Full wwPDB EM Validation Report ⓘ

Oct 31, 2023 – 12:44 PM EDT

PDB ID	:	8FXH
EMDB ID	:	EMD-29533
Title	:	Cryo-EM structure of Stanieria sp. CphA2
Authors	:	Markus, L.M.; Sharon, I.; Strauss, M.; Schmeing, T.M.
Deposited on	:	2023-01-24
Resolution	:	2.80 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 ⓘ 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 ⓘ) were used in the production of this report:

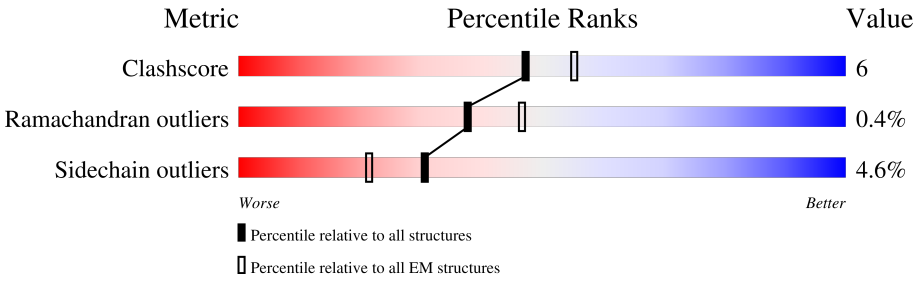
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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)
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	A	642	38% 72% 22%
1	B	642	39% 82% 14%
1	C	642	26% 85% 13%
1	D	642	30% 85% 12%
1	E	642	45% 83% 14%
1	F	642	36% 72% 22%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 30228 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 RimK domain-containing protein ATP-grasp.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	631	Total	C	N	O	S	0	0
			5038	3214	845	965	14		
1	B	631	Total	C	N	O	S	0	0
			5038	3214	845	965	14		
1	C	631	Total	C	N	O	S	0	0
			5038	3214	845	965	14		
1	D	631	Total	C	N	O	S	0	0
			5038	3214	845	965	14		
1	E	631	Total	C	N	O	S	0	0
			5038	3214	845	965	14		
1	F	631	Total	C	N	O	S	0	0
			5038	3214	845	965	14		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	637	GLU	-	expression tag	UNP A0A140K0M0
A	638	ASN	-	expression tag	UNP A0A140K0M0
A	639	LEU	-	expression tag	UNP A0A140K0M0
A	640	TYR	-	expression tag	UNP A0A140K0M0
A	641	PHE	-	expression tag	UNP A0A140K0M0
A	642	GLN	-	expression tag	UNP A0A140K0M0
B	637	GLU	-	expression tag	UNP A0A140K0M0
B	638	ASN	-	expression tag	UNP A0A140K0M0
B	639	LEU	-	expression tag	UNP A0A140K0M0
B	640	TYR	-	expression tag	UNP A0A140K0M0
B	641	PHE	-	expression tag	UNP A0A140K0M0
B	642	GLN	-	expression tag	UNP A0A140K0M0
C	637	GLU	-	expression tag	UNP A0A140K0M0
C	638	ASN	-	expression tag	UNP A0A140K0M0
C	639	LEU	-	expression tag	UNP A0A140K0M0
C	640	TYR	-	expression tag	UNP A0A140K0M0
C	641	PHE	-	expression tag	UNP A0A140K0M0
C	642	GLN	-	expression tag	UNP A0A140K0M0

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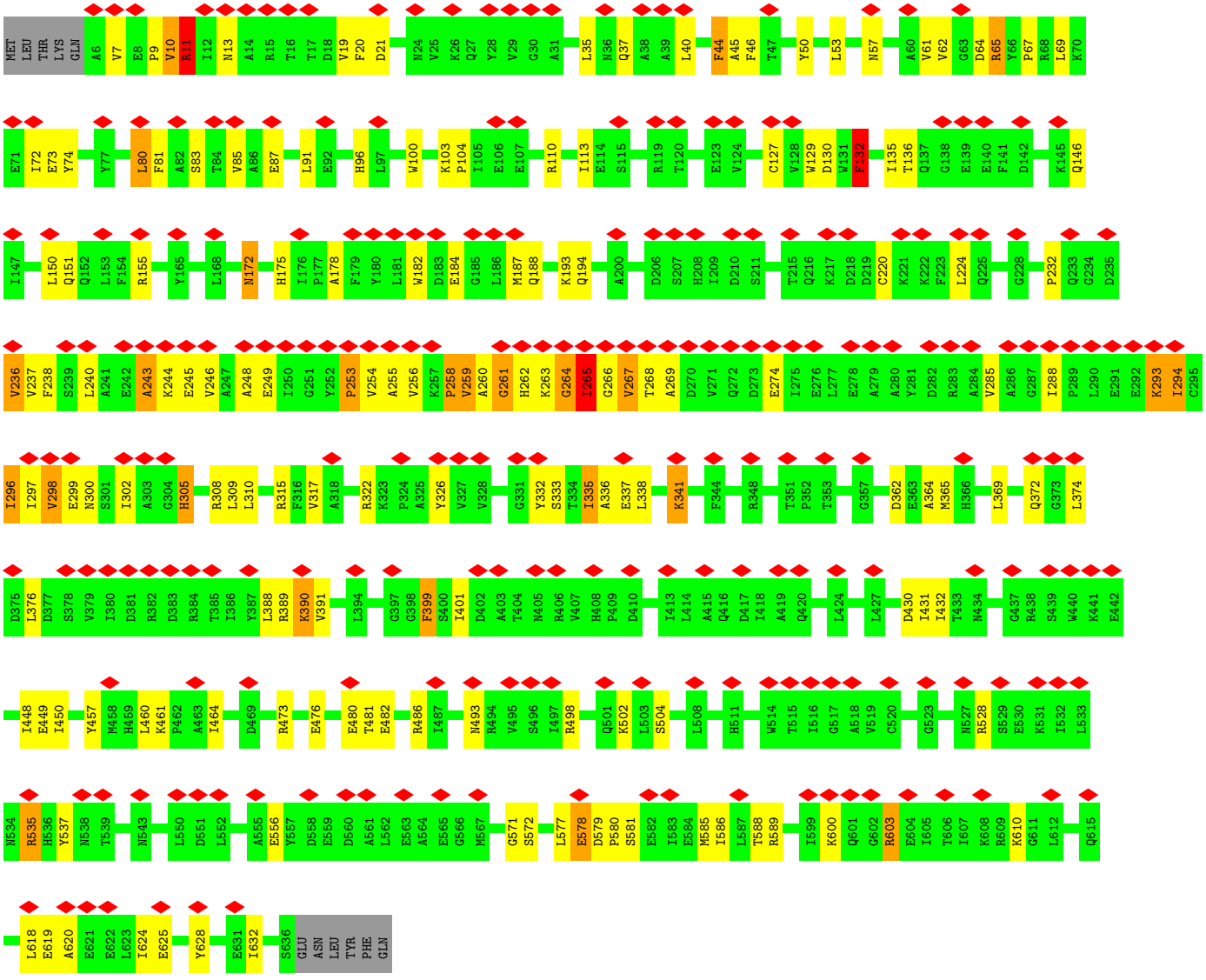
Chain	Residue	Modelled	Actual	Comment	Reference
D	637	GLU	-	expression tag	UNP A0A140K0M0
D	638	ASN	-	expression tag	UNP A0A140K0M0
D	639	LEU	-	expression tag	UNP A0A140K0M0
D	640	TYR	-	expression tag	UNP A0A140K0M0
D	641	PHE	-	expression tag	UNP A0A140K0M0
D	642	GLN	-	expression tag	UNP A0A140K0M0
E	637	GLU	-	expression tag	UNP A0A140K0M0
E	638	ASN	-	expression tag	UNP A0A140K0M0
E	639	LEU	-	expression tag	UNP A0A140K0M0
E	640	TYR	-	expression tag	UNP A0A140K0M0
E	641	PHE	-	expression tag	UNP A0A140K0M0
E	642	GLN	-	expression tag	UNP A0A140K0M0
F	637	GLU	-	expression tag	UNP A0A140K0M0
F	638	ASN	-	expression tag	UNP A0A140K0M0
F	639	LEU	-	expression tag	UNP A0A140K0M0
F	640	TYR	-	expression tag	UNP A0A140K0M0
F	641	PHE	-	expression tag	UNP A0A140K0M0
F	642	GLN	-	expression tag	UNP A0A140K0M0

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.

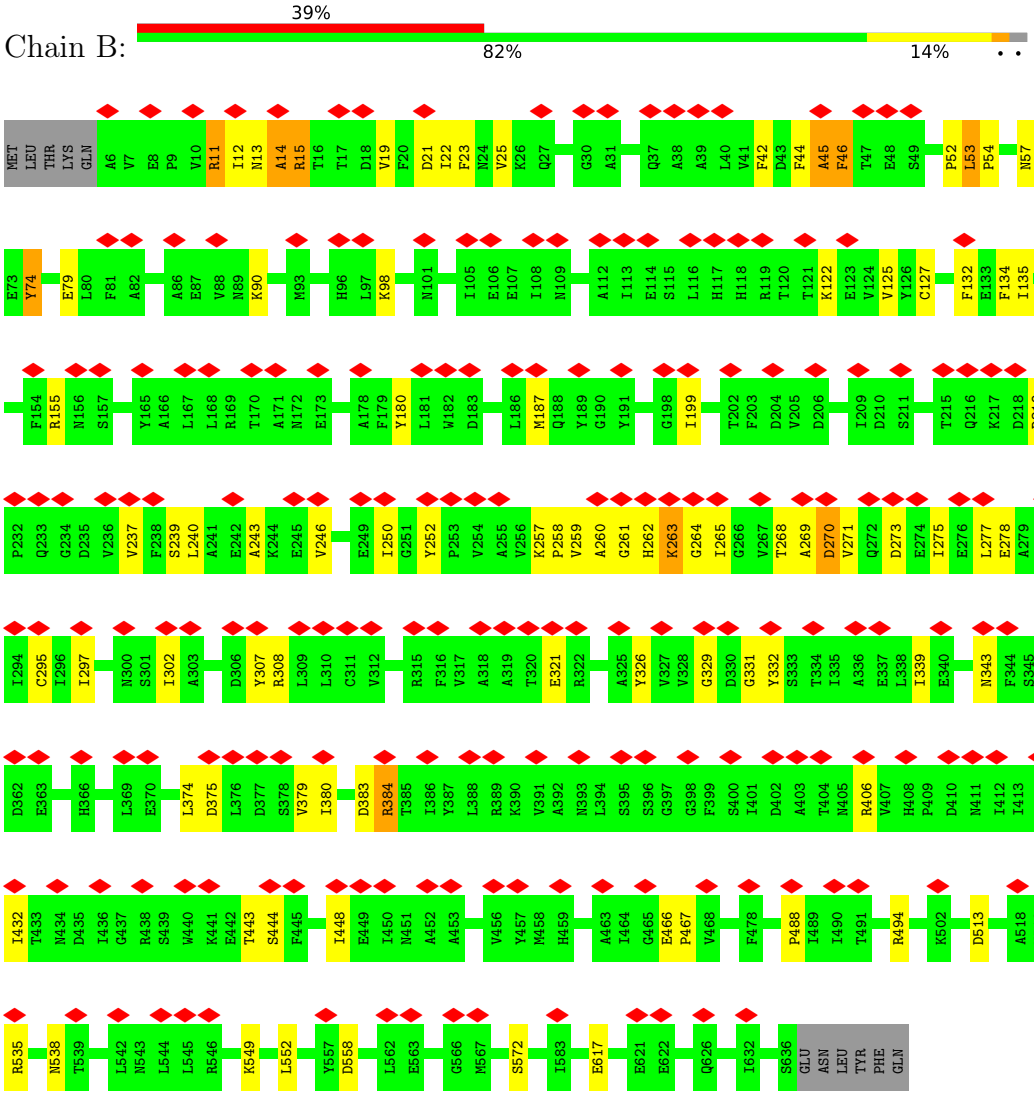
• Molecule 1: RimK domain-containing protein ATP-grasp

Chain A:



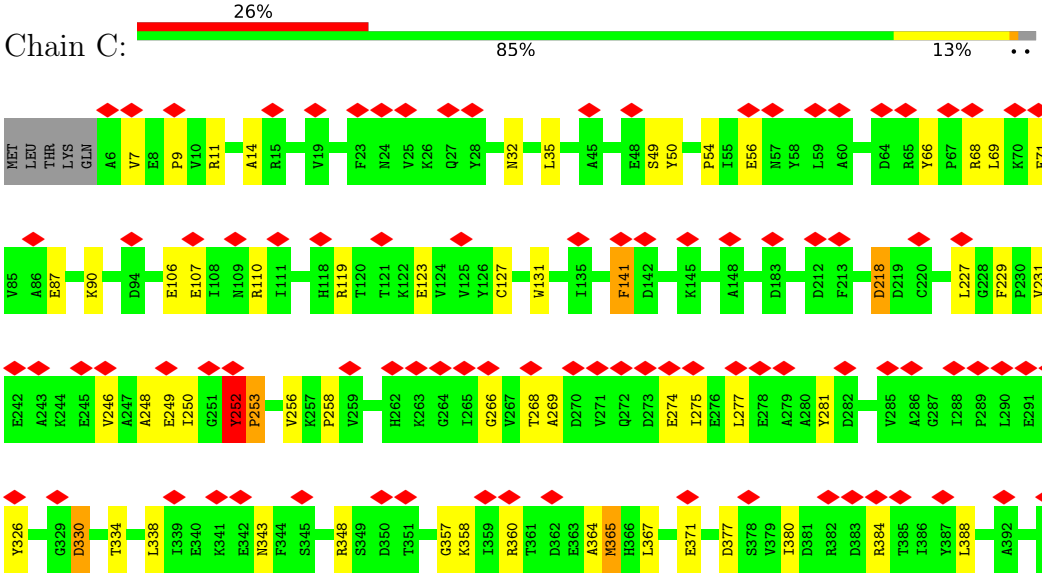
• Molecule 1: RimK domain-containing protein ATP-grasp

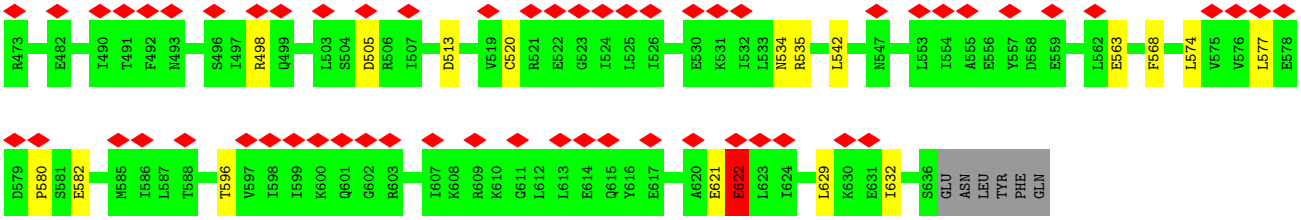
Chain B:



