Full wwPDB EM Validation Report (i)

Dec 10, 2022 – 11:16 pm GMT

PDB ID	:	6R5K
EMDB ID	:	EMD-4728
Title	:	Cryo-EM structure of a poly(A) RNP bound to the Pan2-Pan3 deadenylase
Authors	:	Schaefer, I.B.; Conti, E.
Deposited on	:	2019-03-25
Resolution	:	4.80 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 (i) symbol.

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

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

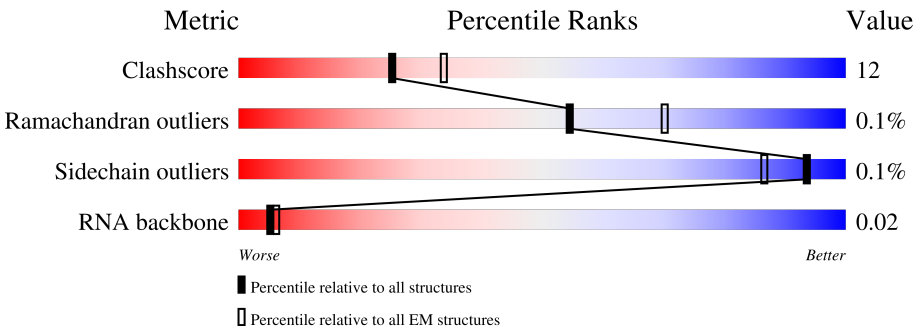
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.80 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
RNA backbone	4643	859

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	1115	8%, 64%, 29%, 7%
2	D	581	21%, 51%, 16%, 33%
2	F	581	8%, 21%, 7%, 72%
2	H	581	10%, 45%, 23%, 32%
3	E	90	•, •, 34%, 32%, •, 26%
4	N	458	•, 72%, 21%, 6%
5	O	689	•, 51%, 14%, 35%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 23508 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 PAN2-PAN3 deadenylation complex catalytic subunit PAN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1040	8053	5094	1357	1563	39	0	0

- Molecule 2 is a protein called Polyadenylate-binding protein, cytoplasmic and nuclear.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	390	2984	1878	517	581	8	0	0
2	F	165	1241	787	209	241	4	0	0
2	H	394	3052	1920	527	597	8	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP P04147
D	-2	PRO	-	expression tag	UNP P04147
D	-1	ASP	-	expression tag	UNP P04147
D	0	SER	-	expression tag	UNP P04147
F	-3	GLY	-	expression tag	UNP P04147
F	-2	PRO	-	expression tag	UNP P04147
F	-1	ASP	-	expression tag	UNP P04147
F	0	SER	-	expression tag	UNP P04147
H	-3	GLY	-	expression tag	UNP P04147
H	-2	PRO	-	expression tag	UNP P04147
H	-1	ASP	-	expression tag	UNP P04147
H	0	SER	-	expression tag	UNP P04147

- Molecule 3 is a RNA chain called poly(A) RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	E	67	1474	670	335	402	67	0	0

- Molecule 4 is a protein called PAN2-PAN3 deadenylation complex subunit PAN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	N	429	3282	2098	551	619	14	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	225	MET	-	initiating methionine	UNP P36102
N	231B	ILE	-	insertion	UNP P36102
N	231C	SER	-	insertion	UNP P36102
N	368	ASN	ASP	conflict	UNP P36102
N	665	GLN	GLU	conflict	UNP P36102
N	680	ALA	-	cloning artifact	UNP P36102

- Molecule 5 is a protein called PAN2-PAN3 deadenylation complex subunit PAN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	O	447	3420	2195	565	646	14	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	680	HIS	-	expression tag	UNP P36102
O	681	HIS	-	expression tag	UNP P36102
O	682	HIS	-	expression tag	UNP P36102
O	683	HIS	-	expression tag	UNP P36102
O	684	HIS	-	expression tag	UNP P36102
O	685	HIS	-	expression tag	UNP P36102
O	686	HIS	-	expression tag	UNP P36102
O	687	HIS	-	expression tag	UNP P36102
O	688	HIS	-	expression tag	UNP P36102
O	689	HIS	-	expression tag	UNP P36102

