of chain
4	j	530	14% • 85%
4	k	530	14% • 85%
4	l	530	5% 14% • 85%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 43436 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 Gag-Pol polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	276	2223	1413	392	409	9	0	0
1	B	252	2038	1294	357	379	8	0	0
1	C	265	2150	1369	378	395	8	0	0
1	D	263	2132	1358	373	393	8	0	0
1	E	269	2180	1389	380	402	9	0	0
1	F	267	2136	1358	377	393	8	0	0
1	G	247	2010	1284	347	371	8	0	0
1	H	264	2136	1361	374	392	9	0	0
1	I	276	2223	1413	392	409	9	0	0
1	J	252	2038	1294	357	379	8	0	0
1	K	265	2150	1369	378	395	8	0	0
1	L	263	2132	1358	373	393	8	0	0
1	M	269	2180	1389	380	402	9	0	0
1	N	267	2136	1358	377	393	8	0	0
1	O	247	2010	1284	347	371	8	0	0
1	P	264	2136	1361	374	392	9	0	0

- Molecule 2 is a DNA chain called EV306.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	W	21	428	203	79	126	20	0	0
2	Y	21	428	203	79	126	20	0	0

- Molecule 3 is a DNA chain called EV272.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	X	19	389	183	75	112	19	0	0
3	Z	19	389	183	75	112	19	0	0

- Molecule 4 is a protein called PC4 and SFRS1-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	a	80	654	407	119	121	7	0	0
4	b	80	644	401	115	121	7	0	0
4	c	80	654	407	119	121	7	0	0
4	d	79	646	402	118	120	6	0	0
4	e	80	654	407	119	121	7	0	0
4	f	79	636	398	112	119	7	0	0
4	g	80	654	407	119	121	7	0	0
4	h	80	644	401	115	121	7	0	0
4	i	80	654	407	119	121	7	0	0
4	j	79	646	402	118	120	6	0	0
4	k	80	654	407	119	121	7	0	0
4	l	79	636	398	112	119	7	0	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

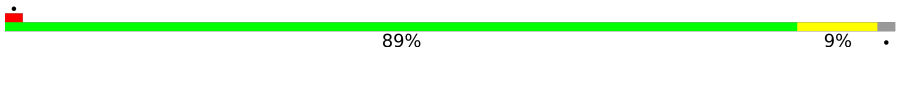
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
5	A	1	1	1	0
5	B	1	1	1	0
5	C	1	1	1	0
5	D	1	1	1	0
5	E	1	1	1	0
5	F	1	1	1	0
5	G	1	1	1	0
5	H	1	1	1	0
5	I	1	1	1	0
5	J	1	1	1	0
5	K	1	1	1	0
5	L	1	1	1	0
5	M	1	1	1	0
5	N	1	1	1	0
5	O	1	1	1	0
5	P	1	1	1	0

3 Residue-property plots (i)

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

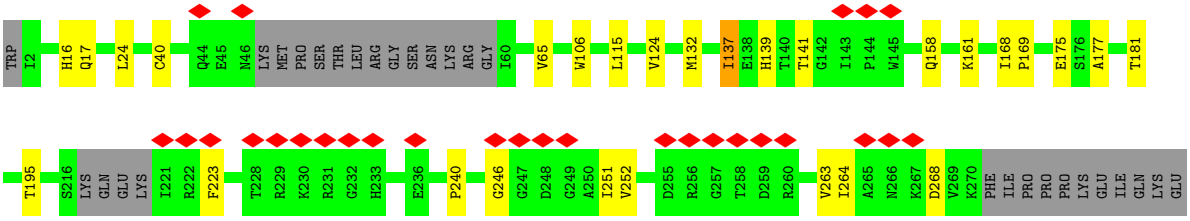
- Molecule 1: Gag-Pol polyprotein

Chain A:



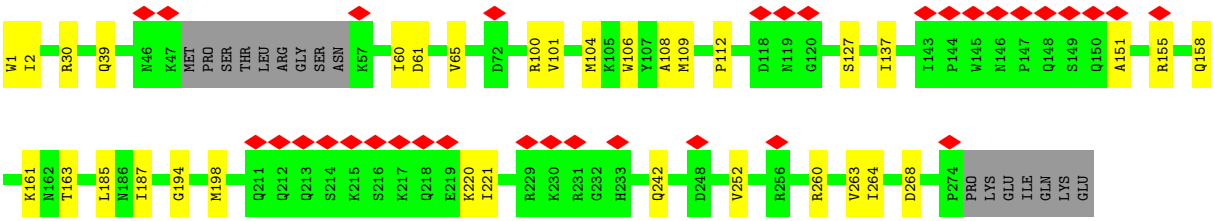
- Molecule 1: Gag-Pol polyprotein

Chain B:



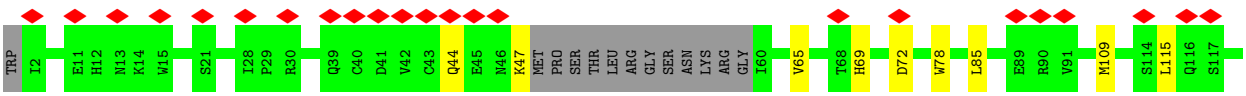
- Molecule 1: Gag-Pol polyprotein

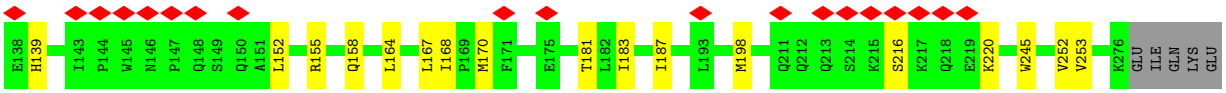
Chain C:



- Molecule 1: Gag-Pol polyprotein

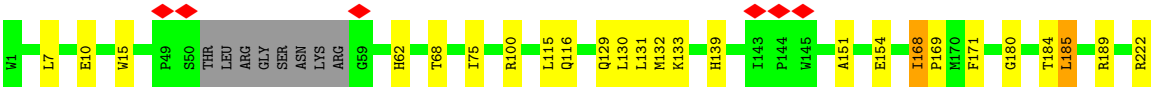
Chain D:

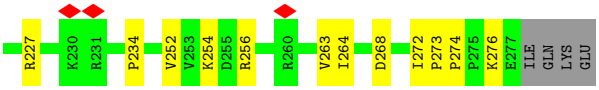




• Molecule 1: Gag-Pol polyprotein

Chain E:



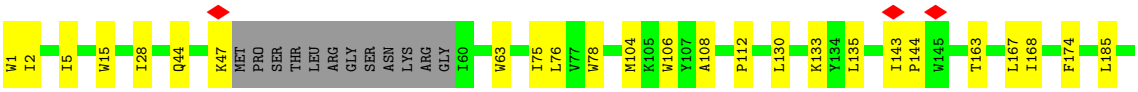


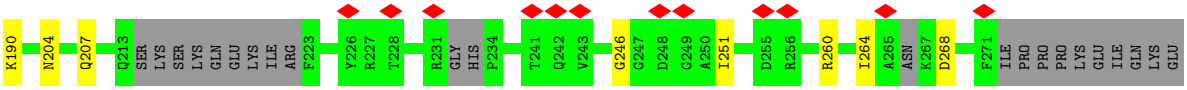
• Molecule 1: Gag-Pol polyprotein

Chain F:

• Molecule 1: Gag-Pol polyprotein

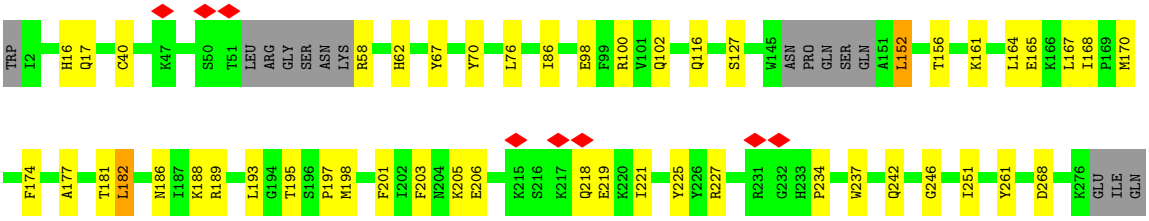
Chain G:





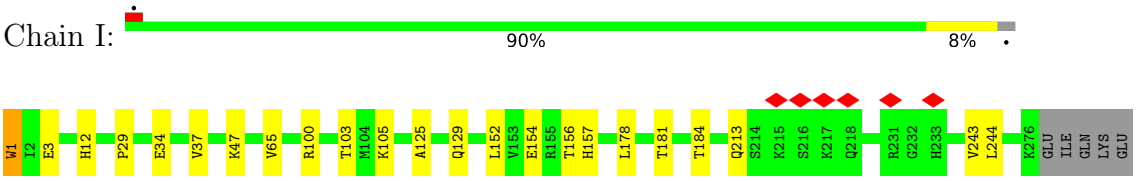
• Molecule 1: Gag-Pol polyprotein

Chain H:



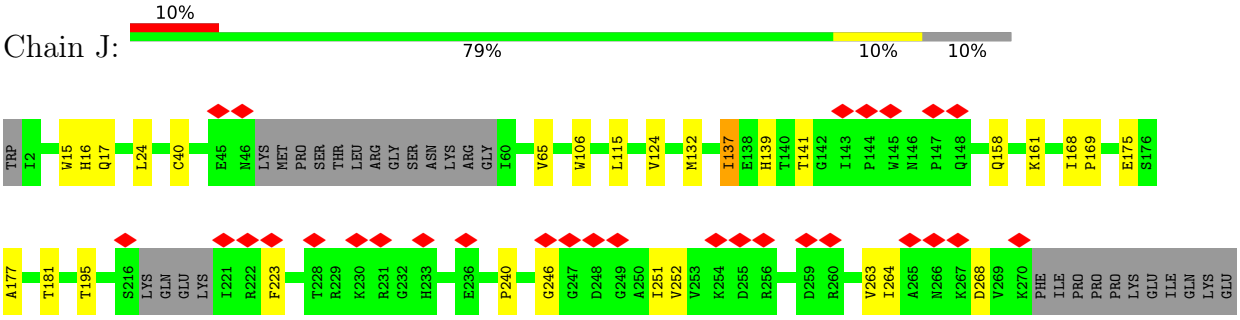
- Molecule 1: Gag-Pol polyprotein

Chain I:



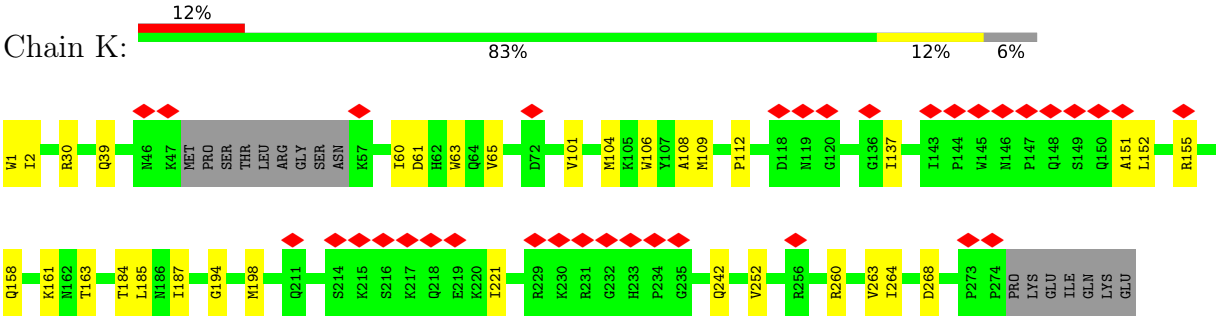
- Molecule 1: Gag-Pol polyprotein

Chain J:



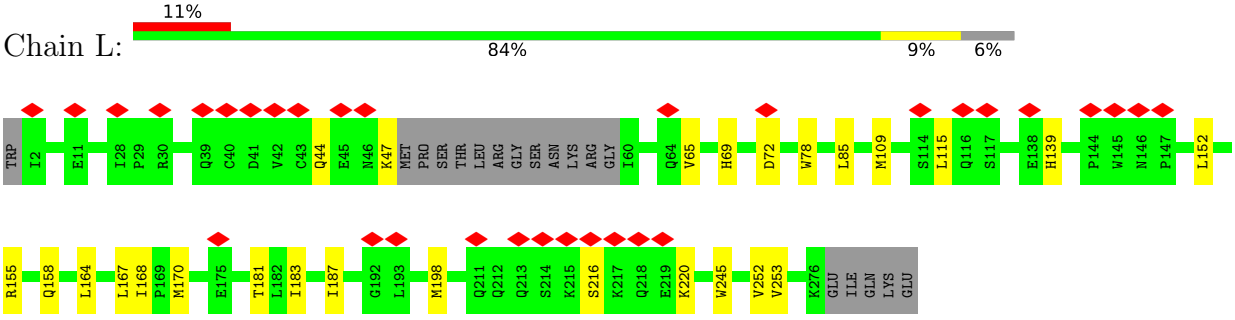
- Molecule 1: Gag-Pol polyprotein

Chain K:



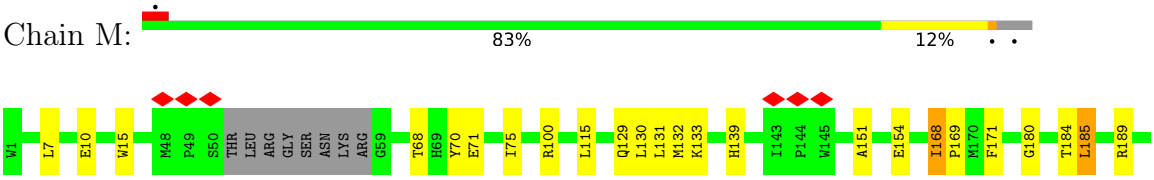
- Molecule 1: Gag-Pol polyprotein

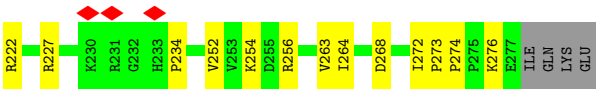
Chain L:



- Molecule 1: Gag-Pol polyprotein

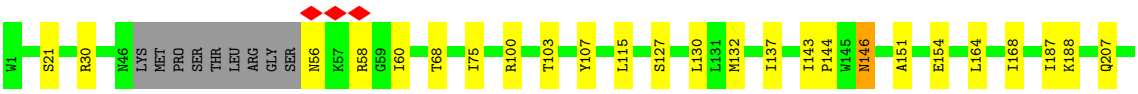
Chain M:

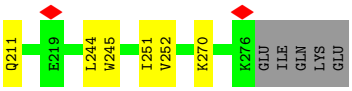




• Molecule 1: Gag-Pol polyprotein

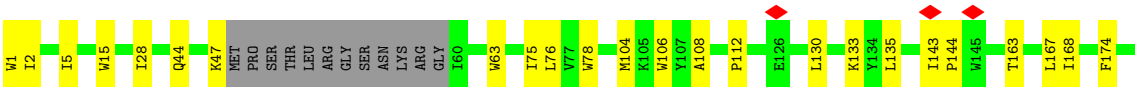
Chain N:

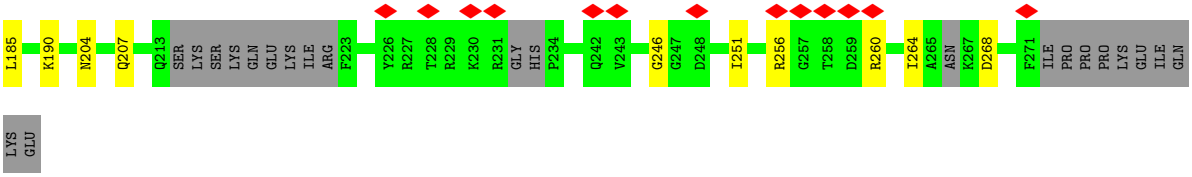




• Molecule 1: Gag-Pol polyprotein

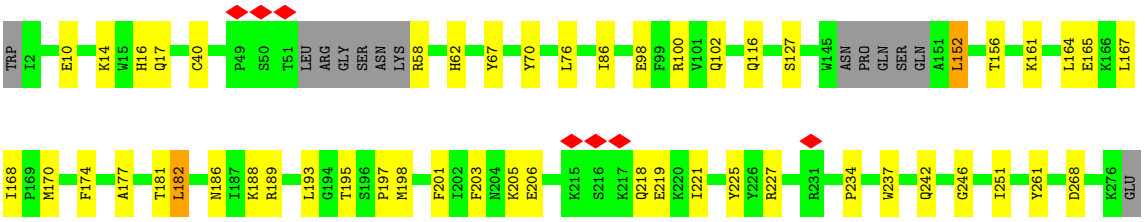
Chain O:





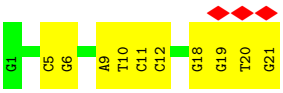
• Molecule 1: Gag-Pol polyprotein

Chain P:



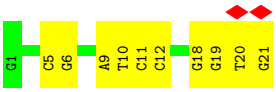
• Molecule 2: EV306

Chain W:



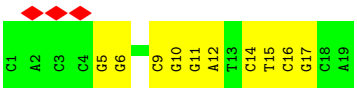
• Molecule 2: EV306

Chain Y:



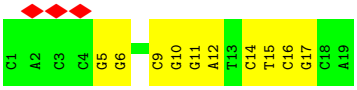
• Molecule 3: EV272

Chain X:



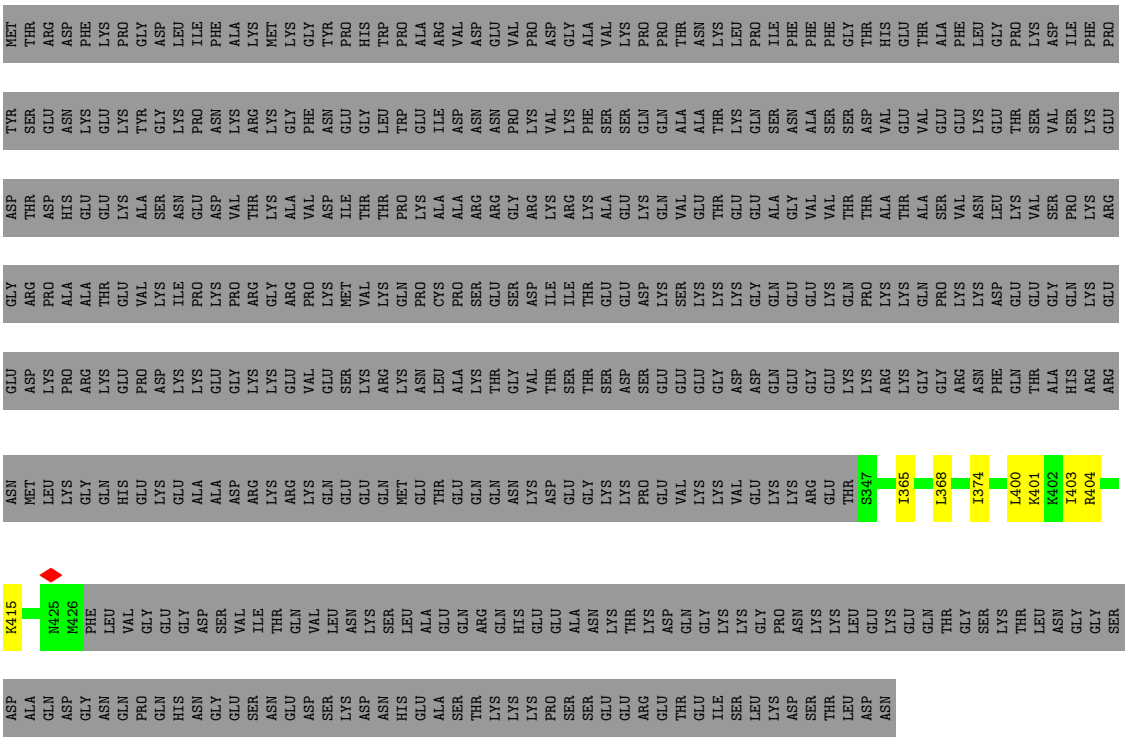
• Molecule 3: EV272

Chain Z:



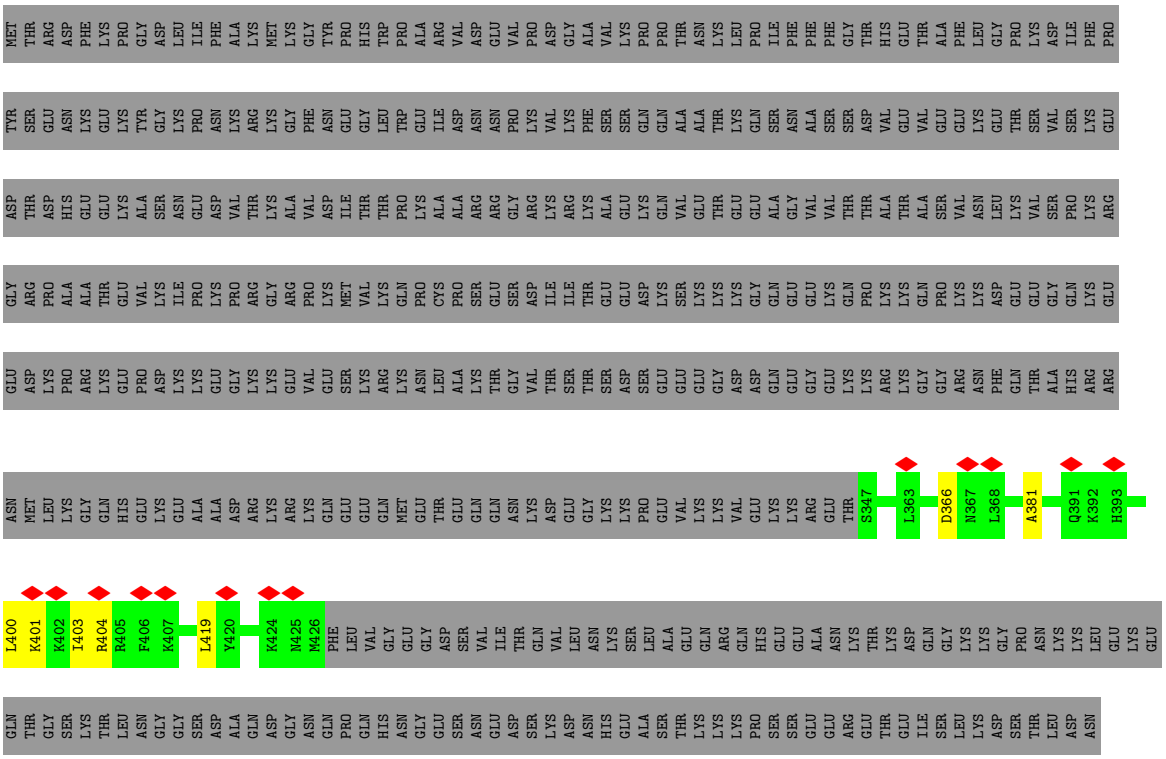
• Molecule 4: PC4 and SFRS1-interacting protein

Chain a:



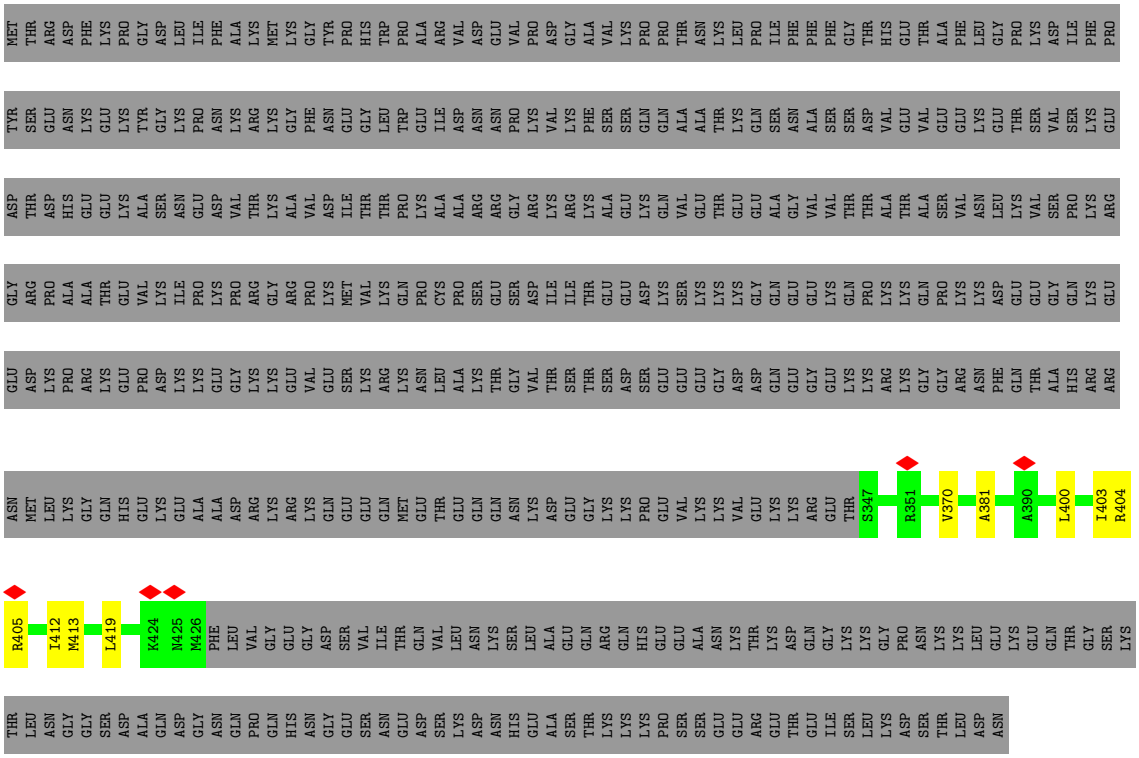
• Molecule 4: PC4 and SFRS1-interacting protein

Chain b:



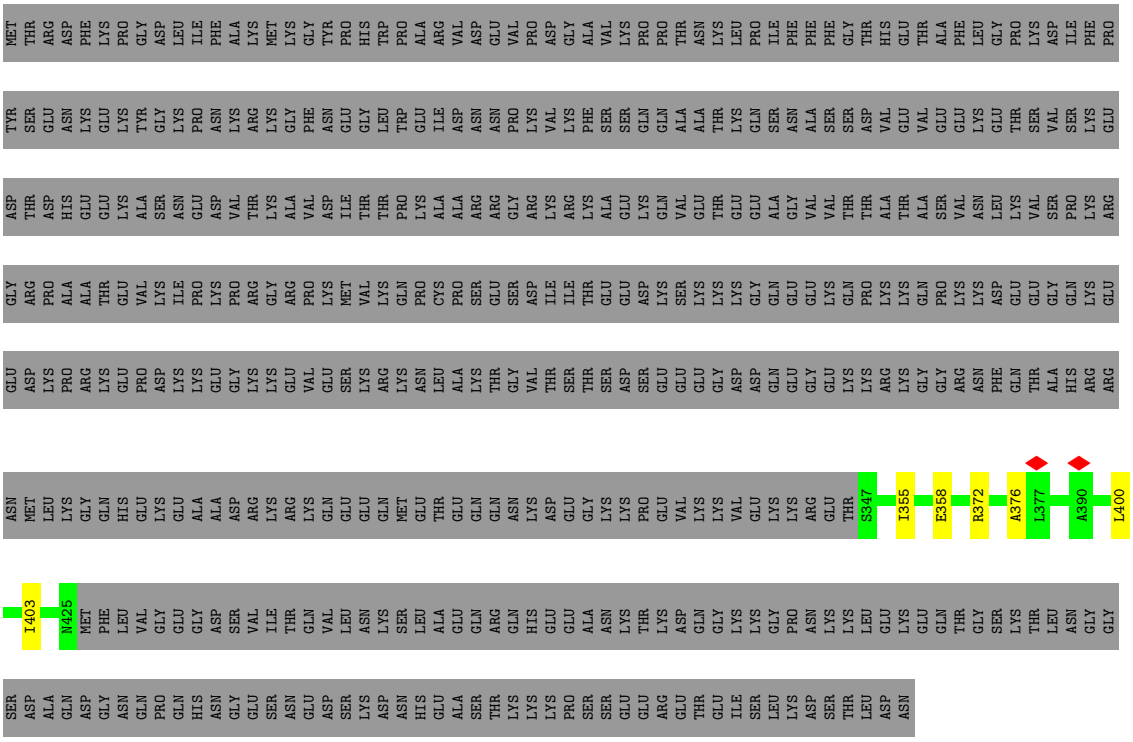
- Molecule 4: PC4 and SFRS1-interacting protein

Chain c:



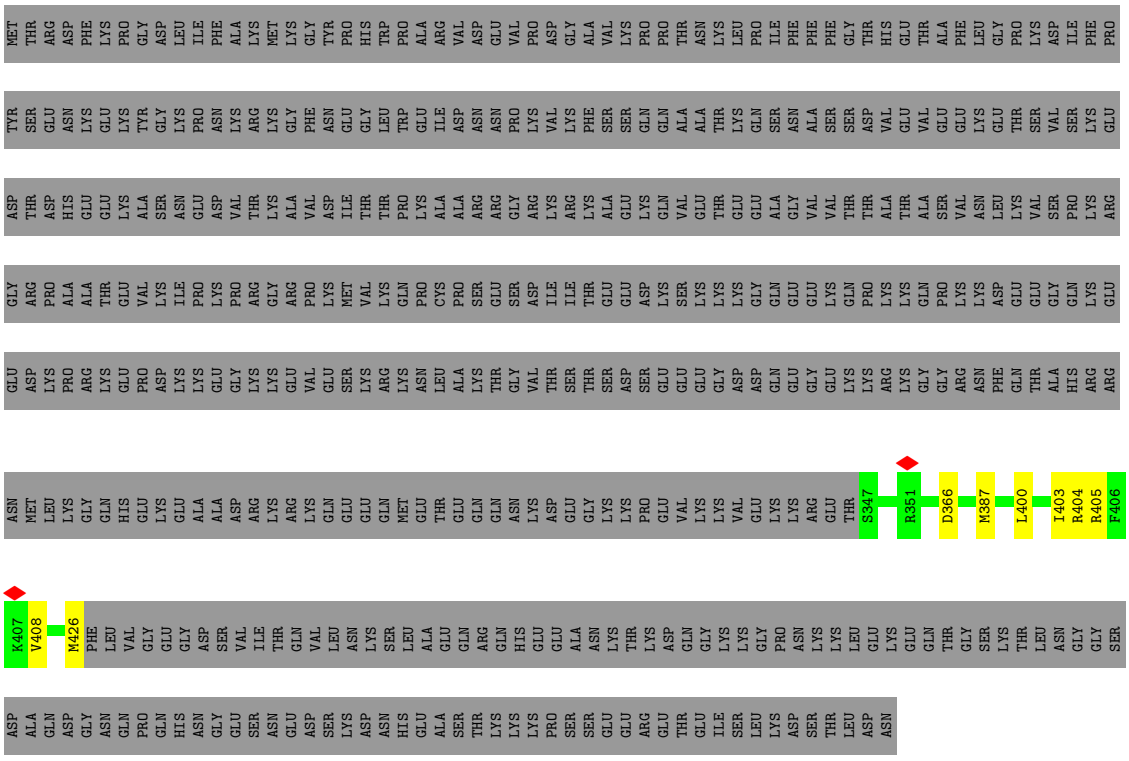
- Molecule 4: PC4 and SFRS1-interacting protein

Chain d: 14% • 85%



- Molecule 4: PC4 and SFRS1-interacting protein

Chain e: 14% • 85%



- Molecule 4: PC4 and SFRS1-interacting protein

Chain f: 8% 14% • 85%

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

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

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

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

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

ASN MET LEU LYS GLY GLN HIS GLU LYS GLU ALA ALA ASP ARG LYS ARG LYS GLN LYS GLU GLN GLN GLN ASN LYS ASP GLU GLY LYS LYS PRO GLU VAL LYS LYS LYS VAL GLU LYS LYS ARG GLU THR M348 D349 S350 R351 L352 Q353 R354 I355 H356 I359 S362

L363 L368 R372 C373 L377 D378 E379 L380 A381 S382 L383 Q384 V385 T386 M387 Q388 Q389 A390 Q391 K392 H393 T394 R405 F406 K407 V408 S409 Q410 V411 L419 Y420 M421 K422 F423 K424 M425 M426 PHE LEU VAL GLY GLU GLY ASP SER VAL ILE THR GLN VAL LEU ASN LYS SER LEU

ALA GLU GLN ARG GLN HIS GLU GLU ALA ASN LYS THR LYS ASP GLN GLY LYS LYS GLY PRO ASN LYS LYS LEU GLU LYS GLU GLN THR GLY SER LYS THR LEU ASN GLY GLY SER ASP ALA GLN ASP GLY ASN GLN PRO GLN HIS ASN GLY GLU SER ASN GLU ASP SER LYS ASP ASN HIS

GLU ALA SER THR LYS LYS LYS PRO SER SER GLU GLU ARG GLU THR GLU ILE SER LEU LYS ASP SER THR LEU ASP ASN

• Molecule 4: PC4 and SFRS1-interacting protein

Chain g: 14% • 85%

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

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

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

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

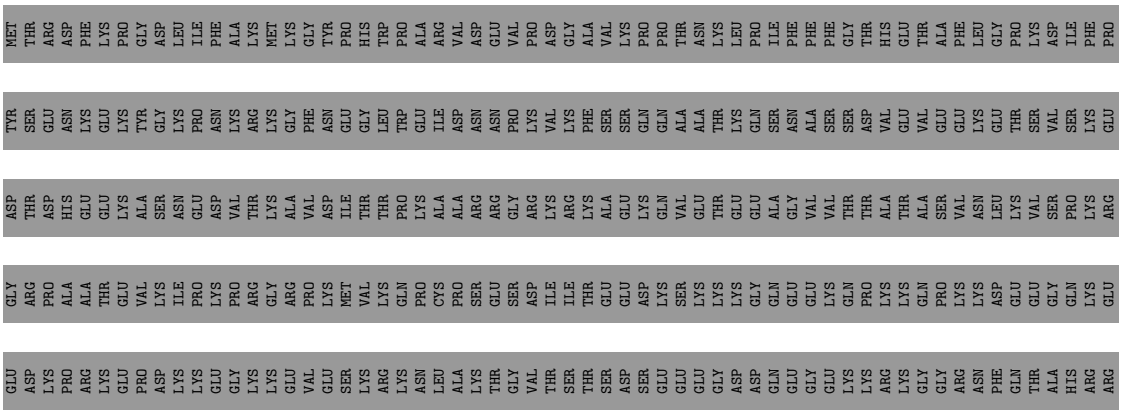
GLU ASP LYS PRO ARG LYS GLU PRO ASP LYS LYS GLU GLY LYS LYS GLU VAL GLU SER LYS ARG LYS ASN LEU ALA LYS THR GLY VAL THR SER THR SER ASP SER GLU GLU GLU GLY ASP ASP GLN GLU GLY GLU LYS LYS ARG LYS GLY GLY ARG ARG ASN PHE GLN THR ALA HIS ARG ARG