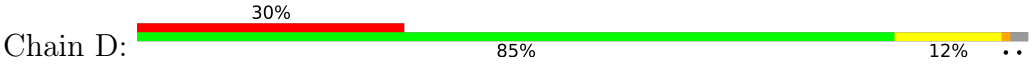
• Molecule 1: RimK domain-containing protein ATP-grasp

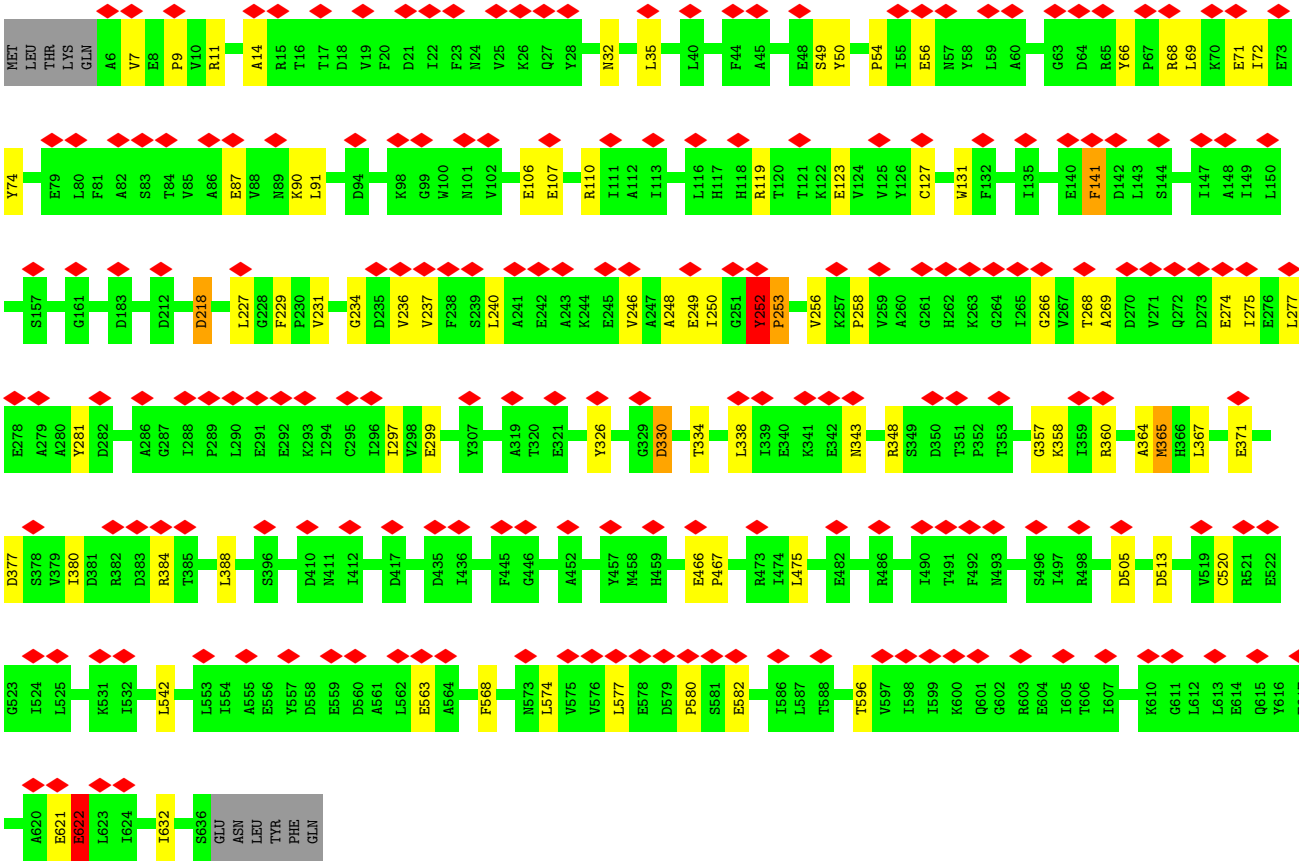
Chain C:



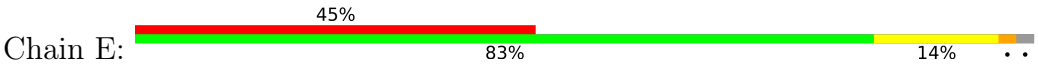


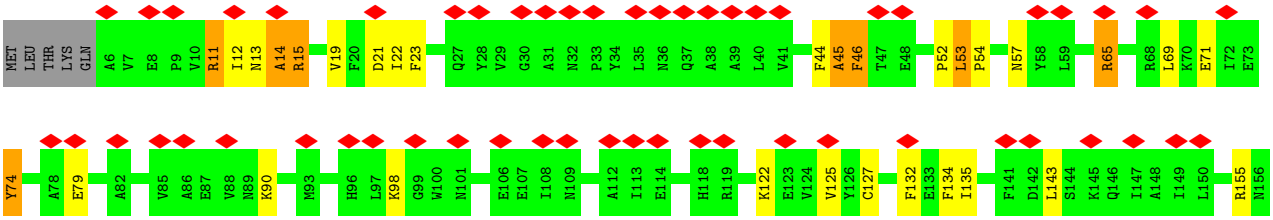
• Molecule 1: RimK domain-containing protein ATP-grasp

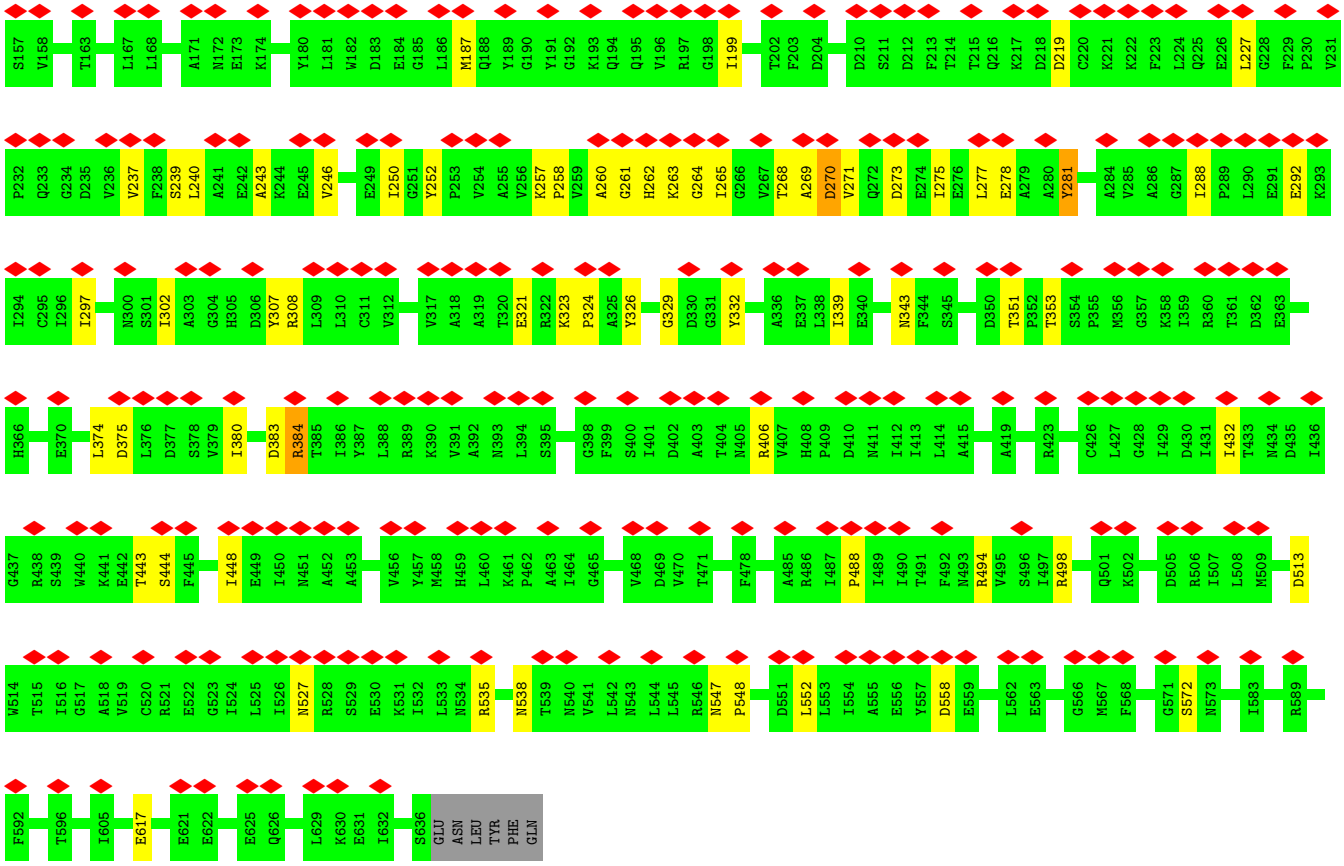




• Molecule 1: RimK domain-containing protein ATP-grasp

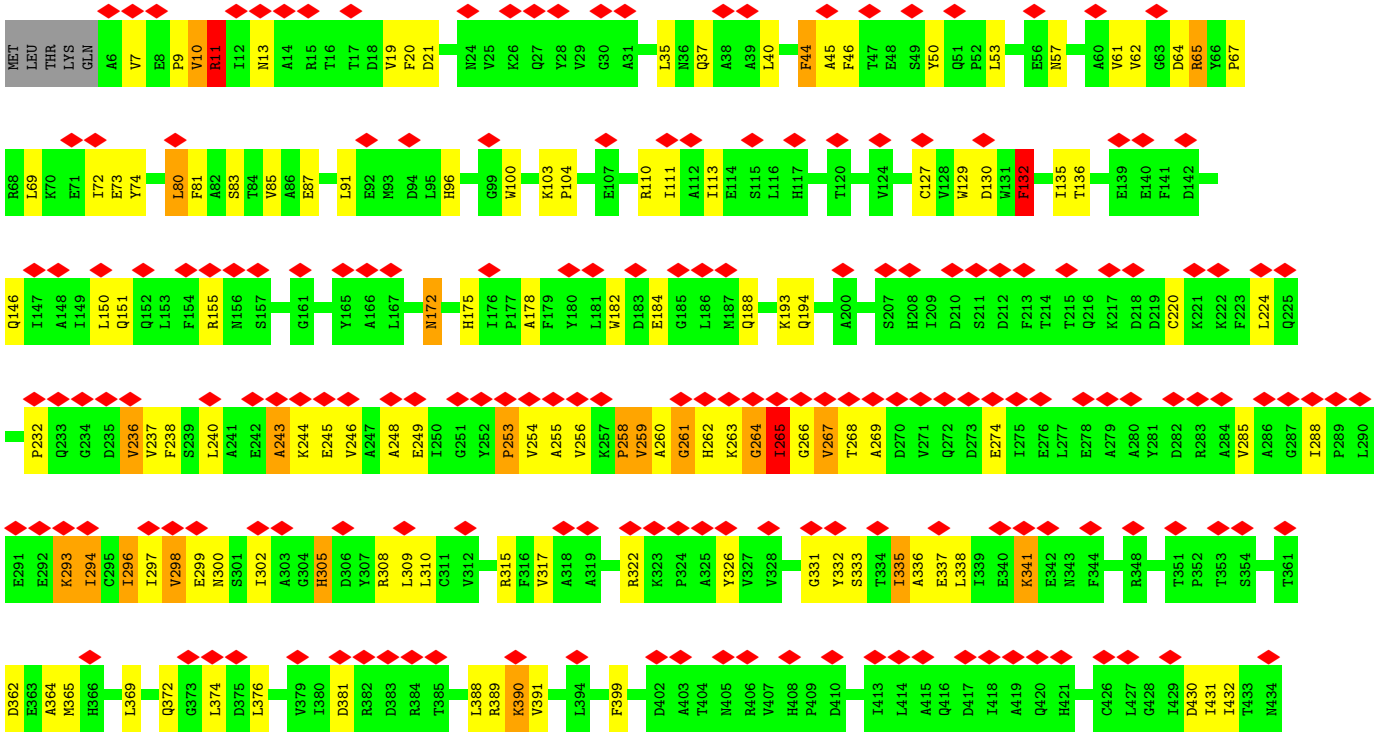


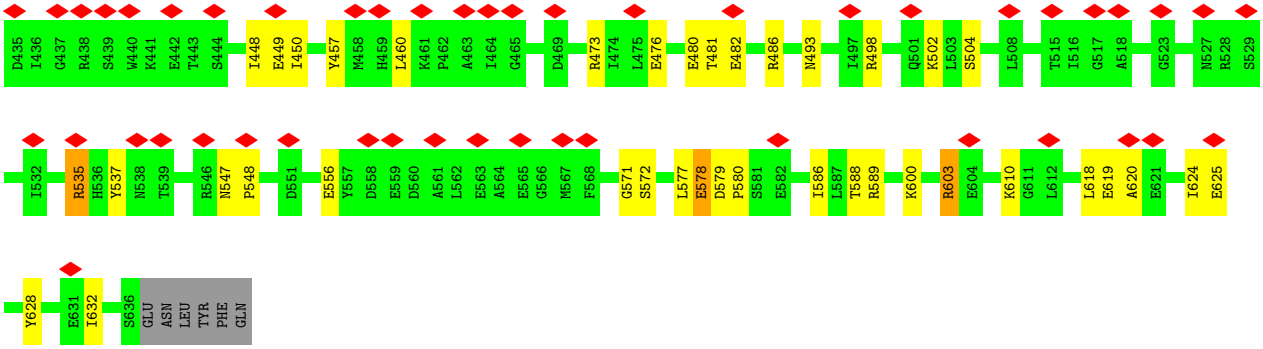




• Molecule 1: RimK domain-containing protein ATP-grasp

Chain F:




D435 I436 G437 R438 S439 W440 K441 E442 T443 S444 I448 E449 I450 Y457 M458 H459 L460 K461 P462 A463 I464 G465 D469 R473 I474 L475 E476 E480 T481 E482 R486 N493 I497 R498 Q501 K502 L503 S504 L508 T515 I516 G517 A518 G523 N527 R528 S529
T532 R535 H536 Y537 N538 T539 R546 N547 P548 D551 E556 Y557 D558 E559 D560 A561 L562 E563 A564 E565 G566 M567 F568 G571 S572 L577 E578 D579 P580 S581 E582 I586 L587 T588 R589 K600 R603 E604 K610 G611 L612 L618 E619 A620 E621 I624 E625
V628 E631 I632 S636 GLU ASN LEU TYR PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	251001	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 ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	-1.0	Depositor
Maximum defocus (nm)	-2.5	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.918	Depositor
Minimum map value	-1.414	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.675, 0.675, 0.675	Depositor

5 Model quality

5.1 Standard geometry

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	0.38	3/5140 (0.1%)	0.92	37/6978 (0.5%)
1	B	0.31	0/5140	0.73	18/6978 (0.3%)
1	C	0.30	0/5140	0.58	6/6978 (0.1%)
1	D	0.30	0/5140	0.58	6/6978 (0.1%)
1	E	0.31	0/5140	0.73	18/6978 (0.3%)
1	F	0.38	3/5140 (0.1%)	0.92	37/6978 (0.5%)
All	All	0.33	6/30840 (0.0%)	0.76	122/41868 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1
1	F	1	1
All	All	2	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	PRO	N-CD	9.54	1.61	1.47
1	F	253	PRO	N-CD	9.53	1.61	1.47
1	A	335	ILE	C-N	-6.01	1.20	1.34
1	F	335	ILE	C-N	-6.00	1.20	1.34
1	A	132	PHE	C-N	-5.68	1.21	1.34
1	F	132	PHE	C-N	-5.67	1.21	1.34

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	264	GLY	N-CA-C	25.32	176.39	113.10
1	F	264	GLY	N-CA-C	25.27	176.29	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	263	LYS	CB-CA-C	18.75	147.89	110.40
1	B	263	LYS	CB-CA-C	18.74	147.87	110.40
1	A	298	VAL	N-CA-C	15.27	152.23	111.00
1	F	298	VAL	N-CA-C	15.27	152.23	111.00
1	B	14	ALA	CB-CA-C	14.86	132.39	110.10
1	E	14	ALA	CB-CA-C	14.84	132.36	110.10
1	A	263	LYS	N-CA-CB	-13.50	86.30	110.60
1	F	263	LYS	N-CA-CB	-13.49	86.31	110.60
1	A	337	GLU	N-CA-CB	-12.98	87.23	110.60
1	F	337	GLU	N-CA-CB	-12.98	87.23	110.60
1	A	332	TYR	CB-CA-C	12.84	136.07	110.40
1	F	332	TYR	CB-CA-C	12.83	136.07	110.40
1	F	262	HIS	CB-CA-C	11.56	133.53	110.40
1	A	262	HIS	CB-CA-C	11.54	133.49	110.40
1	E	264	GLY	N-CA-C	-10.98	85.64	113.10
1	B	264	GLY	N-CA-C	-10.97	85.68	113.10
1	E	45	ALA	CB-CA-C	-10.85	93.83	110.10
1	B	45	ALA	CB-CA-C	-10.84	93.84	110.10
1	B	269	ALA	CB-CA-C	10.69	126.14	110.10
1	E	269	ALA	CB-CA-C	10.67	126.10	110.10
1	F	336	ALA	N-CA-C	9.71	137.22	111.00
1	A	336	ALA	N-CA-C	9.69	137.16	111.00
1	A	263	LYS	N-CA-C	9.37	136.28	111.00
1	F	263	LYS	N-CA-C	9.34	136.22	111.00
1	F	265	ILE	N-CA-C	9.22	135.90	111.00
1	A	265	ILE	N-CA-C	9.21	135.86	111.00
1	B	12	ILE	CB-CA-C	8.80	129.21	111.60
1	E	12	ILE	CB-CA-C	8.79	129.18	111.60
1	F	253	PRO	CA-N-CD	-8.39	99.76	111.50
1	A	253	PRO	CA-N-CD	-8.37	99.78	111.50
1	A	336	ALA	CB-CA-C	-8.19	97.82	110.10
1	F	336	ALA	CB-CA-C	-8.17	97.84	110.10
1	F	298	VAL	CB-CA-C	-8.05	96.11	111.40
1	A	298	VAL	CB-CA-C	-8.04	96.12	111.40
1	B	263	LYS	N-CA-C	-7.79	89.95	111.00
1	E	263	LYS	N-CA-C	-7.78	89.99	111.00
1	E	271	VAL	N-CA-C	7.78	132.01	111.00
1	B	271	VAL	N-CA-C	7.76	131.96	111.00
1	E	270	ASP	CB-CA-C	-7.73	94.94	110.40
1	B	270	ASP	CB-CA-C	-7.71	94.98	110.40
1	A	261	GLY	N-CA-C	-7.64	93.99	113.10
1	F	261	GLY	N-CA-C	-7.63	94.02	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	305	HIS	N-CA-CB	7.50	124.10	110.60
1	F	305	HIS	N-CA-CB	7.49	124.09	110.60
1	B	273	ASP	N-CA-CB	-7.26	97.54	110.60
1	E	273	ASP	N-CA-CB	-7.25	97.56	110.60
1	C	253	PRO	N-CA-C	-7.15	93.51	112.10
1	D	253	PRO	N-CA-C	-7.15	93.50	112.10
1	A	258	PRO	CB-CA-C	-7.01	94.46	112.00
1	F	258	PRO	CB-CA-C	-7.00	94.50	112.00
1	C	248	ALA	CB-CA-C	6.92	120.49	110.10
1	D	248	ALA	CB-CA-C	6.92	120.47	110.10
1	E	13	ASN	N-CA-CB	-6.86	98.25	110.60
1	B	13	ASN	N-CA-CB	-6.86	98.26	110.60
1	F	262	HIS	N-CA-CB	-6.78	98.39	110.60
1	A	262	HIS	N-CA-CB	-6.78	98.40	110.60
1	B	15	ARG	N-CA-CB	6.75	122.76	110.60
1	E	15	ARG	N-CA-CB	6.74	122.73	110.60
1	F	263	LYS	CB-CA-C	6.69	123.79	110.40
1	A	263	LYS	CB-CA-C	6.67	123.73	110.40
1	F	333	SER	N-CA-C	-6.54	93.35	111.00
1	F	258	PRO	N-CA-C	6.52	129.06	112.10
1	A	258	PRO	N-CA-C	6.52	129.05	112.10
1	A	333	SER	N-CA-C	-6.52	93.40	111.00
1	F	296	ILE	N-CA-CB	6.49	125.73	110.80
1	A	296	ILE	N-CA-CB	6.49	125.72	110.80
1	A	305	HIS	N-CA-C	-6.46	93.55	111.00
1	F	305	HIS	N-CA-C	-6.46	93.56	111.00
1	E	14	ALA	N-CA-C	-6.38	93.77	111.00
1	B	14	ALA	N-CA-C	-6.37	93.79	111.00
1	A	262	HIS	N-CA-C	6.33	128.09	111.00
1	F	262	HIS	N-CA-C	6.32	128.06	111.00
1	F	178	ALA	N-CA-CB	-6.14	101.50	110.10
1	A	178	ALA	N-CA-CB	-6.11	101.55	110.10
1	A	243	ALA	CB-CA-C	6.06	119.19	110.10
1	B	269	ALA	N-CA-C	-6.04	94.68	111.00
1	F	243	ALA	CB-CA-C	6.04	119.17	110.10
1	E	269	ALA	N-CA-C	-6.04	94.69	111.00
1	A	13	ASN	N-CA-C	-6.01	94.77	111.00
1	F	13	ASN	N-CA-C	-6.01	94.78	111.00
1	B	271	VAL	N-CA-CB	-5.78	98.79	111.50
1	F	188	GLN	CB-CA-C	-5.76	98.88	110.40
1	E	271	VAL	N-CA-CB	-5.76	98.83	111.50
1	A	188	GLN	CB-CA-C	-5.75	98.90	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	53	LEU	CA-CB-CG	5.67	128.33	115.30
1	F	294	ILE	N-CA-CB	5.66	123.81	110.80
1	C	218	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	294	ILE	N-CA-CB	5.64	123.77	110.80
1	B	53	LEU	CA-CB-CG	5.63	128.26	115.30
1	D	218	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	294	ILE	N-CA-C	-5.58	95.94	111.00
1	F	294	ILE	N-CA-C	-5.58	95.95	111.00
1	F	299	GLU	N-CA-CB	-5.57	100.57	110.60
1	A	11	ARG	N-CA-C	-5.57	95.97	111.00
1	A	299	GLU	N-CA-CB	-5.57	100.58	110.60
1	B	15	ARG	N-CA-C	-5.57	95.97	111.00
1	E	15	ARG	N-CA-C	-5.56	95.98	111.00
1	F	11	ARG	N-CA-C	-5.56	95.99	111.00
1	E	46	PHE	N-CA-CB	-5.49	100.71	110.60
1	B	46	PHE	N-CA-CB	-5.48	100.73	110.60
1	F	259	VAL	N-CA-C	5.41	125.61	111.00
1	A	259	VAL	N-CA-C	5.40	125.58	111.00
1	F	232	PRO	CA-N-CD	-5.38	103.96	111.50
1	A	232	PRO	CA-N-CD	-5.37	103.98	111.50
1	D	622	GLU	N-CA-CB	5.35	120.23	110.60
1	C	622	GLU	N-CA-CB	5.33	120.19	110.60
1	F	293	LYS	C-N-CA	5.29	134.92	121.70
1	A	293	LYS	C-N-CA	5.28	134.89	121.70
1	F	296	ILE	N-CA-C	-5.19	97.00	111.00
1	A	296	ILE	N-CA-C	-5.18	97.00	111.00
1	F	69	LEU	CB-CA-C	-5.16	100.40	110.20
1	F	67	PRO	N-CA-C	-5.16	98.69	112.10
1	A	67	PRO	N-CA-C	-5.14	98.73	112.10
1	A	69	LEU	CB-CA-C	-5.13	100.45	110.20
1	A	299	GLU	N-CA-C	-5.13	97.15	111.00
1	F	299	GLU	N-CA-C	-5.12	97.18	111.00
1	C	505	ASP	CB-CG-OD1	5.04	122.84	118.30
1	C	621	GLU	CB-CA-C	5.03	120.46	110.40
1	D	621	GLU	CB-CA-C	5.02	120.44	110.40
1	D	505	ASP	CB-CG-OD1	5.01	122.81	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	262	HIS	CA
1	F	262	HIS	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	264	GLY	Mainchain
1	F	264	GLY	Mainchain

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	5038	0	4992	100	0
1	B	5038	0	4992	47	0
1	C	5038	0	4992	49	0
1	D	5038	0	4992	49	0
1	E	5038	0	4992	43	0
1	F	5038	0	4992	97	0
All	All	30228	0	29952	385	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 6.