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

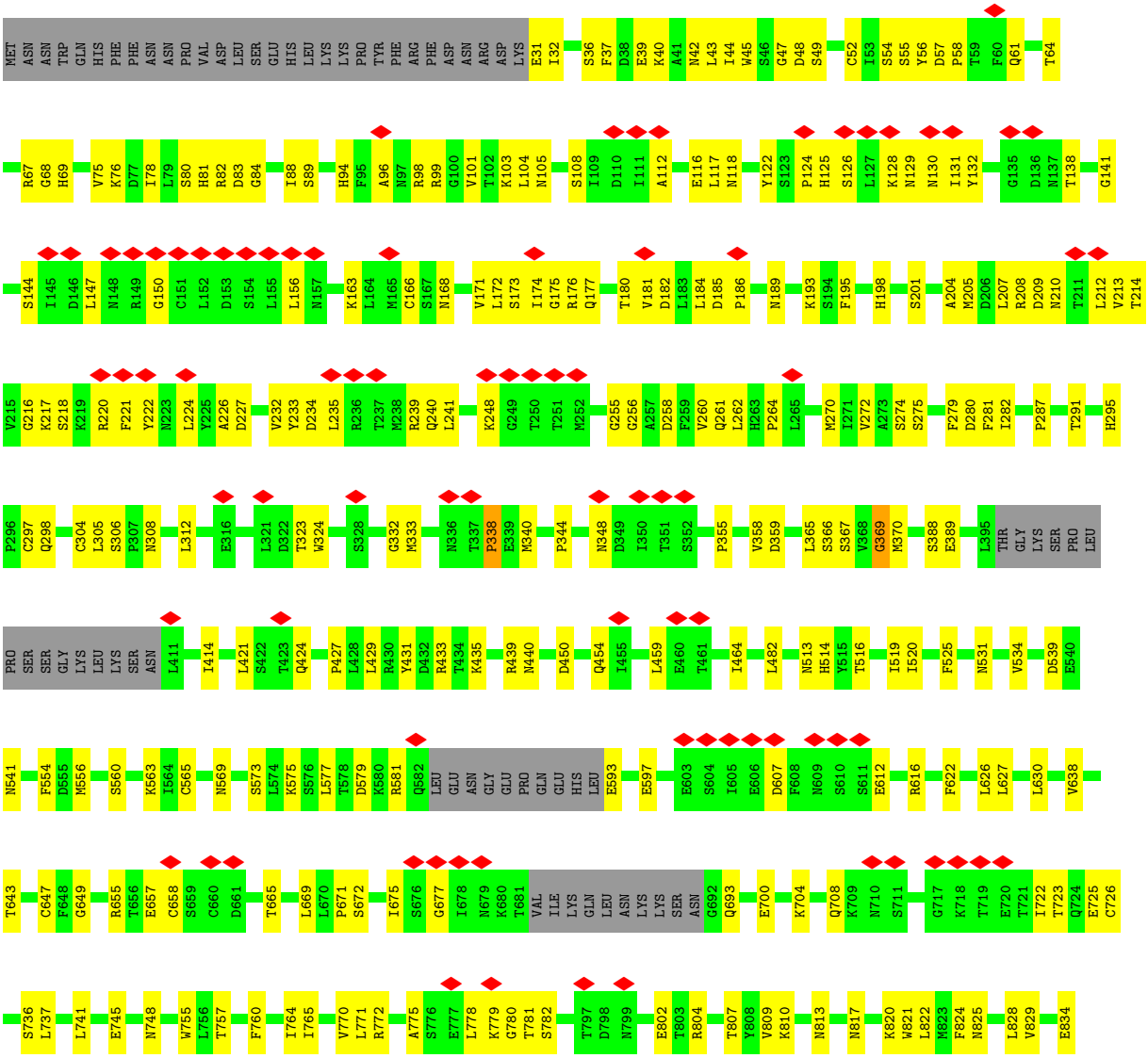
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	E	2	2	2	0

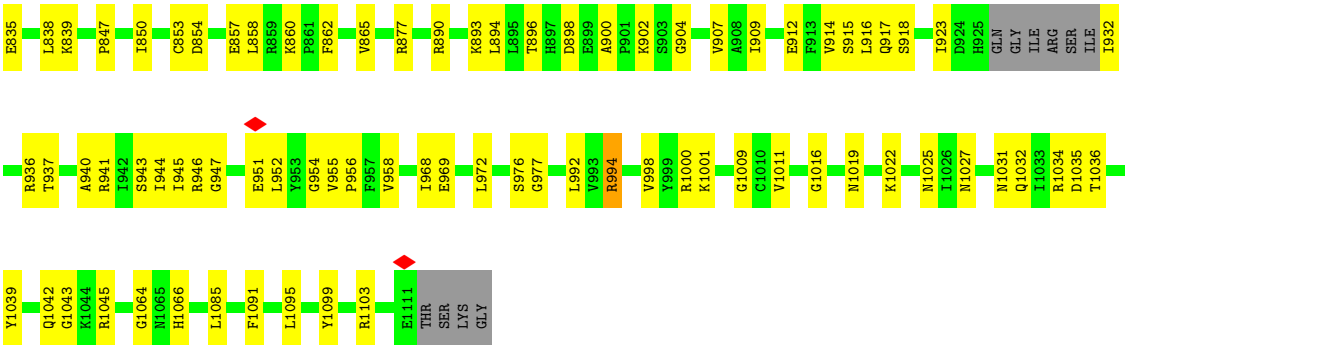
3 Residue-property plots (i)

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: PAN2-PAN3 deadenylation complex catalytic subunit PAN2