ASN MET LEU LYS GLY GLN HIS GLU LYS GLU ALA ALA ASP ARG LYS ARG LYS GLN LYS GLU GLN GLN GLN ASN LYS ASP GLU GLY LYS LYS PRO GLU VAL LYS LYS LYS VAL GLU LYS LYS ARG GLU THR S347 I365 L368 I374 K392 L400 K401 K402 I403

R404 K415 N425 M426 PHE LEU VAL GLY GLU GLY ASP SER VAL ILE THR GLN VAL LEU ASN LYS SER LEU ALA GLU GLN ARG GLN HIS GLU GLU ALA ASN LYS THR LYS ASP GLN GLY LYS LYS GLY PRO ASN LYS LYS LEU GLU LYS GLU GLN THR GLY SER LYS THR LEU ASN GLY

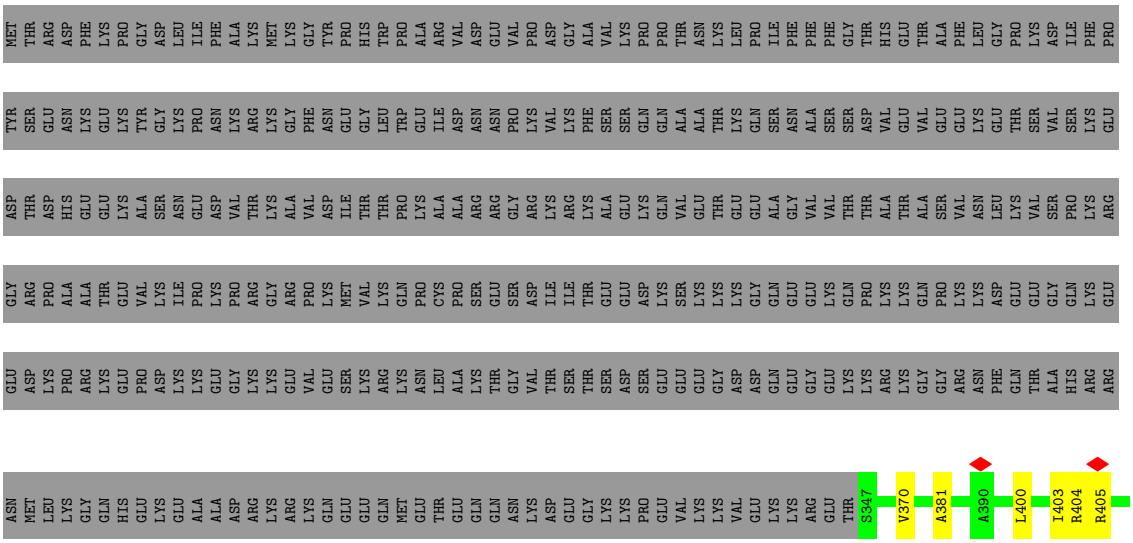
• Molecule 4: PC4 and SFRS1-interacting protein

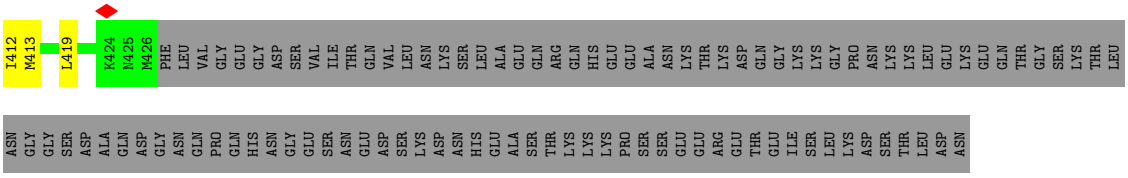
Chain h:



• Molecule 4: PC4 and SFRS1-interacting protein

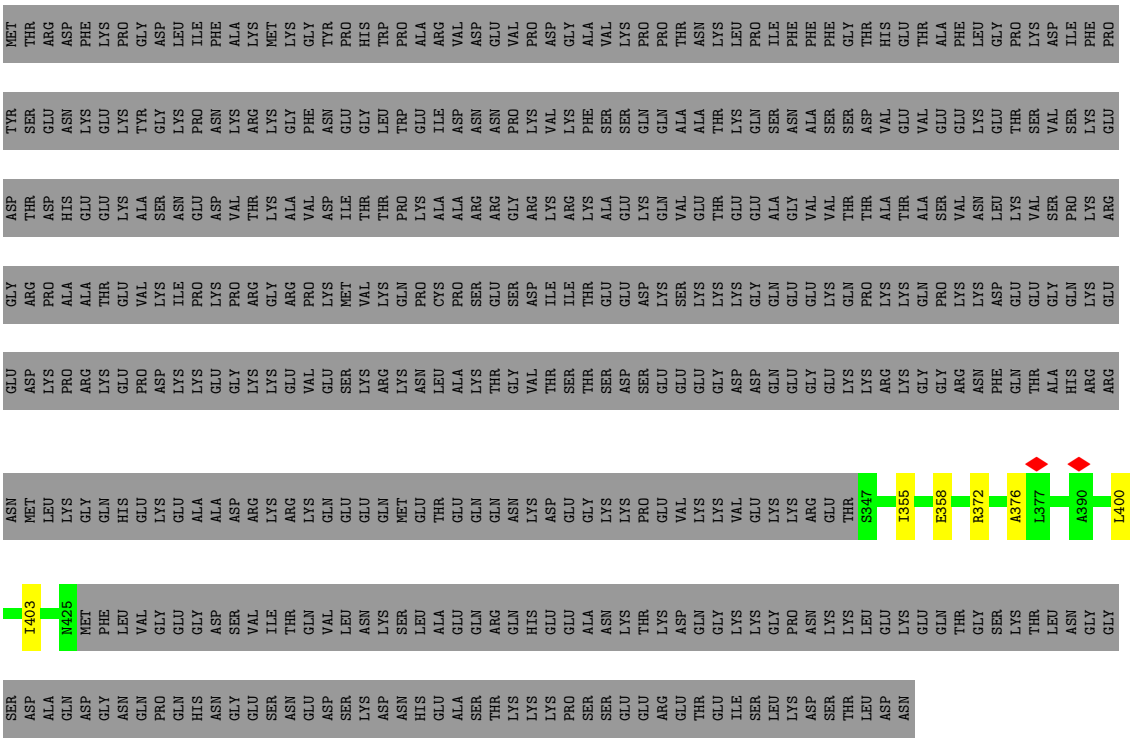
Chain i:





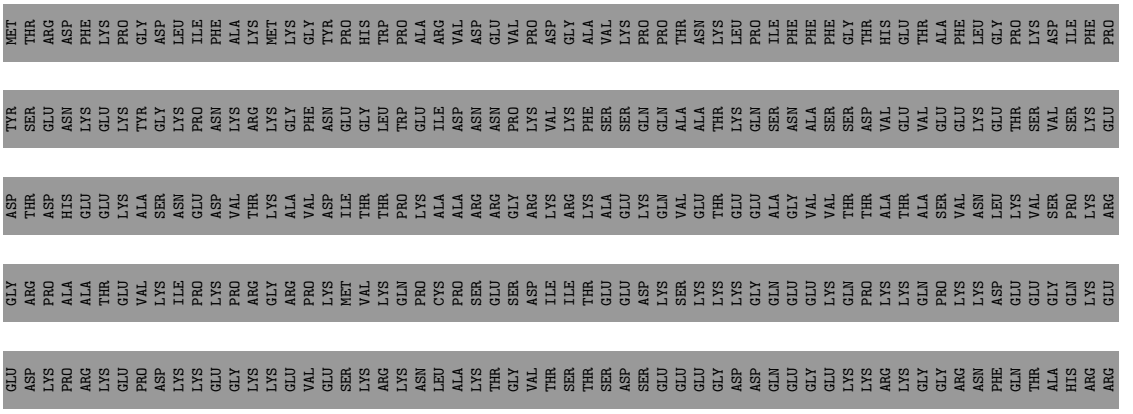
- Molecule 4: PC4 and SFRS1-interacting protein

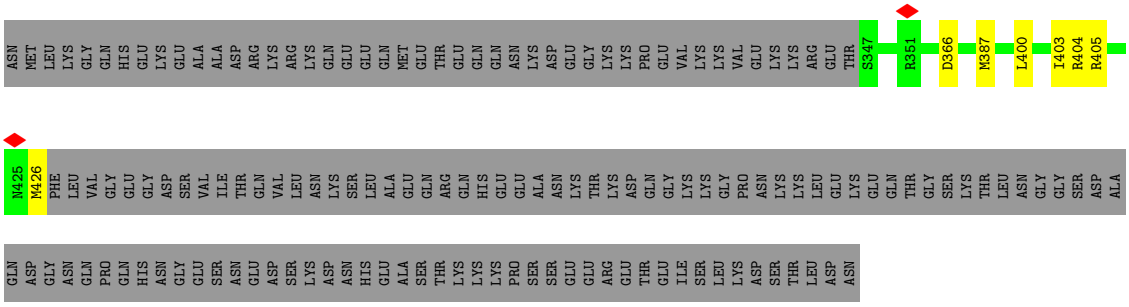
Chain j:



- Molecule 4: PC4 and SFRS1-interacting protein

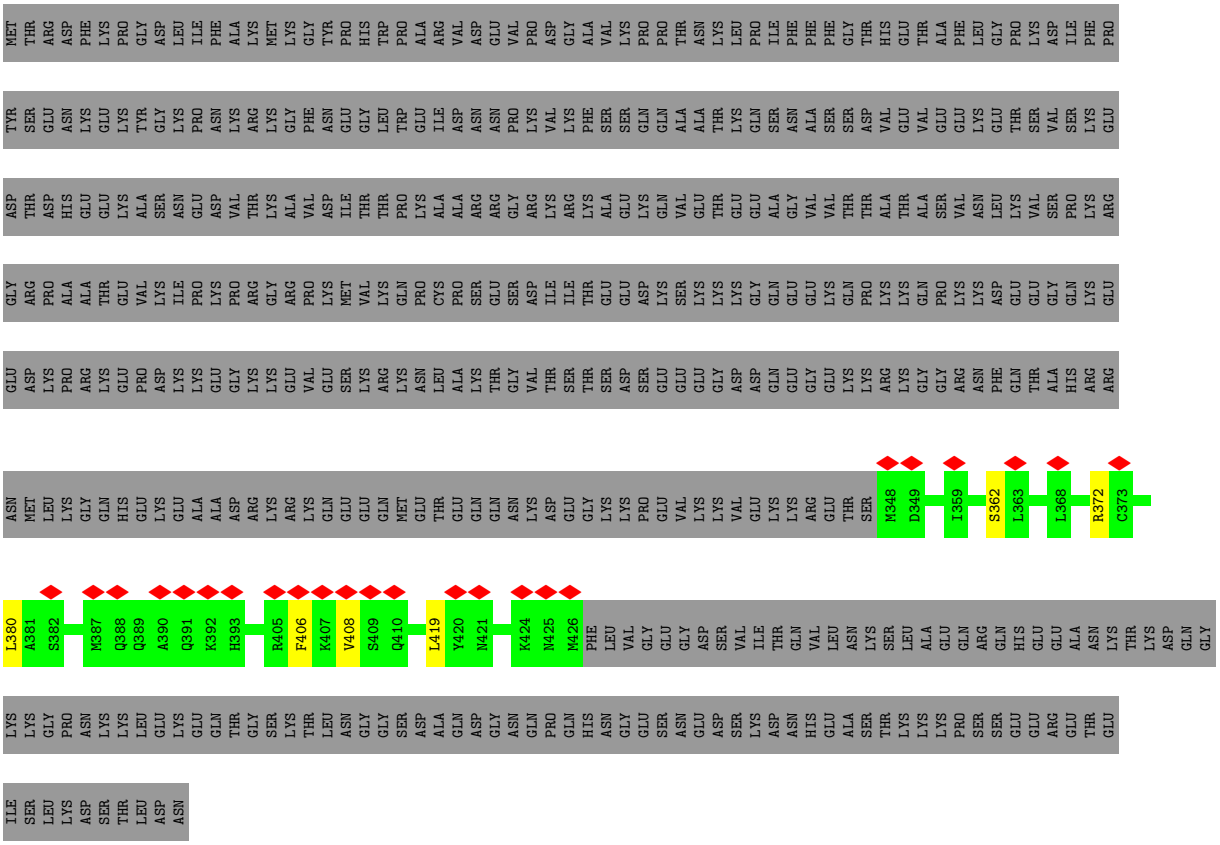
Chain k:





- Molecule 4: PC4 and SFRS1-interacting protein

Chain l:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	167347	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.802	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	418.0, 418.0, 418.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.14	0/2278	0.31	0/3086
1	B	0.10	0/2084	0.25	0/2820
1	C	0.08	0/2202	0.23	0/2980
1	D	0.09	0/2183	0.25	0/2954
1	E	0.10	0/2234	0.25	0/3024
1	F	0.10	0/2187	0.26	0/2964
1	G	0.08	0/2056	0.21	0/2780
1	H	0.09	0/2186	0.25	0/2955
1	I	0.14	0/2278	0.31	0/3086
1	J	0.11	0/2084	0.25	0/2820
1	K	0.08	0/2202	0.23	0/2980
1	L	0.09	0/2183	0.25	0/2954
1	M	0.09	0/2234	0.25	0/3024
1	N	0.10	0/2187	0.25	0/2964
1	O	0.09	0/2056	0.21	0/2780
1	P	0.09	0/2186	0.25	0/2955
2	W	0.20	0/479	0.36	0/738
2	Y	0.20	0/479	0.36	0/738
3	X	0.18	0/436	0.33	0/670
3	Z	0.19	0/436	0.33	0/670
4	a	0.05	0/658	0.16	0/876
4	b	0.05	0/648	0.14	0/865
4	c	0.07	0/658	0.16	0/876
4	d	0.05	0/650	0.15	0/866
4	e	0.07	0/658	0.16	0/876
4	f	0.06	0/640	0.16	0/854
4	g	0.05	0/658	0.16	0/876
4	h	0.05	0/648	0.14	0/865
4	i	0.07	0/658	0.16	0/876
4	j	0.05	0/650	0.15	0/866
4	k	0.07	0/658	0.17	0/876
4	l	0.06	0/640	0.16	0/854

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.10	0/44474	0.24	0/60368

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	2223	0	2188	16	0
1	B	2038	0	1999	15	0
1	C	2150	0	2118	19	0
1	D	2132	0	2107	15	0
1	E	2180	0	2150	32	0
1	F	2136	0	2087	17	0
1	G	2010	0	1970	17	0
1	H	2136	0	2116	39	0
1	I	2223	0	2188	14	0
1	J	2038	0	1999	16	0
1	K	2150	0	2118	20	0
1	L	2132	0	2107	15	0
1	M	2180	0	2150	31	0
1	N	2136	0	2087	16	0
1	O	2010	0	1970	18	0
1	P	2136	0	2116	38	0
2	W	428	0	237	6	0
2	Y	428	0	237	6	0
3	X	389	0	212	7	0
3	Z	389	0	212	7	0
4	a	654	0	691	7	0
4	b	644	0	669	4	0
4	c	654	0	691	5	0
4	d	646	0	682	3	0
4	e	654	0	691	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	f	636	0	664	3	0
4	g	654	0	691	7	0
4	h	644	0	669	4	0
4	i	654	0	691	5	0
4	j	646	0	682	3	0
4	k	654	0	691	5	0
4	l	636	0	664	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
All	All	43436	0	42544	374	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 4.

The worst 5 of 374 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:M:168:ILE:HG13	1:M:169:PRO:HD3	1.65	0.79
1:E:168:ILE:HG13	1:E:169:PRO:HD3	1.65	0.77
1:P:16:HIS:CE1	1:P:40:CYS:SG	2.80	0.75
1:H:16:HIS:CE1	1:H:40:CYS:SG	2.81	0.74
1:H:170:MET:HG3	1:H:177:ALA:HA	1.72	0.70

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	274/281 (98%)	266 (97%)	8 (3%)	0	100	100
1	B	246/281 (88%)	239 (97%)	7 (3%)	0	100	100
1	C	261/281 (93%)	254 (97%)	7 (3%)	0	100	100
1	D	259/281 (92%)	256 (99%)	3 (1%)	0	100	100
1	E	265/281 (94%)	257 (97%)	8 (3%)	0	100	100
1	F	263/281 (94%)	256 (97%)	7 (3%)	0	100	100
1	G	237/281 (84%)	233 (98%)	4 (2%)	0	100	100
1	H	258/281 (92%)	246 (95%)	12 (5%)	0	100	100
1	I	274/281 (98%)	265 (97%)	9 (3%)	0	100	100
1	J	246/281 (88%)	239 (97%)	7 (3%)	0	100	100
1	K	261/281 (93%)	254 (97%)	7 (3%)	0	100	100
1	L	259/281 (92%)	256 (99%)	3 (1%)	0	100	100
1	M	265/281 (94%)	257 (97%)	8 (3%)	0	100	100
1	N	263/281 (94%)	255 (97%)	8 (3%)	0	100	100
1	O	237/281 (84%)	234 (99%)	3 (1%)	0	100	100
1	P	258/281 (92%)	246 (95%)	12 (5%)	0	100	100
4	a	78/530 (15%)	78 (100%)	0	0	100	100
4	b	78/530 (15%)	77 (99%)	1 (1%)	0	100	100
4	c	78/530 (15%)	77 (99%)	1 (1%)	0	100	100
4	d	77/530 (14%)	76 (99%)	1 (1%)	0	100	100
4	e	78/530 (15%)	77 (99%)	1 (1%)	0	100	100
4	f	77/530 (14%)	77 (100%)	0	0	100	100
4	g	78/530 (15%)	78 (100%)	0	0	100	100
4	h	78/530 (15%)	77 (99%)	1 (1%)	0	100	100
4	i	78/530 (15%)	77 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	j	77/530 (14%)	76 (99%)	1 (1%)	0	100	100
4	k	78/530 (15%)	77 (99%)	1 (1%)	0	100	100
4	l	77/530 (14%)	77 (100%)	0	0	100	100
All	All	5058/10856 (47%)	4937 (98%)	121 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	238/246 (97%)	234 (98%)	4 (2%)	53	83
1	B	219/246 (89%)	216 (99%)	3 (1%)	59	85
1	C	230/246 (94%)	228 (99%)	2 (1%)	70	89
1	D	230/246 (94%)	229 (100%)	1 (0%)	84	94
1	E	235/246 (96%)	233 (99%)	2 (1%)	70	89
1	F	226/246 (92%)	219 (97%)	7 (3%)	35	70
1	G	215/246 (87%)	212 (99%)	3 (1%)	59	85
1	H	230/246 (94%)	228 (99%)	2 (1%)	70	89
1	I	238/246 (97%)	234 (98%)	4 (2%)	53	83
1	J	219/246 (89%)	216 (99%)	3 (1%)	59	85
1	K	230/246 (94%)	228 (99%)	2 (1%)	70	89
1	L	230/246 (94%)	229 (100%)	1 (0%)	84	94
1	M	235/246 (96%)	233 (99%)	2 (1%)	70	89
1	N	226/246 (92%)	219 (97%)	7 (3%)	35	70
1	O	215/246 (87%)	212 (99%)	3 (1%)	59	85
1	P	230/246 (94%)	228 (99%)	2 (1%)	70	89
4	a	76/470 (16%)	76 (100%)	0	100	100
4	b	74/470 (16%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	c	76/470 (16%)	76 (100%)	0	100	100
4	d	75/470 (16%)	75 (100%)	0	100	100
4	e	76/470 (16%)	76 (100%)	0	100	100
4	f	73/470 (16%)	73 (100%)	0	100	100
4	g	76/470 (16%)	76 (100%)	0	100	100
4	h	74/470 (16%)	74 (100%)	0	100	100
4	i	76/470 (16%)	76 (100%)	0	100	100
4	j	75/470 (16%)	75 (100%)	0	100	100
4	k	76/470 (16%)	76 (100%)	0	100	100
4	l	73/470 (16%)	73 (100%)	0	100	100
All	All	4546/9576 (48%)	4498 (99%)	48 (1%)	63	87

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	17	GLN
1	M	185	LEU
1	J	65	VAL
1	K	65	VAL
1	N	60	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	157	HIS
1	P	242	GLN
1	N	204	ASN
1	O	212	GLN
1	G	204	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 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.

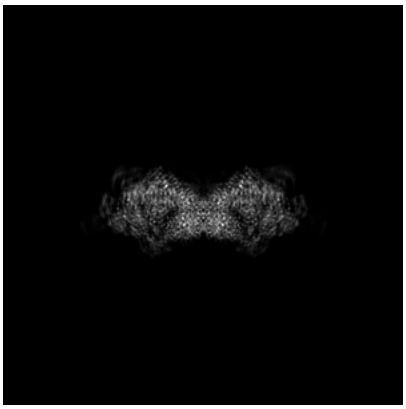
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-54482. These allow visual inspection of the internal detail of the map and identification of artifacts.

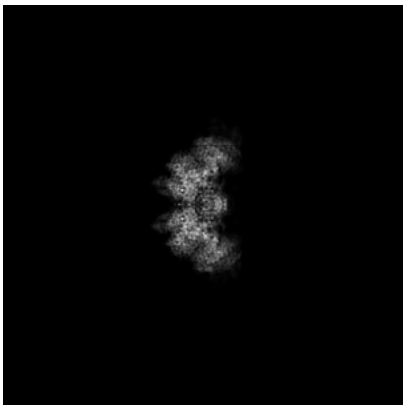
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

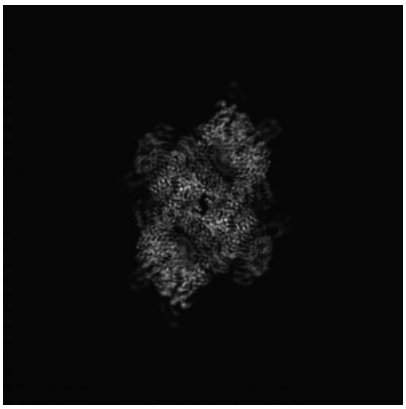
6.1.1 Primary map



X

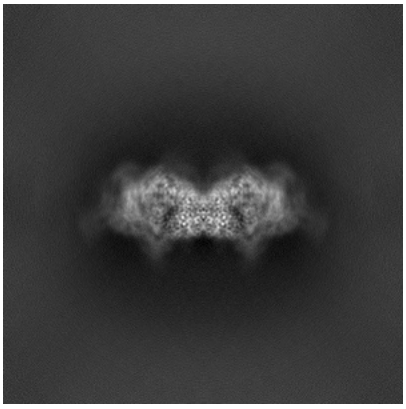


Y

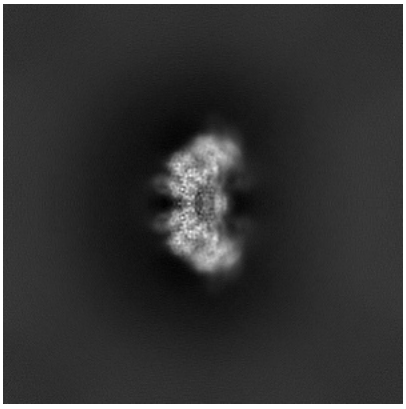


Z

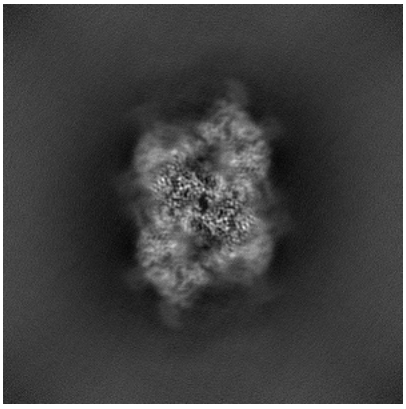
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