All (385) 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:B:383:ASP:HB2	1:B:384:ARG:HH11	1.63	0.64
1:E:383:ASP:HB2	1:E:384:ARG:HH11	1.63	0.64
1:F:53:LEU:HD11	1:F:57:ASN:HB2	1.79	0.64
1:D:330:ASP:HB2	1:D:338:LEU:HD21	1.79	0.63
1:A:53:LEU:HD11	1:A:57:ASN:HB2	1.80	0.63
1:A:236:VAL:HG12	1:A:237:VAL:H	1.63	0.63
1:B:302:ILE:HG23	1:B:432:ILE:HG21	1.80	0.63
1:E:302:ILE:HG23	1:E:432:ILE:HG21	1.80	0.63
1:B:65:ARG:HE	1:B:143:LEU:HD23	1.64	0.63
1:A:10:VAL:HG12	1:A:11:ARG:N	2.14	0.63
1:E:65:ARG:HE	1:E:143:LEU:HD23	1.64	0.63
1:E:71:GLU:OE1	1:E:71:GLU:N	2.32	0.63
1:E:339:ILE:O	1:E:343:ASN:ND2	2.32	0.62
1:C:330:ASP:HB2	1:C:338:LEU:HD21	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ILE:O	1:B:343:ASN:ND2	2.32	0.62
1:E:19:VAL:HG11	1:E:52:PRO:HB3	1.81	0.62
1:F:10:VAL:HG12	1:F:11:ARG:N	2.14	0.62
1:F:236:VAL:HG12	1:F:237:VAL:H	1.63	0.62
1:B:71:GLU:N	1:B:71:GLU:OE1	2.32	0.62
1:D:348:ARG:NH1	1:D:357:GLY:O	2.33	0.62
1:B:19:VAL:HG11	1:B:52:PRO:HB3	1.82	0.62
1:A:10:VAL:HG12	1:A:11:ARG:H	1.65	0.61
1:F:260:ALA:HB1	1:F:288:ILE:HD13	1.82	0.61
1:C:348:ARG:NH1	1:C:357:GLY:O	2.33	0.61
1:F:193:LYS:HE3	1:F:194:GLN:HE21	1.66	0.61
1:A:260:ALA:HB1	1:A:288:ILE:HD13	1.82	0.61
1:F:362:ASP:OD1	1:F:364:ALA:N	2.33	0.61
1:F:603:ARG:HD3	1:F:618:LEU:HD23	1.82	0.61
1:A:193:LYS:HE3	1:A:194:GLN:HE21	1.66	0.61
1:A:362:ASP:OD1	1:A:364:ALA:N	2.33	0.61
1:F:10:VAL:HG12	1:F:11:ARG:H	1.64	0.61
1:A:603:ARG:HD3	1:A:618:LEU:HD23	1.82	0.61
1:B:122:LYS:O	1:B:125:VAL:HG12	2.01	0.60
1:E:122:LYS:O	1:E:125:VAL:HG12	2.01	0.60
1:A:619:GLU:HG2	1:A:620:ALA:H	1.67	0.59
1:D:236:VAL:HG22	1:D:297:ILE:HG12	1.85	0.59
1:F:61:VAL:HG13	1:F:61:VAL:O	2.03	0.59
1:C:236:VAL:HG22	1:C:297:ILE:HG12	1.85	0.59
1:D:348:ARG:HH11	1:D:348:ARG:HB3	1.68	0.58
1:C:268:THR:HG22	1:C:269:ALA:N	2.18	0.58
1:D:11:ARG:HB2	1:D:14:ALA:HB2	1.84	0.58
1:F:619:GLU:HG2	1:F:620:ALA:H	1.67	0.58
1:A:61:VAL:O	1:A:61:VAL:HG13	2.03	0.58
1:F:473:ARG:HA	1:F:476:GLU:OE1	2.04	0.58
1:A:473:ARG:HA	1:A:476:GLU:OE1	2.04	0.58
1:A:53:LEU:HD23	1:A:136:THR:HG23	1.87	0.57
1:C:106:GLU:OE1	1:C:107:GLU:HG2	2.04	0.57
1:C:11:ARG:HB2	1:C:14:ALA:HB2	1.84	0.57
1:C:348:ARG:HB3	1:C:348:ARG:HH11	1.68	0.57
1:D:49:SER:HG	1:D:50:TYR:HD1	1.53	0.57
1:D:106:GLU:OE1	1:D:107:GLU:HG2	2.04	0.57
1:B:443:THR:OG1	1:B:444:SER:N	2.38	0.57
1:E:443:THR:OG1	1:E:444:SER:N	2.38	0.57
1:F:53:LEU:HD23	1:F:136:THR:HG23	1.86	0.57
1:C:256:VAL:HG23	1:C:256:VAL:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:THR:HG22	1:D:269:ALA:N	2.18	0.56
1:F:308:ARG:HB2	1:F:322:ARG:HH21	1.70	0.56
1:D:256:VAL:HG23	1:D:256:VAL:O	2.04	0.56
1:D:66:TYR:HB2	1:D:69:LEU:CD1	2.36	0.56
1:A:308:ARG:HB2	1:A:322:ARG:HH21	1.70	0.55
1:C:66:TYR:HB2	1:C:69:LEU:CD1	2.36	0.55
1:E:270:ASP:OD2	1:E:277:LEU:HD22	2.07	0.55
1:B:275:ILE:HA	1:B:278:GLU:HG2	1.88	0.55
1:A:256:VAL:HA	1:A:298:VAL:O	2.06	0.55
1:B:14:ALA:O	1:B:15:ARG:HG3	2.06	0.55
1:D:119:ARG:O	1:D:123:GLU:HG2	2.07	0.55
1:E:14:ALA:O	1:E:15:ARG:HG3	2.06	0.55
1:E:132:PHE:HA	1:E:135:ILE:HG22	1.88	0.55
1:E:275:ILE:HA	1:E:278:GLU:HG2	1.88	0.55
1:F:256:VAL:HA	1:F:298:VAL:O	2.06	0.55
1:F:35:LEU:O	1:F:589:ARG:NH2	2.40	0.54
1:F:258:PRO:HA	1:F:296:ILE:HG13	1.89	0.54
1:B:132:PHE:HA	1:B:135:ILE:HG22	1.88	0.54
1:B:270:ASP:OD2	1:B:277:LEU:HD22	2.07	0.54
1:C:119:ARG:O	1:C:123:GLU:HG2	2.07	0.54
1:E:240:LEU:HD11	1:E:281:TYR:CZ	2.43	0.54
1:A:266:GLY:O	1:A:267:VAL:HG22	2.08	0.54
1:B:240:LEU:HD11	1:B:281:TYR:CZ	2.43	0.54
1:F:266:GLY:O	1:F:267:VAL:HG22	2.08	0.54
1:E:278:GLU:HA	1:E:281:TYR:CZ	2.43	0.53
1:F:310:LEU:HD23	1:F:317:VAL:HG23	1.91	0.53
1:B:278:GLU:HA	1:B:281:TYR:CZ	2.43	0.53
1:D:334:THR:HB	1:D:377:ASP:HA	1.91	0.53
1:C:577:LEU:HB3	1:C:580:PRO:HG3	1.91	0.53
1:F:297:ILE:HD12	1:F:300:ASN:HD21	1.74	0.53
1:A:258:PRO:HA	1:A:296:ILE:HG13	1.89	0.53
1:F:625:GLU:OE1	1:F:625:GLU:N	2.39	0.53
1:A:35:LEU:O	1:A:589:ARG:NH2	2.40	0.53
1:A:10:VAL:HG12	1:A:11:ARG:HG2	1.91	0.53
1:A:310:LEU:HD23	1:A:317:VAL:HG23	1.91	0.53
1:A:625:GLU:OE1	1:A:625:GLU:N	2.39	0.53
1:C:334:THR:HB	1:C:377:ASP:HA	1.91	0.53
1:F:537:TYR:OH	1:F:556:GLU:O	2.24	0.52
1:A:7:VAL:O	1:A:10:VAL:HG23	2.09	0.52
1:F:10:VAL:HG12	1:F:11:ARG:HG2	1.91	0.52
1:F:61:VAL:HG11	1:F:135:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ILE:HD12	1:A:300:ASN:HD21	1.74	0.52
1:F:7:VAL:O	1:F:10:VAL:HG23	2.09	0.52
1:F:255:ALA:HA	1:F:269:ALA:HB3	1.92	0.52
1:B:237:VAL:HG11	1:B:243:ALA:HB2	1.92	0.52
1:F:256:VAL:HG12	1:F:296:ILE:HG12	1.91	0.52
1:C:106:GLU:CD	1:C:107:GLU:H	2.13	0.52
1:D:577:LEU:HB3	1:D:580:PRO:HG3	1.91	0.51
1:C:49:SER:HG	1:C:50:TYR:HD1	1.59	0.51
1:D:106:GLU:CD	1:D:107:GLU:H	2.13	0.51
1:E:237:VAL:HG11	1:E:243:ALA:HB2	1.92	0.51
1:E:260:ALA:HB3	1:E:292:GLU:HG3	1.93	0.51
1:A:265:ILE:HG22	1:A:266:GLY:N	2.25	0.51
1:D:7:VAL:HG12	1:D:9:PRO:HD3	1.93	0.51
1:A:256:VAL:HG12	1:A:296:ILE:HG12	1.91	0.51
1:C:7:VAL:HG12	1:C:9:PRO:HD3	1.93	0.51
1:F:265:ILE:HG22	1:F:266:GLY:N	2.25	0.51
1:A:61:VAL:HG11	1:A:135:ILE:HD12	1.92	0.51
1:D:582:GLU:OE2	1:D:582:GLU:N	2.33	0.51
1:F:87:GLU:OE2	1:F:87:GLU:HA	2.11	0.51
1:A:255:ALA:HA	1:A:269:ALA:HB3	1.92	0.51
1:C:69:LEU:H	1:C:69:LEU:HD12	1.76	0.51
1:F:430:ASP:OD1	1:F:449:GLU:N	2.40	0.51
1:A:87:GLU:OE2	1:A:87:GLU:HA	2.11	0.51
1:A:240:LEU:HB2	1:A:243:ALA:HB2	1.92	0.51
1:A:537:TYR:OH	1:A:556:GLU:O	2.24	0.51
1:C:246:VAL:O	1:C:249:GLU:HG2	2.11	0.51
1:F:285:VAL:HG22	1:F:285:VAL:O	2.11	0.51
1:A:248:ALA:O	1:A:254:VAL:HG21	2.10	0.51
1:B:278:GLU:HA	1:B:281:TYR:CE2	2.46	0.51
1:B:11:ARG:HE	1:B:14:ALA:HB2	1.77	0.50
1:D:69:LEU:HD12	1:D:69:LEU:H	1.76	0.50
1:E:278:GLU:HA	1:E:281:TYR:CE2	2.46	0.50
1:A:493:ASN:HB2	1:A:577:LEU:HD23	1.93	0.50
1:F:240:LEU:HB2	1:F:243:ALA:HB2	1.92	0.50
1:F:248:ALA:O	1:F:254:VAL:HG21	2.11	0.50
1:F:365:MET:CE	1:F:388:LEU:HD13	2.41	0.50
1:A:246:VAL:HA	1:A:249:GLU:HB3	1.94	0.50
1:A:365:MET:CE	1:A:388:LEU:HD13	2.41	0.50
1:B:261:GLY:O	1:B:262:HIS:CG	2.65	0.50
1:C:250:ILE:HG22	1:C:250:ILE:O	2.12	0.50
1:A:74:TYR:CE2	1:A:80:LEU:HG	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ALA:HB3	1:B:292:GLU:HG3	1.92	0.50
1:A:285:VAL:HG22	1:A:285:VAL:O	2.11	0.50
1:F:493:ASN:HB2	1:F:577:LEU:HD23	1.93	0.50
1:A:300:ASN:HB3	1:A:302:ILE:HG12	1.94	0.50
1:D:246:VAL:O	1:D:249:GLU:HG2	2.11	0.50
1:D:365:MET:SD	1:D:388:LEU:HD23	2.52	0.50
1:F:246:VAL:HA	1:F:249:GLU:HB3	1.94	0.50
1:F:300:ASN:HB3	1:F:302:ILE:HG12	1.94	0.50
1:C:365:MET:SD	1:C:388:LEU:HD23	2.52	0.49
1:E:11:ARG:HE	1:E:14:ALA:HB2	1.76	0.49
1:F:19:VAL:HG23	1:F:20:PHE:CD2	2.47	0.49
1:F:74:TYR:CE2	1:F:80:LEU:HG	2.47	0.49
1:A:91:LEU:HD11	1:A:150:LEU:HB3	1.95	0.49
1:A:335:ILE:HD13	1:A:376:LEU:HB3	1.94	0.49
1:C:367:LEU:O	1:C:371:GLU:HG2	2.12	0.49
1:E:261:GLY:O	1:E:262:HIS:CG	2.65	0.49
1:F:588:THR:O	1:F:588:THR:HG22	2.11	0.49
1:C:131:TRP:CD1	1:C:141:PHE:HE1	2.30	0.49
1:D:54:PRO:HB2	1:D:56:GLU:OE1	2.13	0.49
1:C:343:ASN:OD1	1:C:358:LYS:HE3	2.12	0.49
1:D:513:ASP:OD1	1:D:513:ASP:N	2.45	0.49
1:E:513:ASP:OD1	1:E:513:ASP:N	2.41	0.49
1:F:369:LEU:HD13	1:F:374:LEU:HD13	1.95	0.49
1:A:19:VAL:HG23	1:A:20:PHE:CD2	2.48	0.49
1:D:131:TRP:CD1	1:D:141:PHE:HE1	2.30	0.49
1:A:182:TRP:O	1:A:184:GLU:N	2.45	0.48
1:F:182:TRP:O	1:F:184:GLU:N	2.45	0.48
1:F:335:ILE:HD13	1:F:376:LEU:HB3	1.94	0.48
1:A:430:ASP:OD1	1:A:449:GLU:N	2.40	0.48
1:A:588:THR:O	1:A:588:THR:HG22	2.11	0.48
1:C:240:LEU:HB2	1:C:281:TYR:CZ	2.48	0.48
1:D:250:ILE:O	1:D:250:ILE:HG22	2.12	0.48
1:C:513:ASP:OD1	1:C:513:ASP:N	2.45	0.48
1:D:367:LEU:O	1:D:371:GLU:HG2	2.12	0.48
1:F:91:LEU:HD11	1:F:150:LEU:HB3	1.95	0.48
1:F:96:HIS:ND1	1:F:172:ASN:OD1	2.42	0.48
1:D:240:LEU:HB2	1:D:281:TYR:CZ	2.48	0.48
1:D:364:ALA:HA	1:D:367:LEU:HD13	1.96	0.48
1:C:54:PRO:HB2	1:C:56:GLU:OE1	2.13	0.48
1:A:369:LEU:HD13	1:A:374:LEU:HD13	1.95	0.48
1:F:481:THR:OG1	1:F:482:GLU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:GLU:OE1	1:C:72:ILE:HG13	2.14	0.48
1:D:358:LYS:HE2	1:D:360:ARG:HH12	1.78	0.48
1:F:254:VAL:HG13	1:F:255:ALA:N	2.28	0.48
1:F:372:GLN:OE1	1:F:374:LEU:HG	2.14	0.48
1:A:432:ILE:HG13	1:A:448:ILE:HD11	1.96	0.47
1:D:71:GLU:OE1	1:D:72:ILE:HG13	2.14	0.47
1:A:372:GLN:OE1	1:A:374:LEU:HG	2.14	0.47
1:C:358:LYS:HE2	1:C:360:ARG:HH12	1.78	0.47
1:D:343:ASN:OD1	1:D:358:LYS:HE3	2.12	0.47
1:E:53:LEU:HD21	1:E:57:ASN:HB2	1.95	0.47
1:F:64:ASP:OD2	1:F:65:ARG:NH1	2.48	0.47
1:F:11:ARG:HD2	1:F:129:TRP:CZ2	2.50	0.47
1:B:53:LEU:HD21	1:B:57:ASN:HB2	1.95	0.47
1:A:11:ARG:HD2	1:A:129:TRP:CZ2	2.50	0.47
1:A:254:VAL:HG13	1:A:255:ALA:N	2.28	0.47
1:A:481:THR:OG1	1:A:482:GLU:N	2.46	0.47
1:C:582:GLU:OE2	1:C:582:GLU:N	2.33	0.47
1:F:80:LEU:HD22	1:F:132:PHE:HZ	1.79	0.47