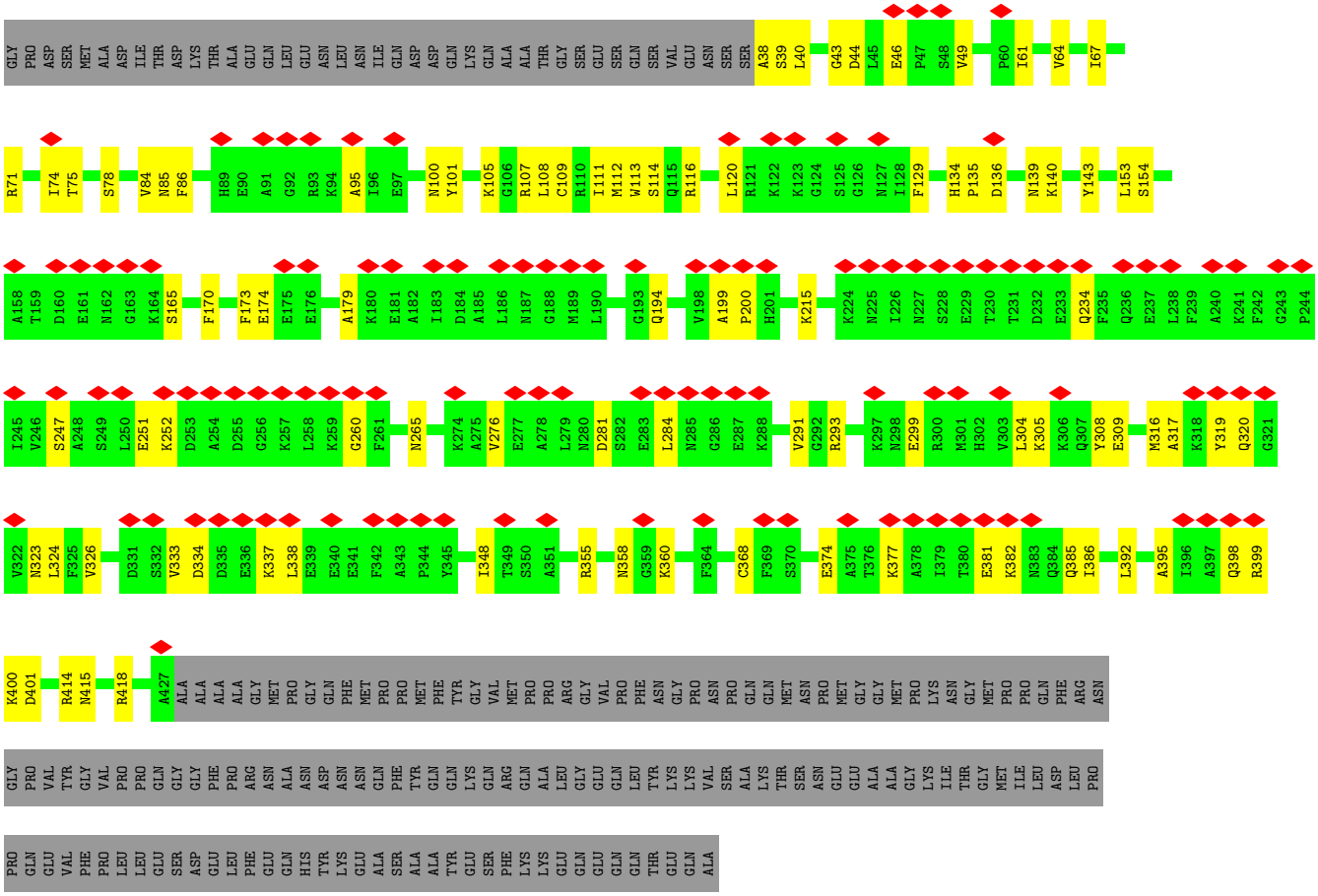
Chain A: 8% 64% 29% 7%





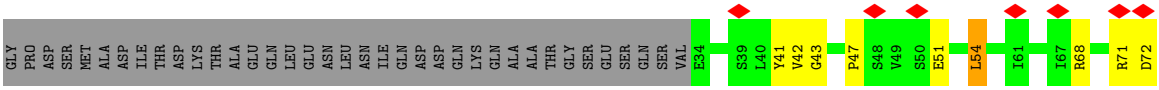
• Molecule 2: Polyadenylate-binding protein, cytoplasmic and nuclear