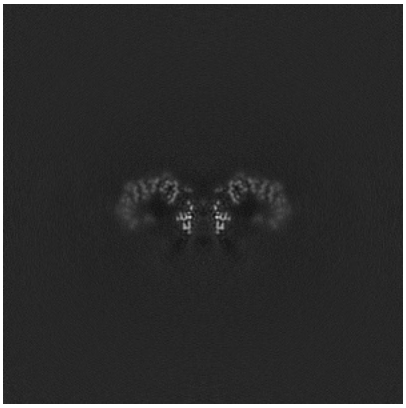
6.2.1 Primary map

X Index: 220

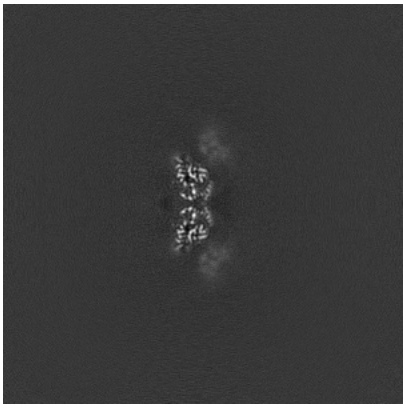
Y Index: 220

Z Index: 220

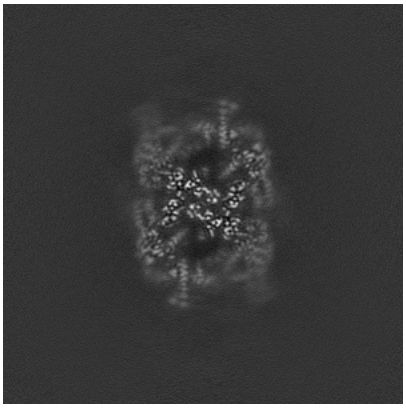
6.2.2 Raw map



X Index: 220



Y Index: 220

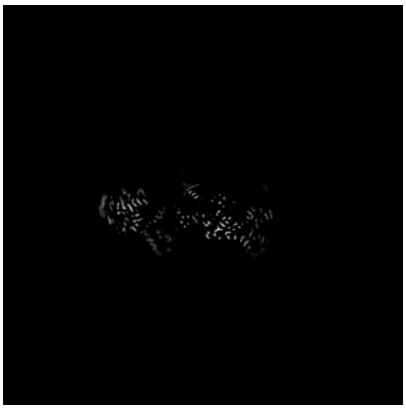


Z Index: 220

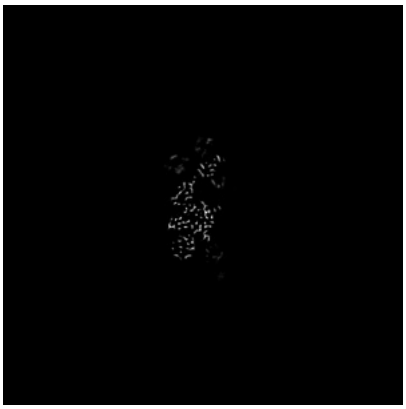
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



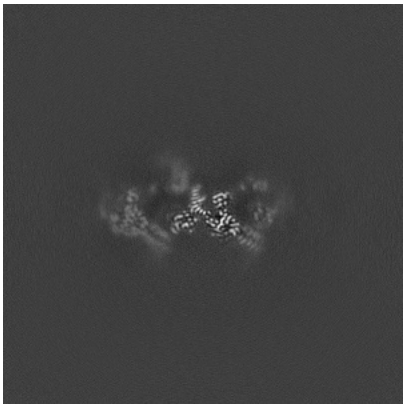
X Index: 199



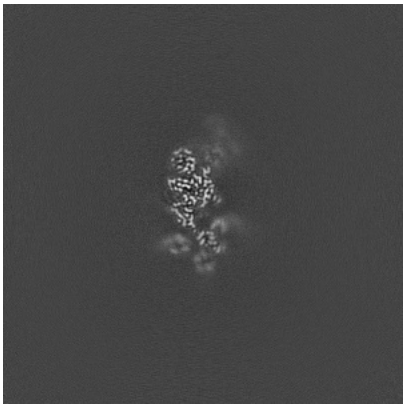
Y Index: 237

Z Index: 222

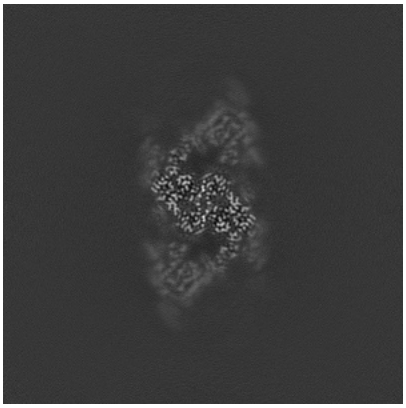
6.3.2 Raw map



X Index: 205



Y Index: 203

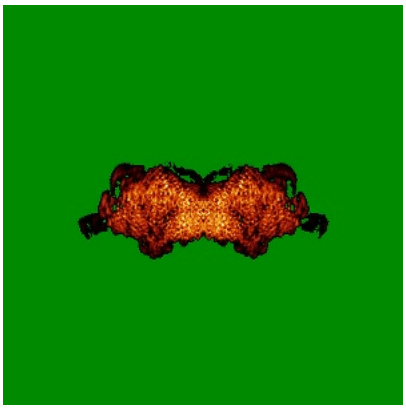


Z Index: 205

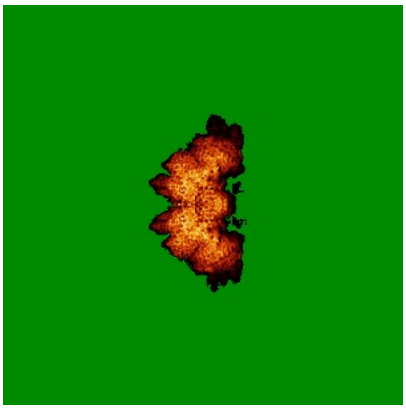
The images above show the largest variance slices of the map in three orthogonal directions.

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

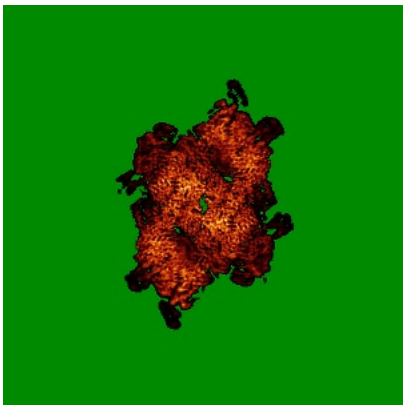
6.4.1 Primary map



X

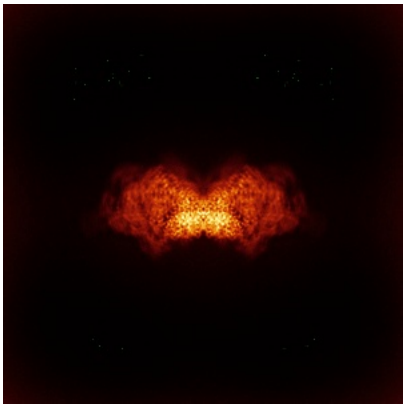


Y

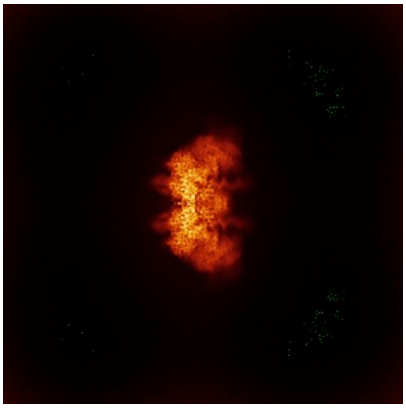


Z

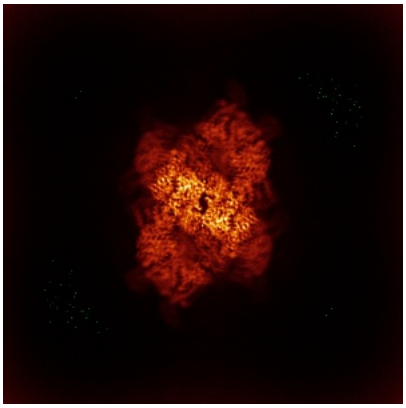
6.4.2 Raw map



X



Y

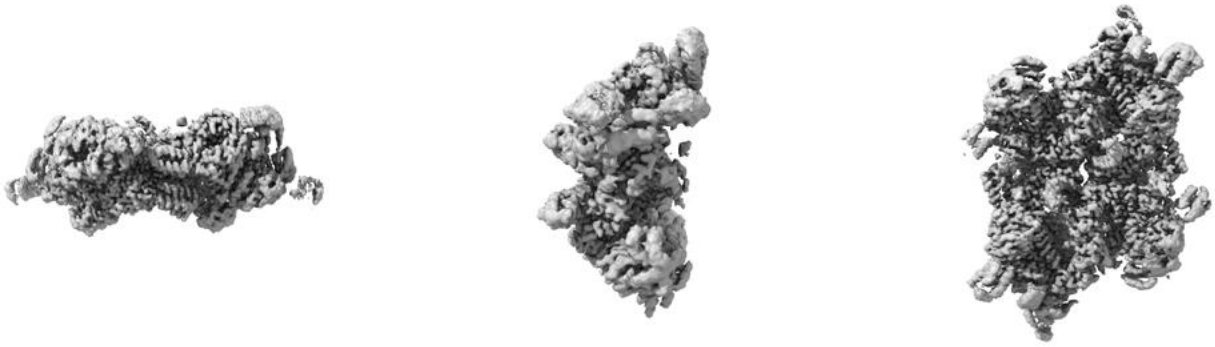


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

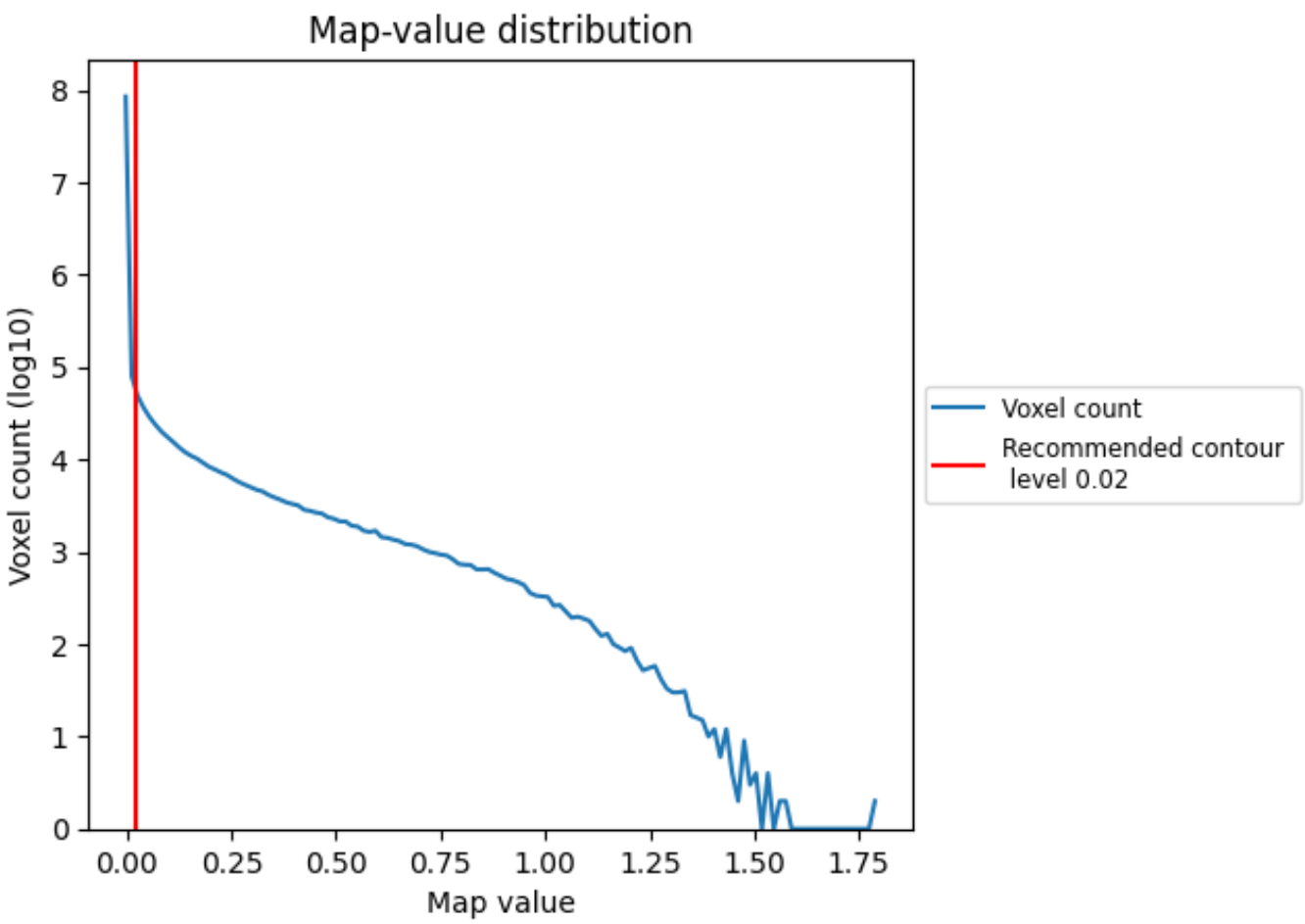
6.6 Mask visualisation (i)