1:A:64:ASP:OD2	1:A:65:ARG:NH1	2.48	0.47
1:C:364:ALA:HA	1:C:367:LEU:HD13	1.96	0.47
1:B:329:GLY:HA3	1:B:380:ILE:HB	1.97	0.47
1:A:127:CYS:SG	1:A:146:GLN:NE2	2.87	0.47
1:F:103:LYS:HD2	1:F:104:PRO:HD2	1.97	0.47
1:A:628:TYR:O	1:A:632:ILE:HG23	2.15	0.46
1:A:265:ILE:HG22	1:A:266:GLY:H	1.81	0.46
1:C:574:LEU:HD13	1:C:596:THR:HB	1.98	0.46
1:F:266:GLY:O	1:F:268:THR:HG23	2.15	0.46
1:A:461:LYS:HE2	1:A:461:LYS:HB2	1.65	0.46
1:D:380:ILE:HD13	1:D:384:ARG:HB3	1.97	0.46
1:F:265:ILE:HG22	1:F:266:GLY:H	1.81	0.46
1:F:628:TYR:O	1:F:632:ILE:HG23	2.15	0.46
1:A:80:LEU:HD22	1:A:132:PHE:HZ	1.79	0.46
1:C:380:ILE:HD13	1:C:384:ARG:HB3	1.97	0.46
1:E:187:MET:HE2	1:E:187:MET:HB2	1.89	0.46
1:A:96:HIS:ND1	1:A:172:ASN:OD1	2.42	0.46
1:D:574:LEU:HD13	1:D:596:THR:HB	1.98	0.46
1:F:127:CYS:SG	1:F:146:GLN:NE2	2.87	0.46
1:A:266:GLY:O	1:A:268:THR:HG23	2.15	0.46
1:B:351:THR:HG22	1:B:353:THR:H	1.81	0.46
1:E:351:THR:HG22	1:E:353:THR:H	1.81	0.46
1:F:432:ILE:HG13	1:F:448:ILE:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ALA:O	1:A:254:VAL:CG2	2.64	0.45
1:E:329:GLY:HA3	1:E:380:ILE:HB	1.97	0.45
1:F:248:ALA:O	1:F:254:VAL:CG2	2.64	0.45
1:A:74:TYR:N	1:A:74:TYR:HD1	2.15	0.45
1:F:74:TYR:HD1	1:F:74:TYR:N	2.15	0.45
1:A:11:ARG:HH22	1:A:130:ASP:N	2.15	0.45
1:A:103:LYS:HD2	1:A:104:PRO:HD2	1.97	0.45
1:D:268:THR:CG2	1:D:269:ALA:N	2.80	0.45
1:B:488:PRO:HB2	1:B:552:LEU:HG	1.99	0.45
1:F:578:GLU:OE1	1:F:579:ASP:HB3	2.17	0.45
1:A:11:ARG:HH12	1:A:130:ASP:HA	1.82	0.45
1:F:11:ARG:HH12	1:F:130:ASP:HA	1.82	0.45
1:A:65:ARG:HD3	1:A:87:GLU:HG3	1.99	0.45
1:A:258:PRO:HD2	1:A:265:ILE:O	2.17	0.45
1:A:365:MET:HB2	1:A:389:ARG:NH2	2.32	0.45
1:F:65:ARG:HD3	1:F:87:GLU:HG3	1.99	0.44
1:F:258:PRO:HD2	1:F:265:ILE:O	2.17	0.44
1:B:246:VAL:HG12	1:B:250:ILE:HG12	2.00	0.44
1:C:234:GLY:HA3	1:C:299:GLU:HG2	1.99	0.44
1:F:365:MET:HB2	1:F:389:ARG:NH2	2.32	0.44
1:C:252:TYR:O	1:C:253:PRO:C	2.56	0.44
1:C:542:LEU:HD12	1:C:568:PHE:CZ	2.52	0.44
1:D:256:VAL:HG22	1:D:268:THR:HB	1.99	0.44
1:F:74:TYR:N	1:F:74:TYR:CD1	2.85	0.44
1:D:234:GLY:HA3	1:D:299:GLU:HG2	1.99	0.44
1:D:252:TYR:O	1:D:253:PRO:C	2.56	0.44
1:D:542:LEU:HD12	1:D:568:PHE:CZ	2.52	0.44
1:A:578:GLU:OE1	1:A:579:ASP:HB3	2.17	0.44
1:B:23:PHE:HE1	1:B:45:ALA:HB2	1.82	0.44
1:E:488:PRO:HB2	1:E:552:LEU:HG	1.99	0.44
1:A:74:TYR:N	1:A:74:TYR:CD1	2.85	0.44
1:B:53:LEU:HD23	1:B:54:PRO:N	2.33	0.44
1:B:199:ILE:O	1:B:199:ILE:HG23	2.18	0.44
1:B:307:TYR:CE1	1:B:321:GLU:HB2	2.53	0.44
1:E:307:TYR:CE1	1:E:321:GLU:HB2	2.53	0.44
1:A:502:LYS:HB3	1:A:502:LYS:HE3	1.68	0.44
1:E:23:PHE:HE1	1:E:45:ALA:HB2	1.82	0.44
1:E:53:LEU:HD23	1:E:54:PRO:N	2.33	0.44
1:E:199:ILE:HG23	1:E:199:ILE:O	2.18	0.44
1:B:513:ASP:OD1	1:B:513:ASP:N	2.41	0.43
1:D:229:PHE:O	1:D:231:VAL:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:ARG:HH22	1:F:130:ASP:N	2.15	0.43
1:A:175:HIS:HB2	1:A:482:GLU:OE1	2.18	0.43
1:B:180:TYR:HD1	1:B:187:MET:HE2	1.83	0.43
1:B:549:LYS:HE3	1:B:549:LYS:HB3	1.88	0.43
1:A:44:PHE:HD1	1:A:45:ALA:H	1.66	0.43
1:A:187:MET:HE2	1:A:187:MET:HB2	1.89	0.43
1:C:229:PHE:O	1:C:231:VAL:HG13	2.18	0.43
1:C:256:VAL:HG22	1:C:268:THR:HB	1.98	0.43
1:A:236:VAL:HG12	1:A:237:VAL:N	2.33	0.43
1:E:246:VAL:HG12	1:E:250:ILE:HG12	1.99	0.43
1:F:309:LEU:HD11	1:F:431:ILE:HD13	2.01	0.43
1:E:79:GLU:N	1:E:79:GLU:OE1	2.52	0.43
1:F:175:HIS:HB2	1:F:482:GLU:OE1	2.18	0.43
1:A:309:LEU:HD11	1:A:431:ILE:HD13	2.01	0.43
1:C:268:THR:CG2	1:C:269:ALA:N	2.80	0.43
1:D:348:ARG:HH12	1:D:358:LYS:HA	1.84	0.43
1:B:21:ASP:OD1	1:B:22:ILE:N	2.52	0.43
1:C:258:PRO:HD2	1:C:266:GLY:O	2.19	0.43
1:B:268:THR:OG1	1:B:268:THR:O	2.36	0.43
1:D:258:PRO:HD2	1:D:266:GLY:O	2.19	0.43
1:D:274:GLU:O	1:D:275:ILE:HB	2.19	0.43
1:E:21:ASP:OD1	1:E:22:ILE:N	2.52	0.43
1:A:72:ILE:HD12	1:A:73:GLU:N	2.34	0.42
1:A:91:LEU:O	1:A:151:GLN:NE2	2.35	0.42
1:C:274:GLU:O	1:C:275:ILE:HB	2.19	0.42
1:A:259:VAL:O	1:A:261:GLY:O	2.38	0.42
1:F:245:GLU:O	1:F:249:GLU:N	2.49	0.42
1:E:69:LEU:HB3	1:E:74:TYR:OH	2.20	0.42
1:A:293:LYS:O	1:A:294:ILE:C	2.57	0.42
1:F:502:LYS:HE3	1:F:502:LYS:HB3	1.68	0.42
1:F:72:ILE:HD12	1:F:73:GLU:N	2.34	0.42
1:F:293:LYS:O	1:F:294:ILE:C	2.57	0.42
1:F:535:ARG:HH11	1:F:535:ARG:HG2	1.84	0.42
1:B:384:ARG:HD3	1:B:384:ARG:N	2.34	0.42
1:E:384:ARG:HD3	1:E:384:ARG:N	2.34	0.42
1:F:62:VAL:HG22	1:F:65:ARG:O	2.19	0.42
1:F:547:ASN:HA	1:F:548:PRO:HD3	1.90	0.42
1:A:62:VAL:HG22	1:A:65:ARG:O	2.19	0.42
1:B:79:GLU:N	1:B:79:GLU:OE1	2.52	0.42
1:B:237:VAL:HG22	1:B:239:SER:H	1.84	0.42
1:E:547:ASN:HA	1:E:548:PRO:HD3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:244:LYS:HE2	1:F:274:GLU:HB2	2.02	0.42
1:F:259:VAL:O	1:F:261:GLY:O	2.38	0.42
1:A:19:VAL:HG12	1:A:50:TYR:HB2	2.02	0.42
1:C:348:ARG:HH12	1:C:358:LYS:HA	1.84	0.42
1:A:600:LYS:HD2	1:A:624:ILE:CG2	2.50	0.42
1:F:9:PRO:O	1:F:11:ARG:O	2.38	0.42
1:A:9:PRO:O	1:A:11:ARG:O	2.38	0.42
1:A:85:VAL:CG1	1:A:113:ILE:HD13	2.50	0.42
1:D:330:ASP:H	1:D:380:ILE:HD11	1.85	0.42
1:A:244:LYS:HE3	1:A:244:LYS:HB3	1.94	0.41
1:A:245:GLU:O	1:A:249:GLU:N	2.49	0.41
1:D:348:ARG:NH1	1:D:348:ARG:HB3	2.35	0.41
1:E:268:THR:O	1:E:268:THR:OG1	2.36	0.41
1:F:486:ARG:NH2	1:F:571:GLY:HA3	2.35	0.41
1:A:220:CYS:SG	1:A:450:ILE:HD11	2.60	0.41
1:A:244:LYS:HE2	1:A:274:GLU:HB2	2.02	0.41
1:B:262:HIS:O	1:B:263:LYS:C	2.58	0.41
1:C:330:ASP:H	1:C:380:ILE:HD11	1.85	0.41
1:D:68:ARG:NH1	1:D:87:GLU:OE1	2.53	0.41
1:D:475:LEU:HD23	1:D:475:LEU:HA	1.90	0.41
1:F:44:PHE:HD1	1:F:45:ALA:H	1.66	0.41
1:F:331:GLY:N	1:F:381:ASP:HA	2.36	0.41
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.89	0.41
1:A:457:TYR:HA	1:A:460:LEU:HD12	2.02	0.41
1:A:586:ILE:HD12	1:A:586:ILE:HA	1.85	0.41
1:B:69:LEU:HB3	1:B:74:TYR:OH	2.20	0.41
1:F:600:LYS:HD2	1:F:624:ILE:CG2	2.50	0.41
1:A:390:LYS:HG3	1:A:391:VAL:H	1.85	0.41
1:E:258:PRO:HB3	1:E:288:ILE:HG12	2.02	0.41
1:E:323:LYS:HA	1:E:324:PRO:HD3	1.94	0.41
1:F:224:LEU:HD23	1:F:224:LEU:HA	1.89	0.41
1:A:486:ARG:NH2	1:A:571:GLY:HA3	2.35	0.41
1:B:297:ILE:O	1:B:297:ILE:HG22	2.21	0.41
1:C:498:ARG:HE	1:C:498:ARG:HB3	1.65	0.41
1:D:91:LEU:HD23	1:D:91:LEU:HA	1.92	0.41
1:A:11:ARG:NH1	1:A:130:ASP:HA	2.36	0.41
1:A:399:PHE:CD1	1:A:399:PHE:N	2.89	0.41
1:A:535:ARG:HH11	1:A:535:ARG:HG2	1.84	0.41
1:C:32:ASN:OD1	1:C:35:LEU:N	2.53	0.41
1:F:338:LEU:HA	1:F:341:LYS:HE3	2.03	0.41
1:F:577:LEU:HD22	1:F:580:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:534:ASN:OD1	1:C:535:ARG:N	2.54	0.41
1:F:457:TYR:HA	1:F:460:LEU:HD12	2.03	0.41
1:F:586:ILE:HD11	1:F:589:ARG:HE	1.85	0.41
1:B:187:MET:HE2	1:B:187:MET:HB2	2.00	0.41
1:B:258:PRO:CG	1:B:265:ILE:HG22	2.51	0.41
1:B:432:ILE:HD12	1:B:448:ILE:HD11	2.02	0.41
1:D:32:ASN:OD1	1:D:35:LEU:N	2.53	0.41
1:E:237:VAL:HG22	1:E:239:SER:H	1.84	0.41
1:E:258:PRO:CG	1:E:265:ILE:HG22	2.51	0.41
1:E:498:ARG:H	1:E:498:ARG:HG2	1.65	0.41
1:F:85:VAL:CG1	1:F:113:ILE:HD13	2.50	0.41
1:F:220:CYS:SG	1:F:450:ILE:HD11	2.60	0.41
1:A:338:LEU:HA	1:A:341:LYS:HE3	2.03	0.41
1:B:25:VAL:HG12	1:B:42:PHE:HB3	2.03	0.41
1:B:331:GLY:C	1:B:379:VAL:HG11	2.42	0.41
1:C:68:ARG:NH1	1:C:87:GLU:OE1	2.53	0.41
1:E:432:ILE:HD12	1:E:448:ILE:HD11	2.02	0.41
1:F:91:LEU:O	1:F:151:GLN:NE2	2.35	0.41
1:F:390:LYS:HG3	1:F:391:VAL:H	1.86	0.41
1:F:449:GLU:OE2	1:F:449:GLU:HA	2.21	0.41
1:A:401:ILE:HG12	1:A:464:ILE:HD12	2.03	0.40
1:B:259:VAL:HG22	1:B:295:CYS:O	2.22	0.40
1:C:629:LEU:HD23	1:C:629:LEU:HA	1.96	0.40
1:F:11:ARG:NH1	1:F:130:ASP:HA	2.36	0.40
1:A:103:LYS:HD2	1:A:103:LYS:HA	1.81	0.40
1:A:528:ARG:HE	1:A:528:ARG:HB3	1.75	0.40
1:A:581:SER:O	1:A:585:MET:HG2	2.21	0.40
1:A:586:ILE:HD11	1:A:589:ARG:HE	1.85	0.40
1:C:238:PHE:HB3	1:C:294:ILE:CG1	2.52	0.40
1:C:632:ILE:HD12	1:C:632:ILE:O	2.21	0.40
1:F:236:VAL:HG12	1:F:237:VAL:N	2.33	0.40
1:A:577:LEU:HD22	1:A:580:PRO:HB3	2.02	0.40
1:B:258:PRO:HB3	1:B:288:ILE:HG12	2.03	0.40
1:B:466:GLU:HA	1:B:467:PRO:HD3	1.95	0.40
1:D:466:GLU:HA	1:D:467:PRO:HD3	1.97	0.40
1:D:632:ILE:HD12	1:D:632:ILE:O	2.21	0.40
1:E:297:ILE:O	1:E:297:ILE:HG22	2.21	0.40
1:F:111:ILE:HD13	1:F:111:ILE:HA	1.88	0.40
1:F:260:ALA:CB	1:F:288:ILE:HD13	2.51	0.40
1:C:622:GLU:OE1	1:C:622:GLU:HA	2.21	0.40
1:D:622:GLU:OE1	1:D:622:GLU:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:19:VAL:HG12	1:F:50:TYR:HB2	2.02	0.40
1:F:586:ILE:HA	1:F:586:ILE:HD12	1.85	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	A	629/642 (98%)	563 (90%)	61 (10%)	5 (1%)	19	49
1	B	629/642 (98%)	584 (93%)	44 (7%)	1 (0%)	47	78
1	C	629/642 (98%)	586 (93%)	42 (7%)	1 (0%)	47	78
1	D	629/642 (98%)	585 (93%)	43 (7%)	1 (0%)	47	78
1	E	629/642 (98%)	584 (93%)	44 (7%)	1 (0%)	47	78
1	F	629/642 (98%)	563 (90%)	61 (10%)	5 (1%)	19	49
All	All	3774/3852 (98%)	3465 (92%)	295 (8%)	14 (0%)	38	66