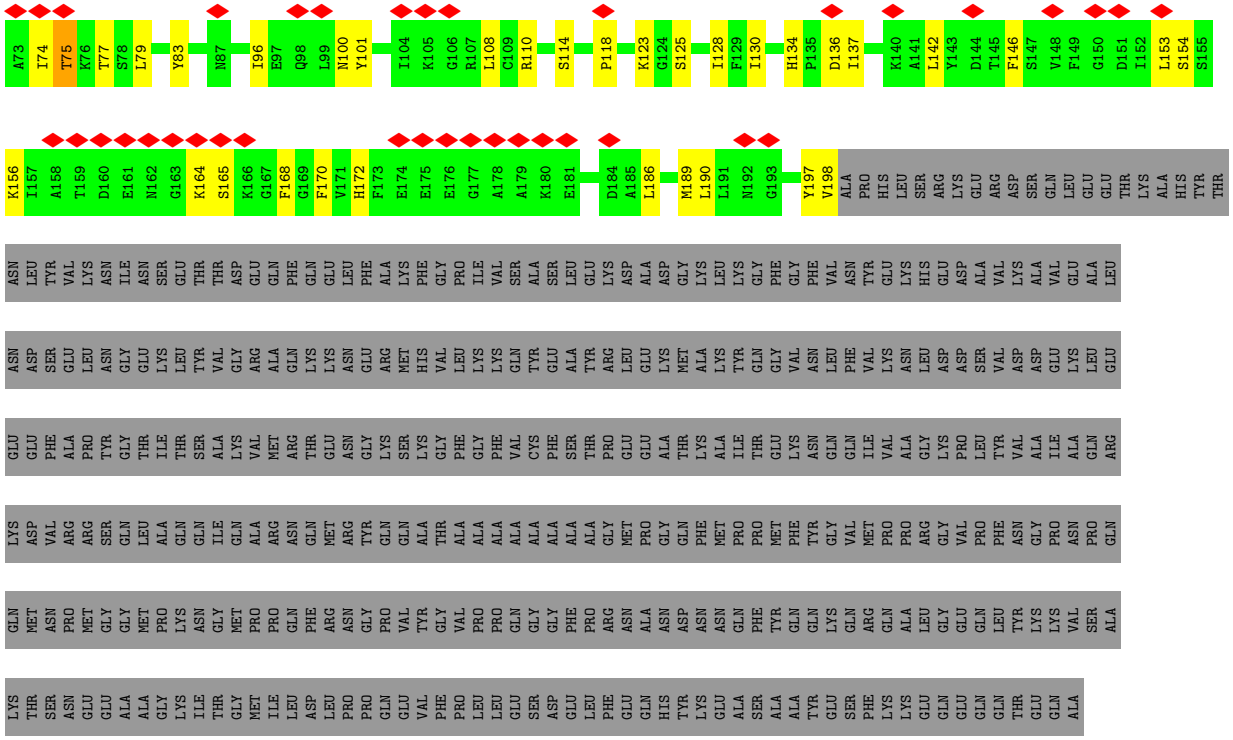
Chain D:



• Molecule 2: Polyadenylate-binding protein, cytoplasmic and nuclear

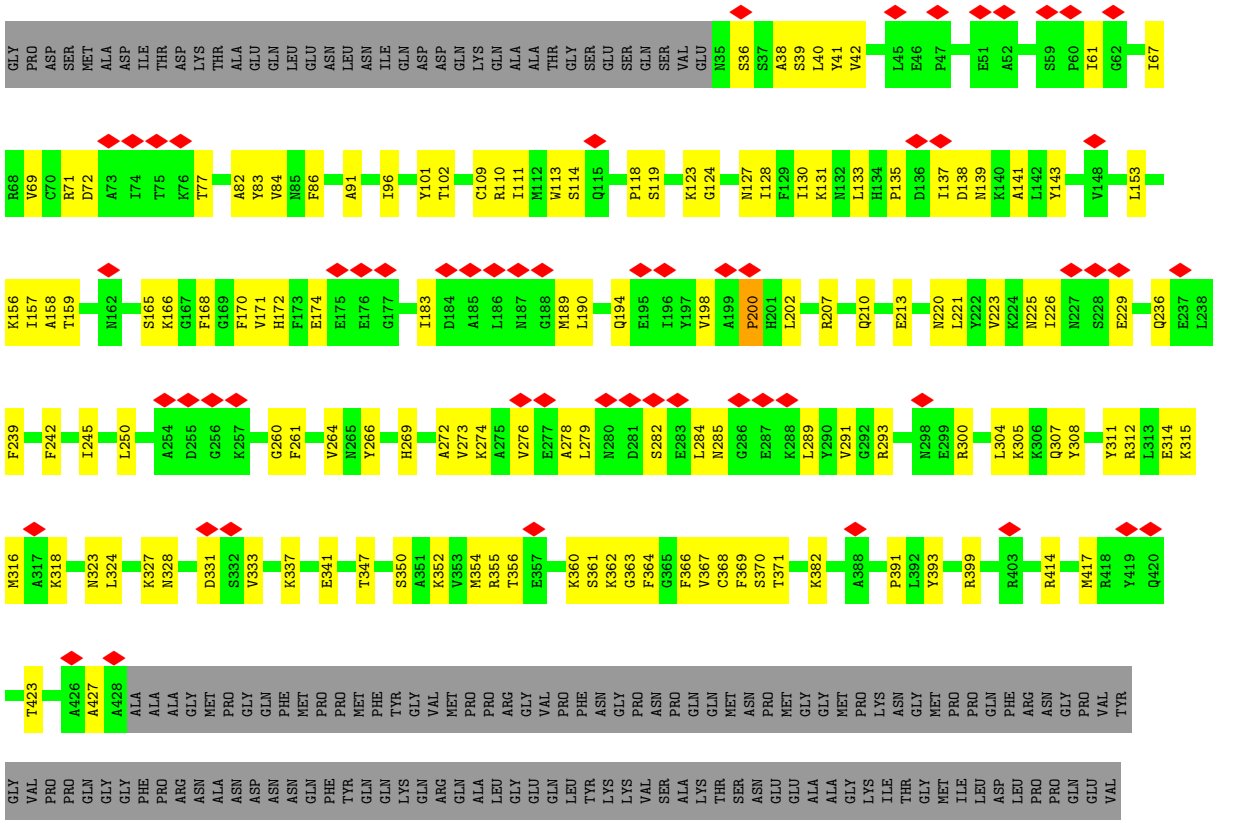
Chain F:

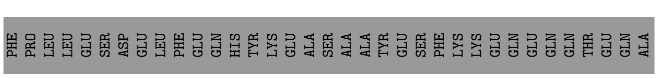




- Molecule 2: Polyadenylate-binding protein, cytoplasmic and nuclear

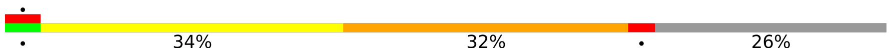
Chain H:

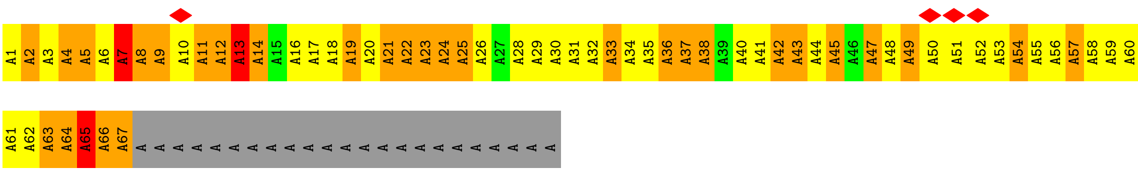




• Molecule 3: poly(A) RNA

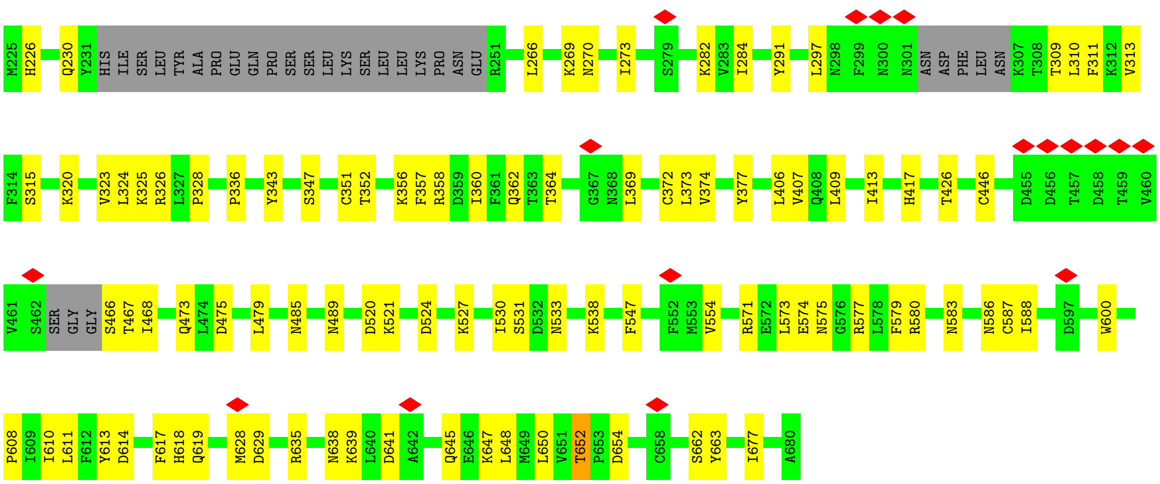
Chain E:





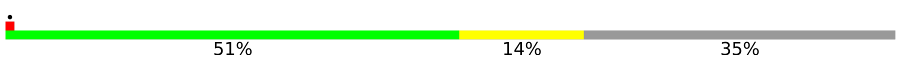
• Molecule 4: PAN2-PAN3 deadenylation complex subunit PAN3

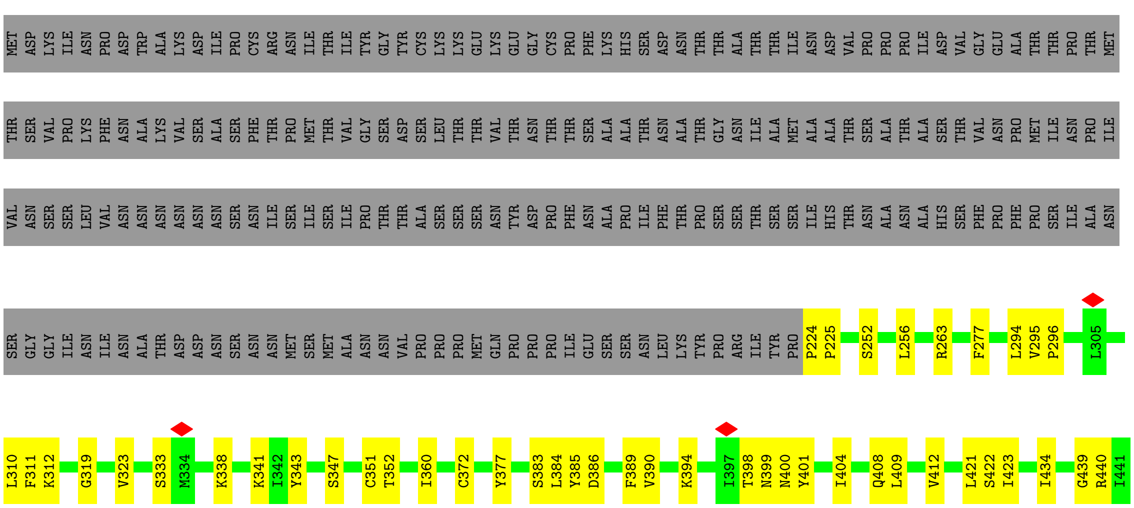
Chain N:

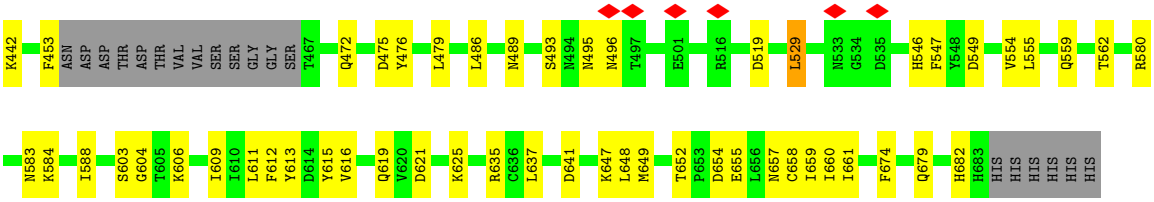


• Molecule 5: PAN2-PAN3 deadenylation complex subunit PAN3

Chain O:






K442
F453
ASN
ASP
ASP
THR
ASP
THR
VAL
VAL
SER
SER
GLY
GLY
SER
T467
Q472
D475
Y476
L479
L486
N489
S493
N494
N495
N496
T497
E501
R516
D519
L529
N533
G534
D535
H546
F547
Y548
D549
V554
L555
Q559
T562
R580
N583
K584
I588
S603
G604
T605
K606
I609
I610
L611
F612
Y613
D614
Y615
V616
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V620
D621
K625
R635
C636
L637
D641
K647
L648
M649
T652
P653
D654
E655
L656
N657
C658
I659
I660
I661
F674
Q679
H682
H683
HIS
HIS
HIS
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HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	29165	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	304.128, 304.128, 304.128	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.056, 1.056, 1.056	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: MG

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	0.33	0/8223	0.64	3/11171 (0.0%)
2	D	0.31	0/3034	0.60	2/4091 (0.0%)
2	F	0.33	0/1265	0.74	3/1712 (0.2%)
2	H	0.34	0/3104	0.62	1/4183 (0.0%)
3	E	0.49	1/1674 (0.1%)	1.14	6/2609 (0.2%)
4	N	0.33	0/3351	0.64	1/4559 (0.0%)
5	O	0.33	0/3498	0.65	3/4773 (0.1%)
All	All	0.34	1/24149 (0.0%)	0.69	19/33098 (0.1%)

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	0	9
2	D	0	2
2	F	0	2
2	H	0	2
5	O	0	5
All	All	0	20

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	13	A	N7-C5	-5.30	1.36	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	224	LEU	CA-CB-CG	7.74	133.09	115.30
3	E	65	A	O5'-P-OP1	-7.45	99.00	105.70
5	O	225	PRO	N-CA-CB	6.75	111.40	103.30
2	D	200	PRO	N-CA-CB	6.34	110.90	103.30
1	A	338	PRO	N-CA-CB	6.32	110.88	103.30
5	O	224	PRO	N-CA-CB	6.14	110.66	103.30
3	E	11	A	C2-N3-C4	6.11	113.65	110.60
3	E	57	A	P-O3'-C3'	5.99	126.89	119.70
4	N	652	THR	C-N-CD	-5.85	107.72	120.60
3	E	7	A	P-O3'-C3'	5.70	126.53	119.70
2	H	200	PRO	N-CA-CB	5.66	110.09	103.30
2	F	118	PRO	N-CA-CB	5.58	109.99	103.30
3	E	13	A	C5-N7-C8	5.49	106.64	103.90
2	D	40	LEU	CA-CB-CG	5.33	127.55	115.30
1	A	209	ASP	CB-CG-OD1	5.08	122.88	118.30
2	F	54	LEU	CA-CB-CG	5.08	126.98	115.30
2	F	190	LEU	CA-CB-CG	5.03	126.88	115.30
5	O	555	LEU	CA-CB-CG	5.02	126.85	115.30
3	E	11	A	N3-C4-N9	5.00	131.40	127.40

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	TYR	Peptide
1	A	304	CYS	Peptide
1	A	369	GLY	Peptide
1	A	37	PHE	Peptide
1	A	424	GLN	Peptide
1	A	58	PRO	Peptide
1	A	607	ASP	Peptide
1	A	890	ARG	Peptide
1	A	994	ARG	Peptide
2	D	154	SER	Peptide
2	D	401	ASP	Peptide
2	F	125	SER	Peptide
2	F	74	ILE	Peptide
2	H	300	ARG	Mainchain,Peptide
5	O	277	PHE	Peptide
5	O	319	GLY	Peptide
5	O	383	SER	Peptide
5	O	529	LEU	Peptide
5	O	612	PHE	Peptide

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	8053	0	7627	215	0
2	D	2984	0	2865	64	0
2	F	1241	0	1167	27	0
2	H	3052	0	2950	104	0
3	E	1474	0	737	41	0
4	N	3282	0	2992	69	0
5	O	3420	0	3129	57	0
6	E	2	0	0	0	0
All	All	23508	0	21467	515	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 12.