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

7 Map analysis (i)

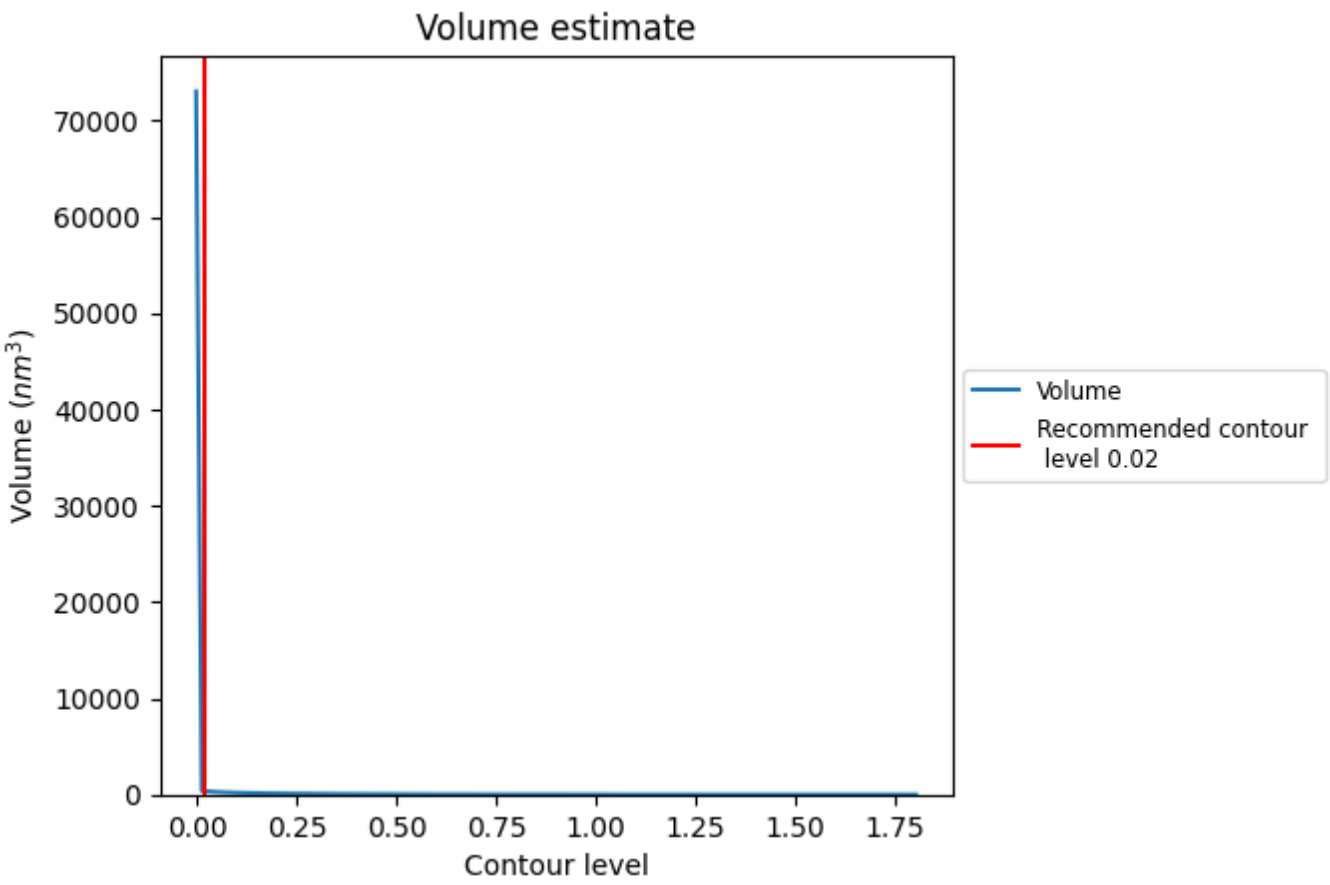
This section contains the results of statistical analysis of the map.

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.

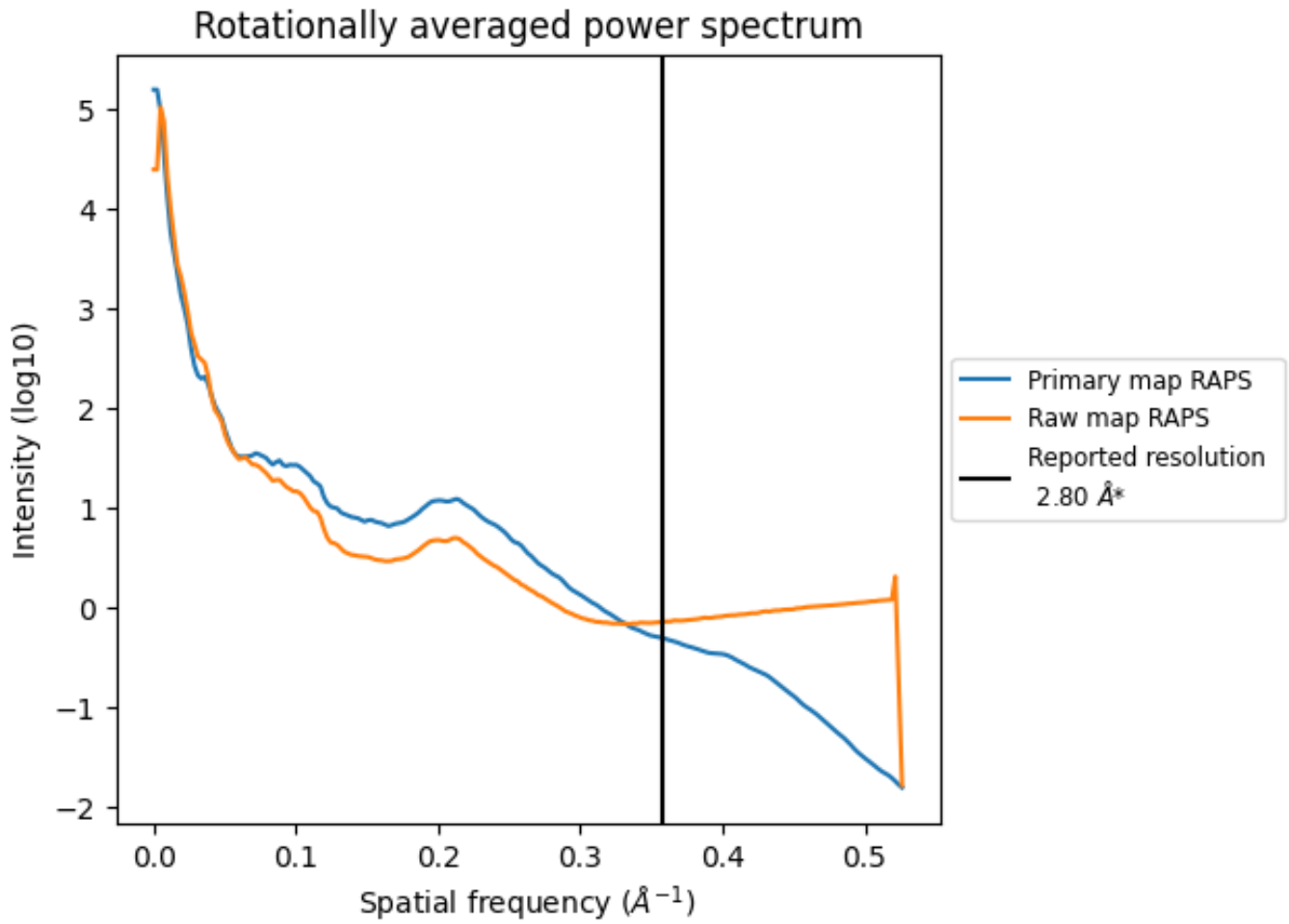
7.2 Volume estimate (i)



The volume at the recommended contour level is 361 nm^3; this corresponds to an approximate mass of 326 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)