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	PRO
1	F	253	PRO
1	A	236	VAL
1	F	236	VAL
1	C	252	TYR
1	D	252	TYR
1	A	10	VAL
1	F	10	VAL
1	A	265	ILE
1	F	265	ILE

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Mol	Chain	Res	Type
1	B	257	LYS
1	E	257	LYS
1	A	267	VAL
1	F	267	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	547/558 (98%)	516 (94%)	31 (6%)	20	50
1	B	547/558 (98%)	519 (95%)	28 (5%)	24	55
1	C	547/558 (98%)	531 (97%)	16 (3%)	42	76
1	D	547/558 (98%)	531 (97%)	16 (3%)	42	76
1	E	547/558 (98%)	519 (95%)	28 (5%)	24	55
1	F	547/558 (98%)	516 (94%)	31 (6%)	20	50
All	All	3282/3348 (98%)	3132 (95%)	150 (5%)	31	60

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	21	ASP
1	A	37	GLN
1	A	40	LEU
1	A	44	PHE
1	A	46	PHE
1	A	65	ARG
1	A	80	LEU
1	A	81	PHE
1	A	83	SER
1	A	100	TRP
1	A	110	ARG
1	A	132	PHE
1	A	155	ARG

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Mol	Chain	Res	Type
1	A	172	ASN
1	A	238	PHE
1	A	265	ILE
1	A	305	HIS
1	A	315	ARG
1	A	326	TYR
1	A	341	LYS
1	A	390	LYS
1	A	399	PHE
1	A	480	GLU
1	A	498	ARG
1	A	504	SER
1	A	535	ARG
1	A	572	SER
1	A	578	GLU
1	A	603	ARG
1	A	610	LYS
1	B	11	ARG
1	B	44	PHE
1	B	46	PHE
1	B	65	ARG
1	B	74	TYR
1	B	90	LYS
1	B	98	LYS
1	B	127	CYS
1	B	134	PHE
1	B	155	ARG
1	B	219	ASP
1	B	227	LEU
1	B	252	TYR
1	B	281	TYR
1	B	308	ARG
1	B	326	TYR
1	B	332	TYR
1	B	374	LEU
1	B	375	ASP
1	B	384	ARG
1	B	406	ARG
1	B	494	ARG
1	B	527	ASN
1	B	535	ARG
1	B	538	ASN

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Mol	Chain	Res	Type
1	B	558	ASP
1	B	572	SER
1	B	617	GLU
1	C	74	TYR
1	C	90	LYS
1	C	110	ARG
1	C	127	CYS
1	C	141	PHE
1	C	218	ASP
1	C	227	LEU
1	C	237	VAL
1	C	252	TYR
1	C	277	LEU
1	C	326	TYR
1	C	330	ASP
1	C	365	MET
1	C	520	CYS
1	C	563	GLU
1	C	622	GLU
1	D	74	TYR
1	D	90	LYS
1	D	110	ARG
1	D	127	CYS
1	D	141	PHE
1	D	218	ASP
1	D	227	LEU
1	D	237	VAL
1	D	252	TYR
1	D	277	LEU
1	D	326	TYR
1	D	330	ASP
1	D	365	MET
1	D	520	CYS
1	D	563	GLU
1	D	622	GLU
1	E	11	ARG
1	E	44	PHE
1	E	46	PHE
1	E	65	ARG
1	E	74	TYR
1	E	90	LYS
1	E	98	LYS

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Mol	Chain	Res	Type
1	E	127	CYS
1	E	134	PHE
1	E	155	ARG
1	E	219	ASP
1	E	227	LEU
1	E	252	TYR
1	E	281	TYR
1	E	308	ARG
1	E	326	TYR
1	E	332	TYR
1	E	374	LEU
1	E	375	ASP
1	E	384	ARG
1	E	406	ARG
1	E	494	ARG
1	E	527	ASN
1	E	535	ARG
1	E	538	ASN
1	E	558	ASP
1	E	572	SER
1	E	617	GLU
1	F	11	ARG
1	F	21	ASP
1	F	37	GLN
1	F	40	LEU
1	F	44	PHE
1	F	46	PHE
1	F	65	ARG
1	F	80	LEU
1	F	81	PHE
1	F	83	SER
1	F	100	TRP
1	F	110	ARG
1	F	132	PHE
1	F	155	ARG
1	F	172	ASN
1	F	238	PHE
1	F	265	ILE
1	F	305	HIS
1	F	315	ARG
1	F	326	TYR
1	F	341	LYS

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Mol	Chain	Res	Type
1	F	390	LYS
1	F	399	PHE
1	F	480	GLU
1	F	498	ARG
1	F	504	SER
1	F	535	ARG
1	F	572	SER
1	F	578	GLU
1	F	603	ARG
1	F	610	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	GLN
1	B	343	ASN
1	B	416	GLN
1	C	416	GLN
1	D	416	GLN
1	E	416	GLN
1	F	194	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	335:ILE	C	336:ALA	N	1.20
1	F	335:ILE	C	336:ALA	N	1.20

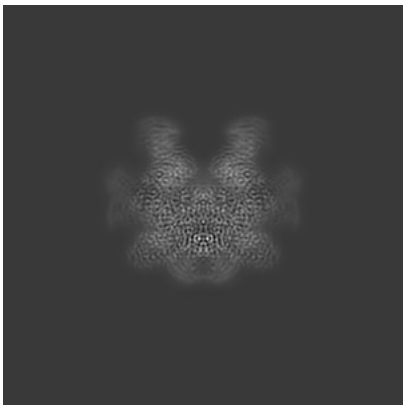
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29533. These allow visual inspection of the internal detail of the map and identification of artifacts.

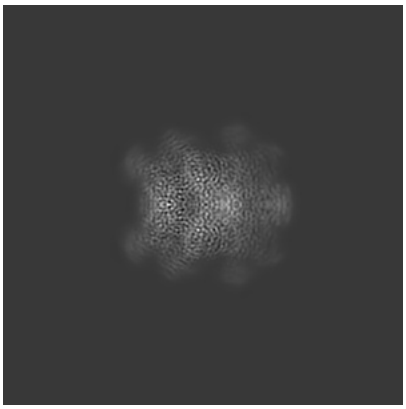
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

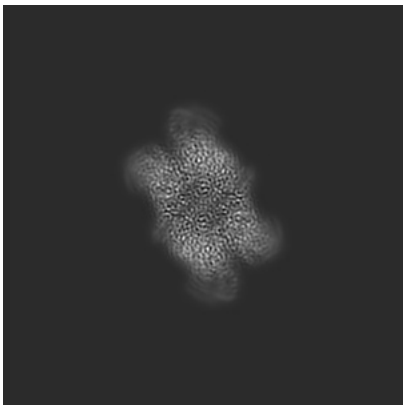
6.1.1 Primary map



X

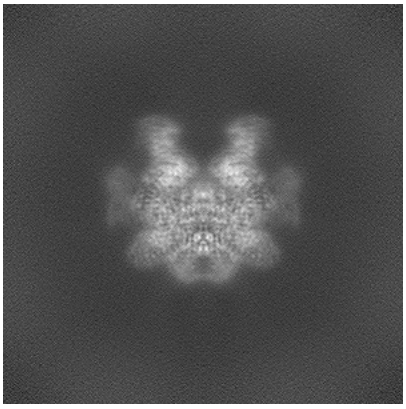


Y

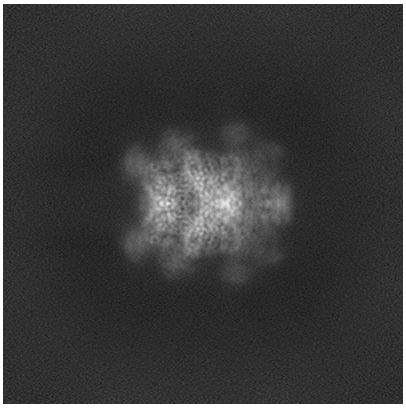


Z

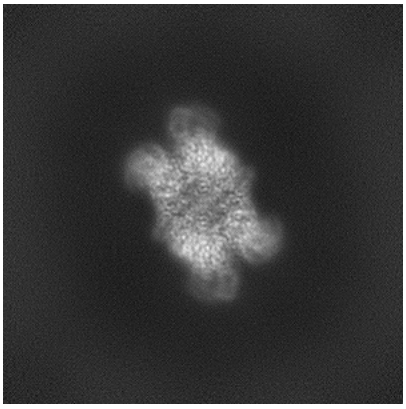
6.1.2 Raw map



X



Y



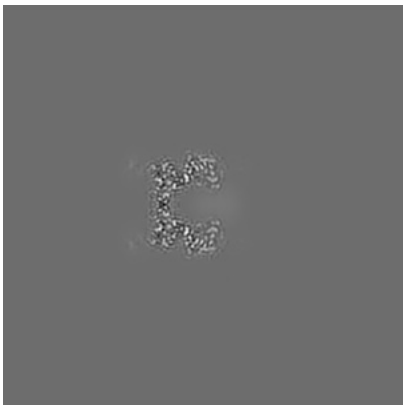
Z

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

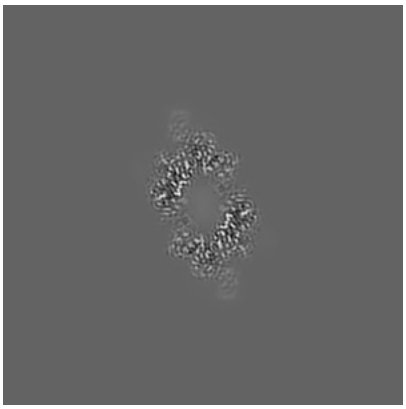
6.2 Central slices (i)

6.2.1 Primary map

X Index: 256

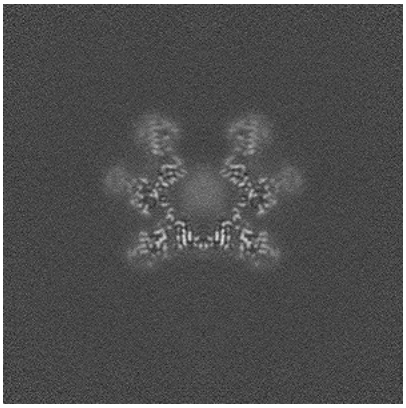


Y Index: 256

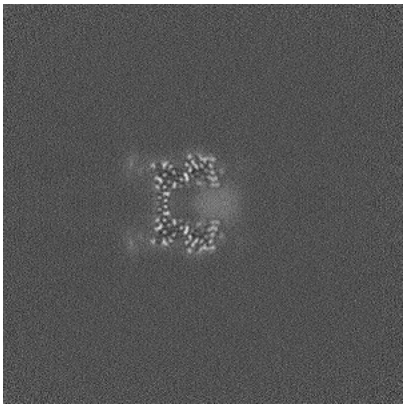


Z Index: 256

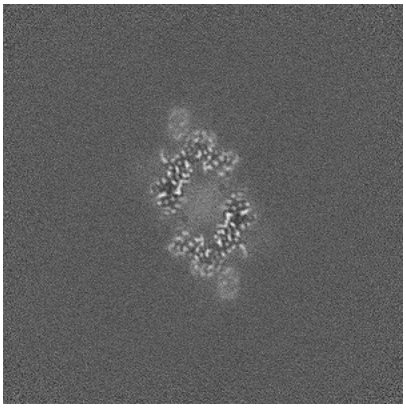
6.2.2 Raw map



X Index: 256



Y Index: 256



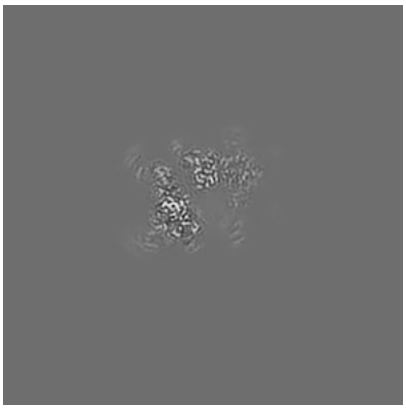
Z Index: 256

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

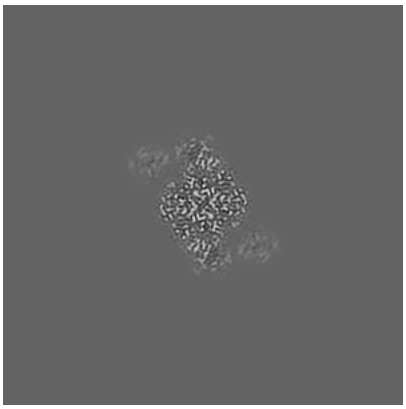
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 259

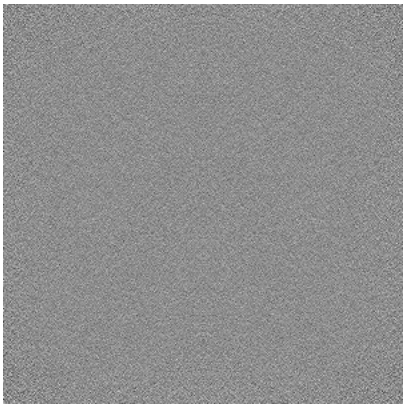


Y Index: 231

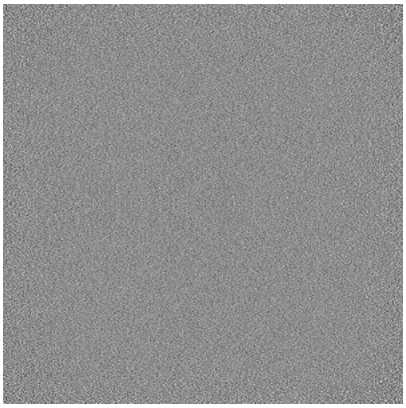


Z Index: 211

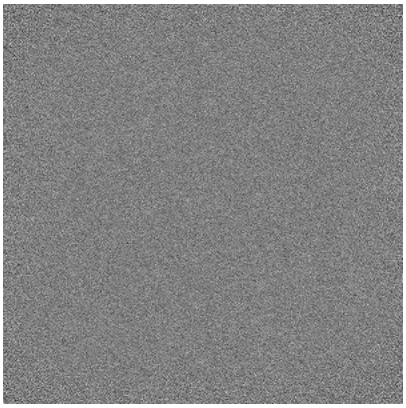
6.3.2 Raw map



X Index: 0



Y Index: 0

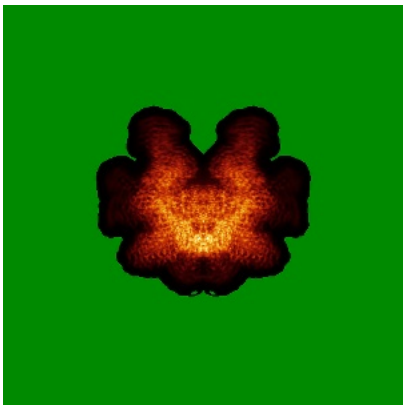


Z Index: 0

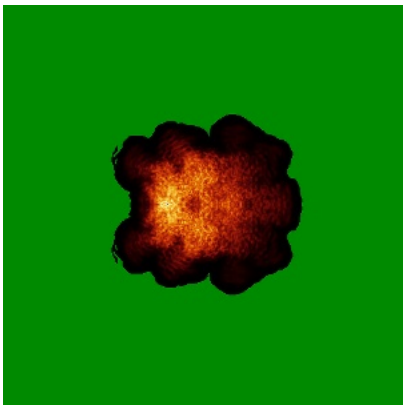
The images above show the largest variance slices of the map in three orthogonal directions.