All (515) 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:A:43:LEU:HA	1:A:56:TYR:O	1.63	0.98
5:O:360:ILE:HA	5:O:372:CYS:O	1.66	0.95
2:F:130:ILE:O	2:F:168:PHE:HA	1.69	0.92
2:H:305:LYS:O	2:H:308:TYR:HB3	1.77	0.85
2:H:304:LEU:O	2:H:307:GLN:HB3	1.82	0.79
2:H:274:LYS:O	2:H:278:ALA:HB3	1.83	0.77
2:H:139:ASN:O	2:H:143:TYR:HB2	1.88	0.73
2:D:398:GLN:HG2	2:D:399:ARG:HG2	1.71	0.73
1:A:810:LYS:HA	1:A:820:LYS:O	1.88	0.73
4:N:610:ILE:O	4:N:613:TYR:HB3	1.88	0.72
1:A:208:ARG:HH12	1:A:264:PRO:HA	1.54	0.72
2:H:41:TYR:O	2:H:111:ILE:HA	1.90	0.70
2:F:154:SER:O	2:F:172:HIS:HB3	1.92	0.69
1:A:44:ILE:O	1:A:55:SER:HA	1.94	0.68
5:O:647:LYS:HA	5:O:661:ILE:O	1.94	0.68
2:D:38:ALA:N	2:D:114:SER:HG	1.92	0.68
2:H:350:SER:O	2:H:367:VAL:HA	1.94	0.67
2:F:42:VAL:HA	2:F:110:ARG:HB3	1.76	0.67
4:N:583:ASN:O	4:N:587:CYS:HB2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:33:A:N7	2:H:131:LYS:NZ	2.43	0.67
5:O:648:LEU:O	5:O:660:ILE:HA	1.95	0.67
2:D:75:THR:HA	4:N:336:PRO:HD2	1.77	0.67
2:D:129:PHE:HA	2:D:170:PHE:HA	1.77	0.67
2:H:38:ALA:HB3	2:H:86:PHE:HB2	1.77	0.66
1:A:280:ASP:HA	1:A:291:THR:O	1.95	0.66
1:A:367:SER:H	4:N:574:GLU:HG3	1.60	0.66
2:H:223:VAL:O	2:H:261:PHE:HA	1.96	0.66
2:H:423:THR:O	2:H:427:ALA:HB2	1.97	0.65
4:N:351:CYS:SG	4:N:352:THR:N	2.69	0.65
1:A:778:LEU:HD23	1:A:780:GLY:H	1.60	0.65
4:N:466:SER:HB3	4:N:468:ILE:HG12	1.79	0.65
1:A:205:MET:HA	1:A:213:VAL:O	1.97	0.64
1:A:560:SER:HB3	1:A:563:LYS:HB3	1.79	0.64
1:A:1011:VAL:HG12	1:A:1032:GLN:HG3	1.79	0.64
1:A:198:HIS:HB3	1:A:218:SER:HB2	1.80	0.64
2:H:223:VAL:HG22	2:H:291:VAL:HG22	1.80	0.64
4:N:588:ILE:HG21	4:N:677:ILE:HG13	1.80	0.63
1:A:807:THR:HB	1:A:824:PHE:HB2	1.80	0.63
3:E:5:A:N6	2:H:362:LYS:O	2.32	0.63
1:A:81:HIS:ND1	1:A:83:ASP:OD1	2.31	0.62
4:N:230:GLN:O	4:N:571:ARG:NH1	2.32	0.62
3:E:36:A:HO2'	2:H:83:TYR:HH	1.45	0.62
2:D:360:LYS:HB3	2:H:124:GLY:HA3	1.81	0.62
2:D:414:ARG:HH12	2:H:36:SER:HA	1.65	0.62
1:A:99:ARG:HH22	4:N:647:LYS:HG2	1.65	0.61
2:H:312:ARG:NH2	2:H:316:MET:SD	2.70	0.61
1:A:42:ASN:HA	1:A:333:MET:HB2	1.81	0.61
2:F:156:LYS:HB3	2:F:170:PHE:HB2	1.82	0.61
1:A:262:LEU:HD23	1:A:270:MET:HB3	1.81	0.61
1:A:174:ILE:O	1:A:181:VAL:HA	2.01	0.61
2:F:123:LYS:H	2:H:362:LYS:HE3	1.66	0.61
2:H:42:VAL:HG22	2:H:111:ILE:HG12	1.81	0.60
2:D:101:TYR:HB2	2:D:140:LYS:HB3	1.84	0.60
4:N:356:LYS:NZ	4:N:357:PHE:O	2.35	0.60
1:A:32:ILE:HA	1:A:48:ASP:HA	1.84	0.60
1:A:204:ALA:O	1:A:214:THR:HA	2.01	0.60
1:A:1043:GLY:HA3	3:E:63:A:H62	1.66	0.60
1:A:57:ASP:HB2	1:A:61:GLN:HB3	1.83	0.60
1:A:450:ASP:O	1:A:454:GLN:NE2	2.35	0.60