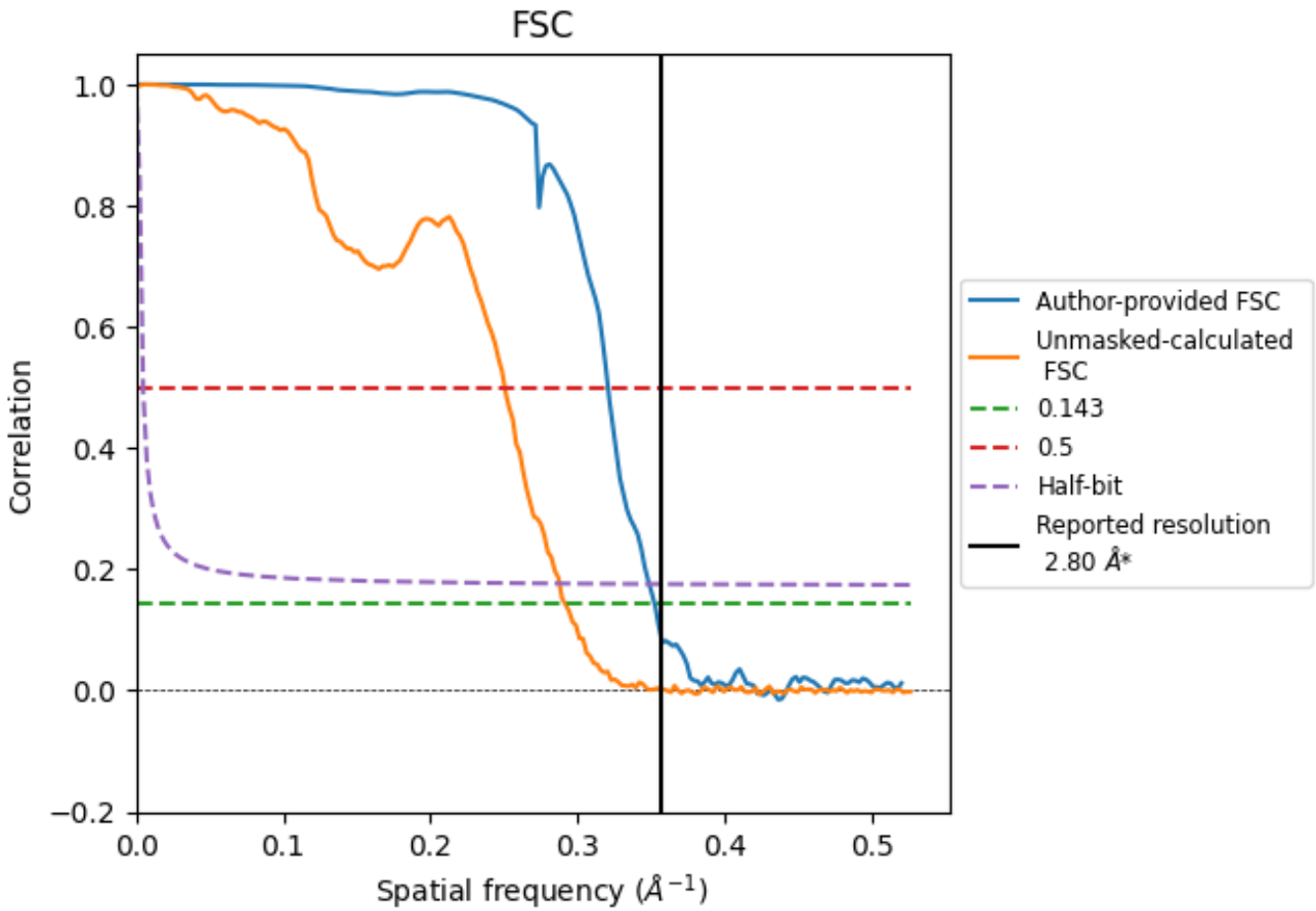


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

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 0.357 Å^{-1}

8.2 Resolution estimates (i)

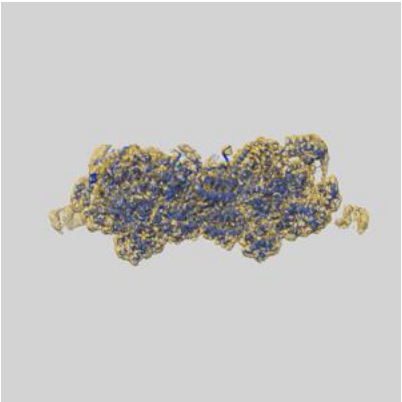
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.84	3.12	2.87
Unmasked-calculated*	3.43	3.99	3.47

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.43 differs from the reported value 2.8 by more than 10 %

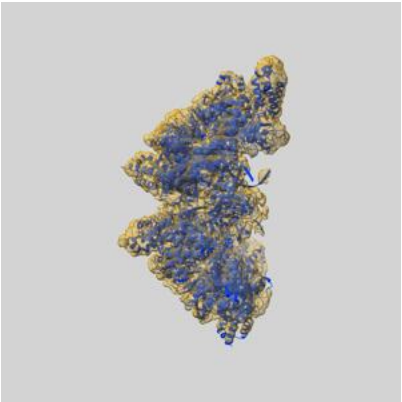
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-54482 and PDB model 9S29. Per-residue inclusion information can be found in section 3 on page 8.

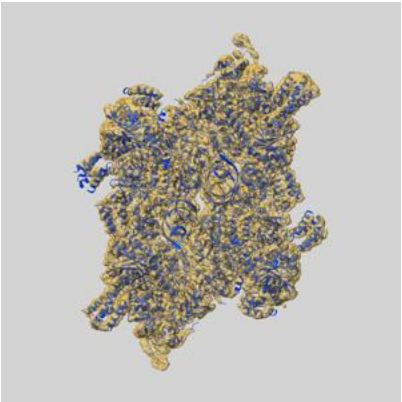
9.1 Map-model overlay (i)



X



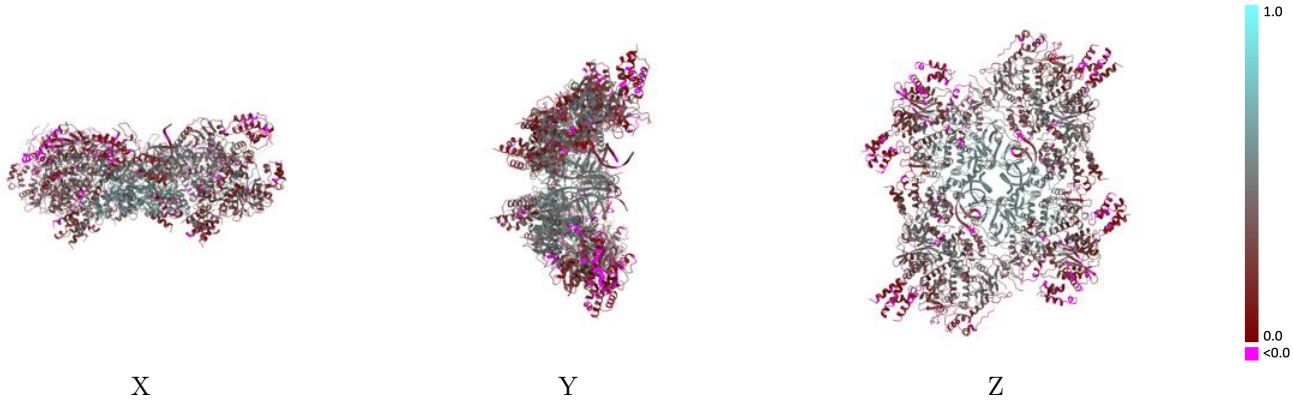
Y



Z

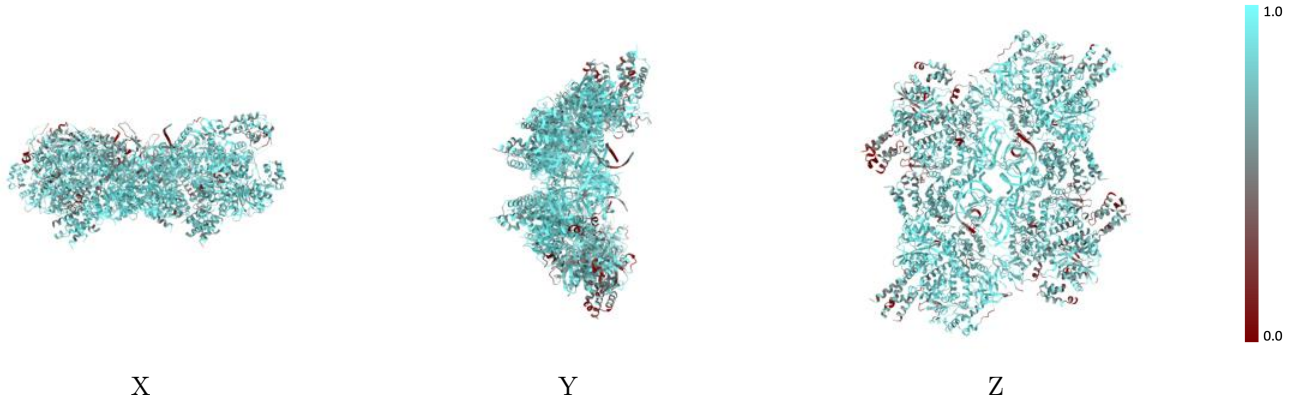
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



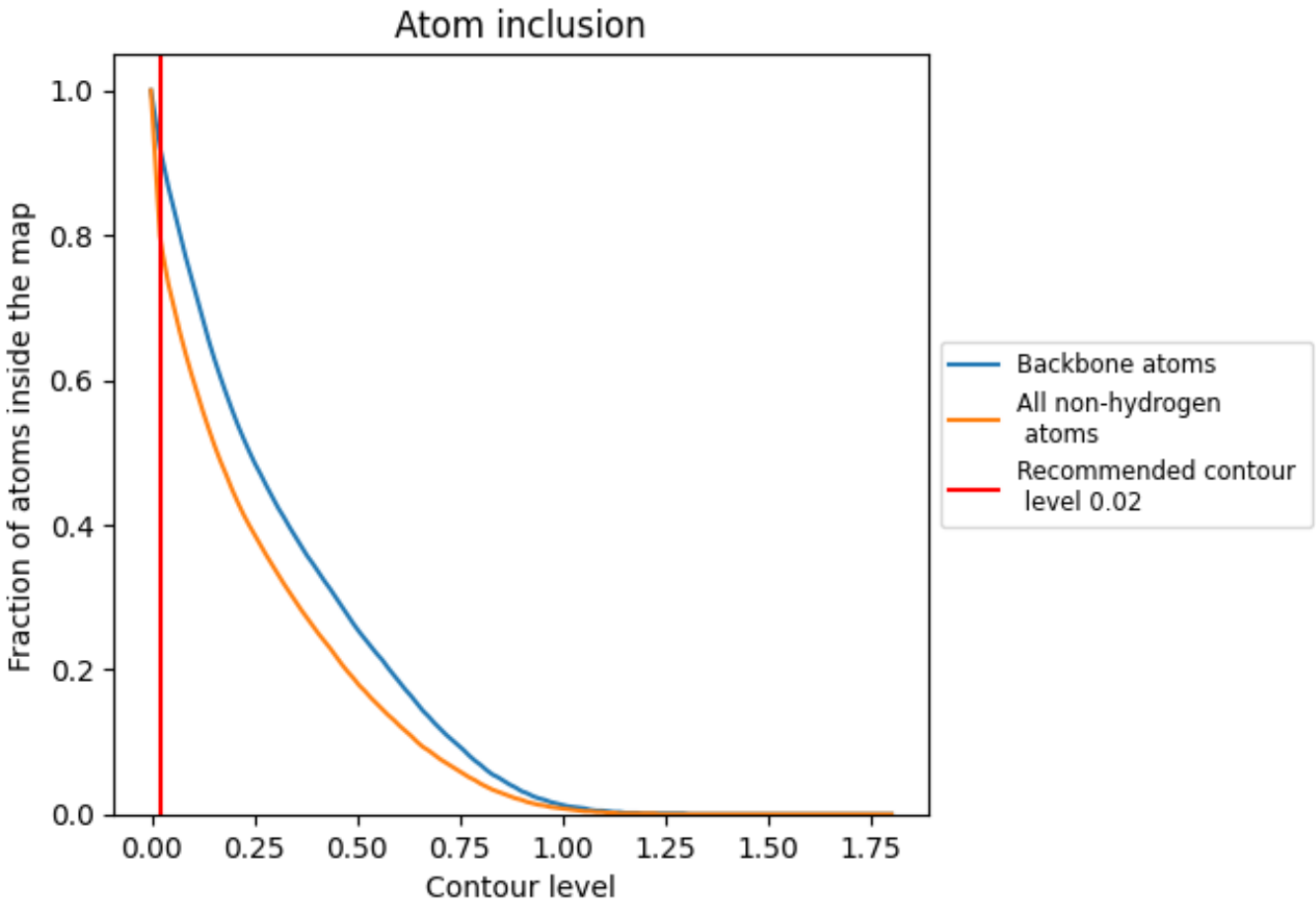
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 92% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7990	0.3370
A	0.9350	0.5340
B	0.7930	0.4150
C	0.7360	0.3110
D	0.7000	0.2360
E	0.8860	0.4050
F	0.8830	0.4150
G	0.7950	0.2740
H	0.8340	0.3080
I	0.9400	0.5360
J	0.8030	0.4170
K	0.7380	0.3090
L	0.7310	0.2410
M	0.8860	0.4040
N	0.8860	0.4160
O	0.8060	0.2760
P	0.8490	0.3090
W	0.8480	0.4750
X	0.8300	0.4400
Y	0.8970	0.4810
Z	0.8360	0.4500
a	0.7030	0.2410
b	0.6280	0.0860
c	0.7290	0.2510
d	0.7390	0.1920
e	0.7920	0.3120
f	0.3400	0.0560
g	0.7220	0.2380
h	0.5460	0.0670
i	0.7650	0.2570
j	0.7540	0.2000
k	0.7820	0.3020
l	0.5010	0.0650