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

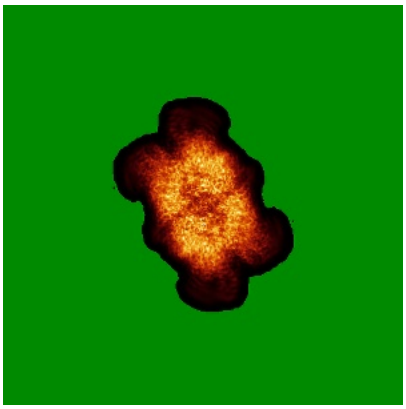
6.4.1 Primary map



X

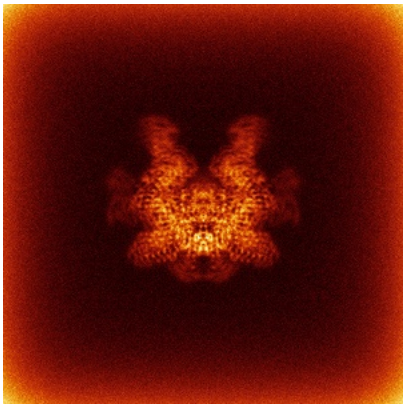


Y

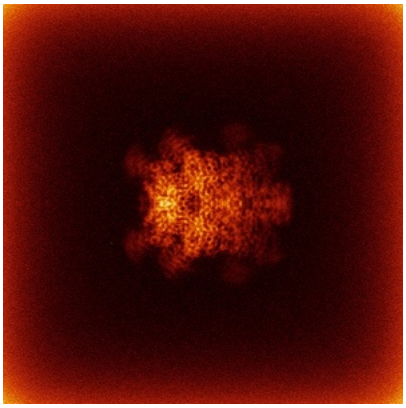


Z

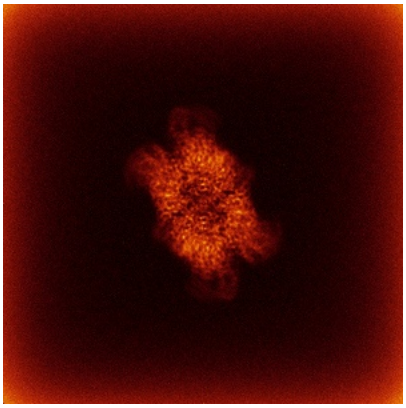
6.4.2 Raw map



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 0.08. 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.

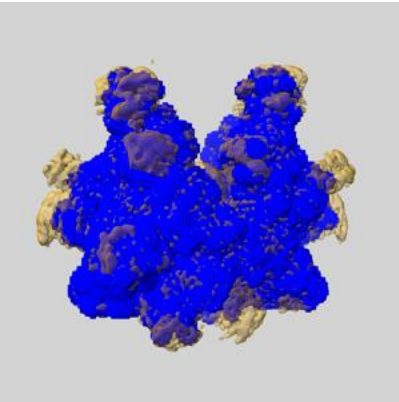
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

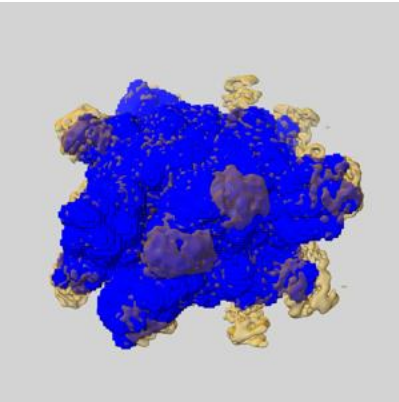
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

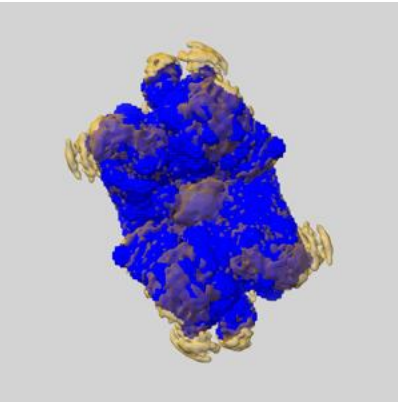
6.6.1 emd_29533_msk_1.map (i)



X



Y

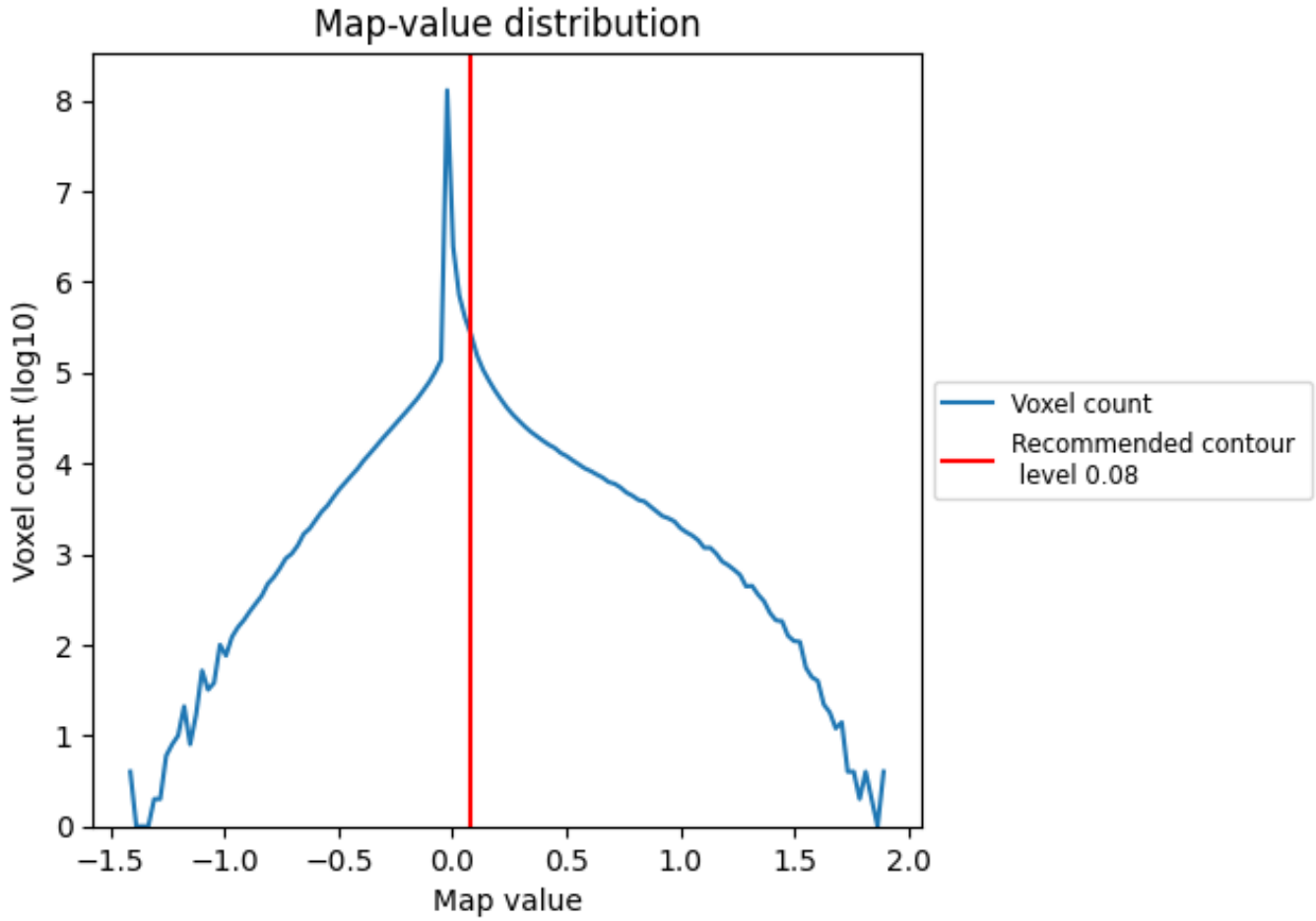


Z

7 Map analysis

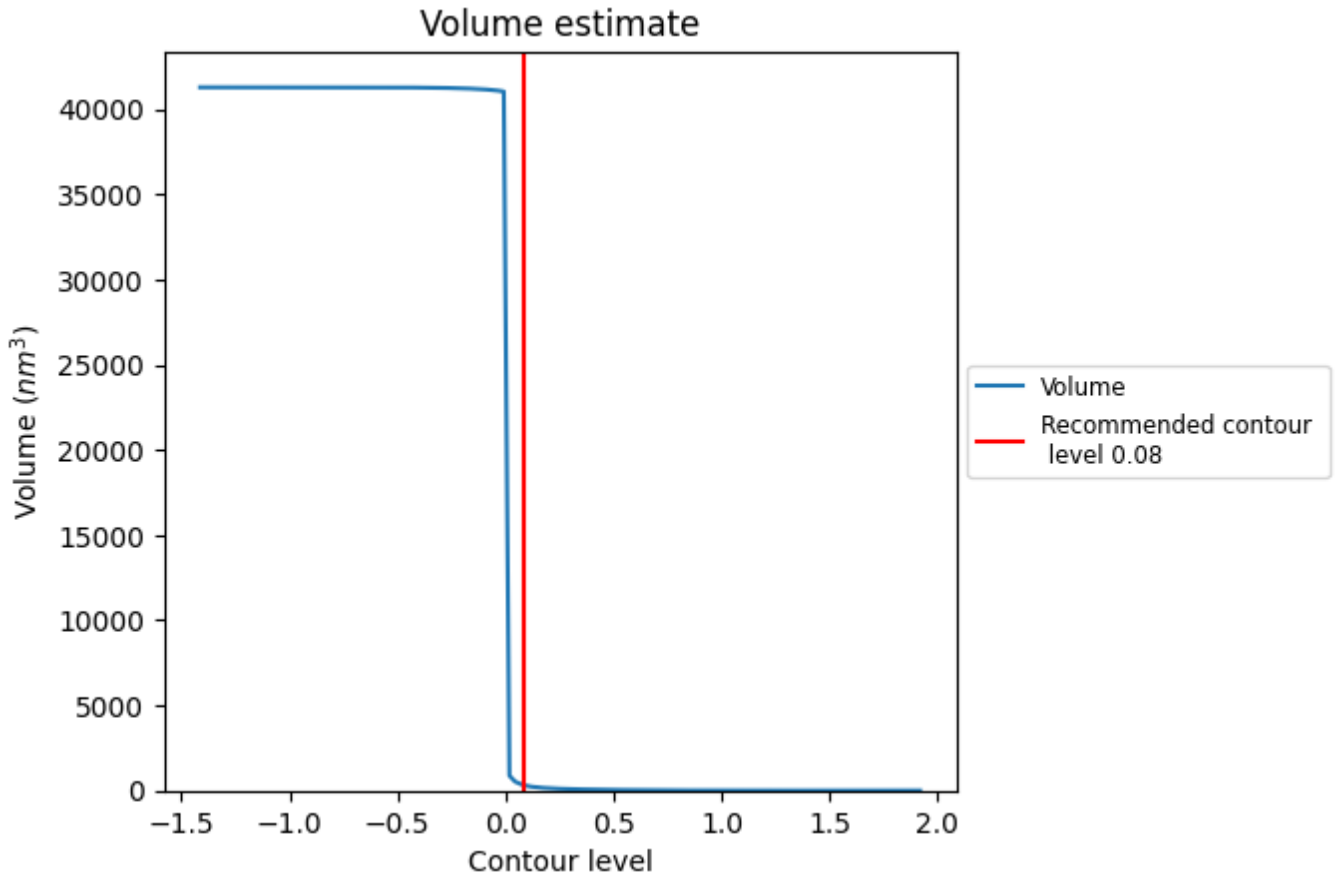
This section contains the results of statistical analysis of the map.

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.

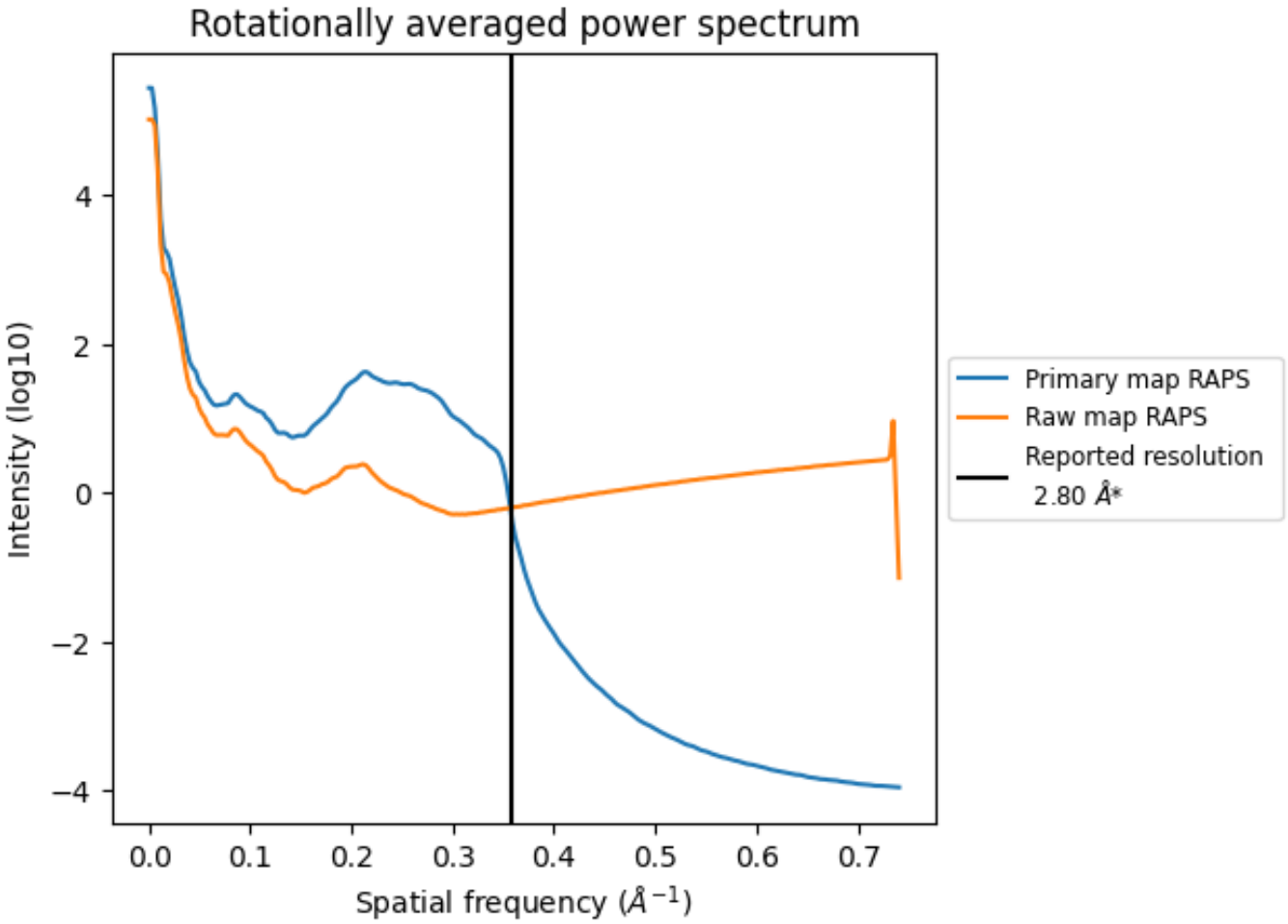
7.2 Volume estimate



The volume at the recommended contour level is 342 nm^3; this corresponds to an approximate mass of 309 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)

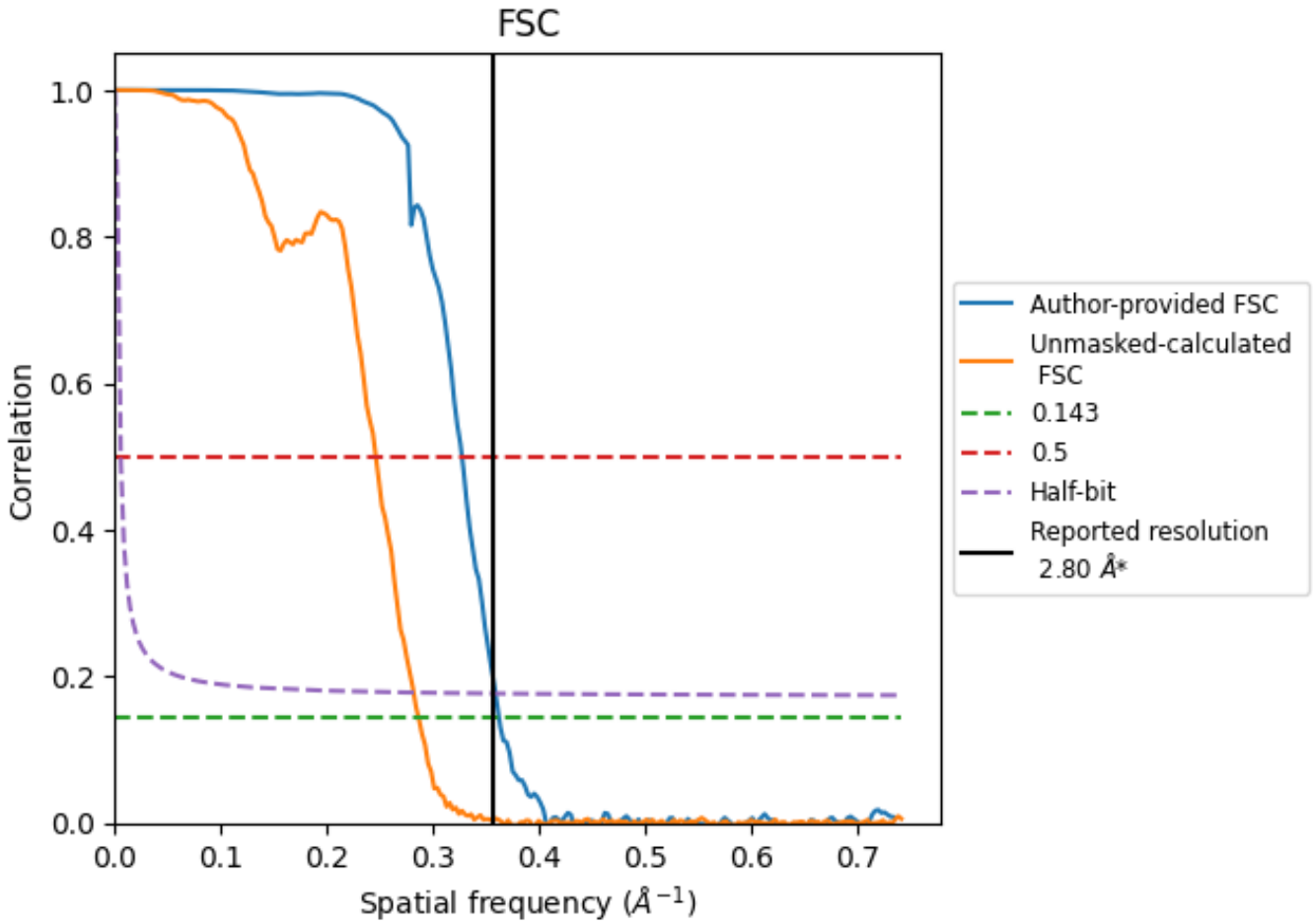


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation

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 0.357 Å^{-1}

8.2 Resolution estimates (i)

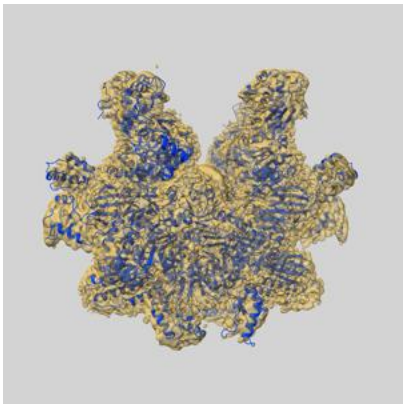
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.76	3.06	2.79
Unmasked-calculated*	3.49	4.07	3.55

*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 3.49 differs from the reported value 2.8 by more than 10 %

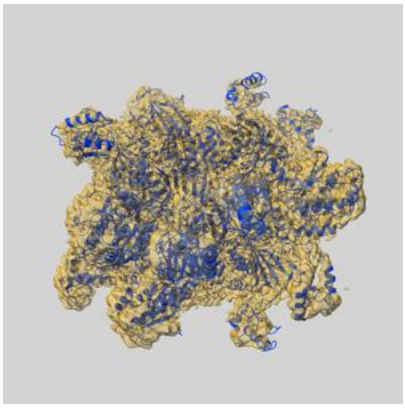
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29533 and PDB model 8FXH. Per-residue inclusion information can be found in section 3 on page 5.

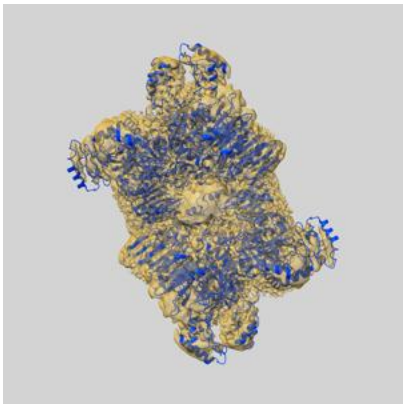
9.1 Map-model overlay



X



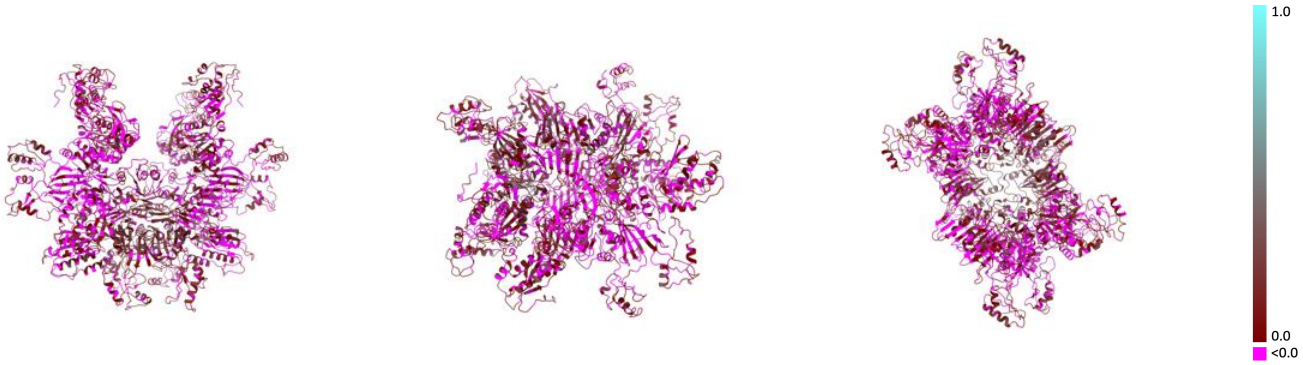
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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.

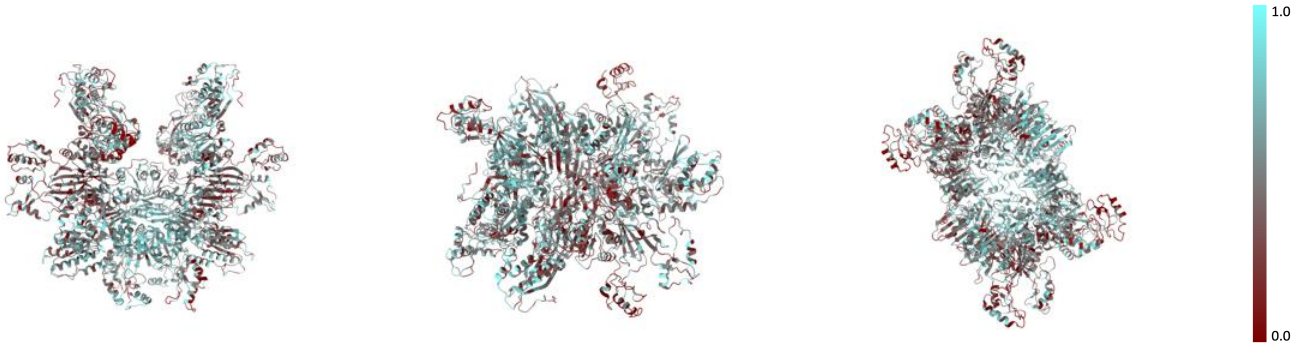
9.2 Q-score mapped to coordinate model (i)



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.

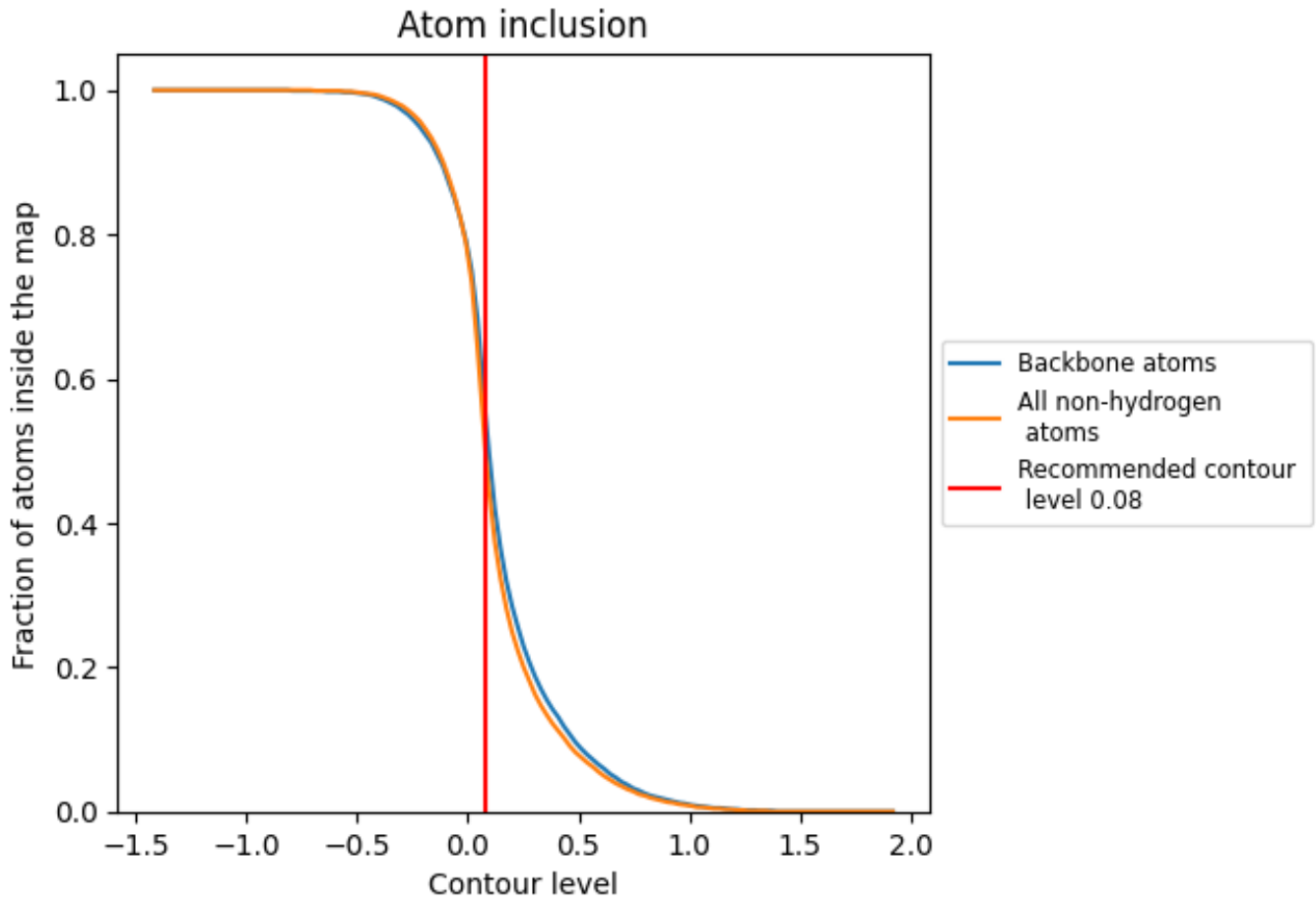
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 55% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4980	0.0460
A	0.4790	0.0280
B	0.4860	0.0310
C	0.5560	0.0880
D	0.5310	0.0760
E	0.4430	0.0070
F	0.4940	0.0480