5:O:323:VAL:HG23	5:O:377:TYR:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1085:LEU:HB3	1:A:1091:PHE:HB3	1.84	0.59
1:A:81:HIS:H	1:A:98:ARG:HH21	1.49	0.59
1:A:193:LYS:NZ	1:A:233:TYR:OH	2.35	0.59
3:E:1:A:N3	3:E:3:A:N6	2.50	0.59
1:A:39:GLU:HG2	1:A:98:ARG:HH22	1.68	0.59
2:H:135:PRO:HG3	2:H:207:ARG:HD2	1.83	0.59
1:A:94:HIS:HE2	1:A:96:ALA:HB2	1.67	0.59
2:H:347:THR:HB	2:H:370:SER:HB3	1.84	0.59
5:O:394:LYS:NZ	5:O:495:ASN:O	2.35	0.59
1:A:802:GLU:OE1	1:A:804:ARG:NH2	2.35	0.59
2:H:139:ASN:O	2:H:143:TYR:CB	2.50	0.59
1:A:103:LYS:NZ	1:A:147:LEU:O	2.35	0.58
2:D:317:ALA:O	2:D:320:GLN:NE2	2.36	0.58
1:A:915:SER:HA	1:A:937:THR:HA	1.85	0.58
1:A:912:GLU:HB2	1:A:941:ARG:HB3	1.85	0.58
5:O:333:SER:HB3	5:O:453:PHE:HA	1.85	0.58
5:O:615:TYR:O	5:O:619:GLN:NE2	2.37	0.58
1:A:308:ASN:ND2	1:A:332:GLY:O	2.37	0.58
2:D:323:ASN:ND2	3:E:45:A:N7	2.52	0.58
1:A:435:LYS:O	1:A:616:ARG:NH2	2.36	0.57
4:N:635:ARG:HG2	4:N:639:LYS:HE2	1.86	0.57
2:F:96:ILE:HG12	2:F:100:ASN:HD22	1.69	0.57
2:H:337:LYS:NZ	2:H:341:GLU:OE2	2.38	0.57
5:O:613:TYR:HA	5:O:616:VAL:HG12	1.86	0.57
2:D:139:ASN:O	2:D:143:TYR:HB2	2.04	0.57
2:F:153:LEU:N	2:F:172:HIS:O	2.36	0.57
4:N:652:THR:OG1	4:N:654:ASP:N	2.37	0.57
1:A:565:CYS:SG	1:A:1027:ASN:ND2	2.78	0.57
1:A:573:SER:OG	1:A:994:ARG:NH2	2.37	0.57
2:H:128:ILE:HG12	2:H:172:HIS:HB2	1.87	0.57
1:A:575:LYS:O	1:A:579:ASP:N	2.37	0.57
2:H:282:SER:HB3	2:H:289:LEU:HD12	1.86	0.57
2:D:415:ASN:OD1	2:D:418:ARG:NH2	2.38	0.57
2:F:72:ASP:HB3	2:F:75:THR:HG21	1.87	0.57
5:O:351:CYS:SG	5:O:352:THR:N	2.78	0.57
1:A:82:ARG:NH1	1:A:128:LYS:O	2.37	0.56
1:A:163:LYS:HE3	1:A:177:GLN:HA	1.87	0.56
1:A:367:SER:OG	4:N:638:ASN:ND2	2.38	0.56
1:A:622:PHE:O	1:A:626:LEU:HB2	2.05	0.56
2:D:381:GLU:HG3	2:D:382:LYS:HG2	1.87	0.56
3:E:64:A:H1'	3:E:65:A:H2'	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1031:ASN:OD1	1:A:1034:ARG:NH2	2.38	0.56
3:E:42:A:OP2	3:E:43:A:N6	2.38	0.56
2:H:327:LYS:HA	2:H:364:PHE:HA	1.87	0.56
3:E:24:A:N6	2:H:250:LEU:O	2.38	0.56
1:A:172:LEU:HD22	1:A:184:LEU:HB2	1.87	0.56
2:D:247:SER:HB3	2:D:265:ASN:HD22	1.70	0.56
4:N:406:LEU:HD12	4:N:409:LEU:HD11	1.87	0.56
4:N:521:LYS:NZ	4:N:547:PHE:O	2.33	0.56
1:A:116:GLU:OE2	1:A:118:ASN:ND2	2.37	0.55
2:H:130:ILE:HB	2:H:171:VAL:HB	1.88	0.55
1:A:612:GLU:OE2	1:A:616:ARG:NH1	2.39	0.55
2:H:236:GLN:NE2	2:H:245:ILE:O	2.40	0.55
4:N:362:GLN:HE21	4:N:369:LEU:HB3	1.70	0.55
1:A:39:GLU:HG3	1:A:40:LYS:HG3	1.87	0.55
3:E:3:A:H5'	2:H:360:LYS:HD2	1.87	0.55
3:E:14:A:O5'	2:H:399:ARG:NH1	2.40	0.55
2:F:130:ILE:HG23	2:F:197:TYR:H	1.71	0.55
2:H:221:LEU:HB2	2:H:264:VAL:HB	1.88	0.55
1:A:204:ALA:HB1	1:A:260:VAL:H	1.71	0.55
1:A:877:ARG:HA	1:A:894:LEU:HD23	1.88	0.55
4:N:358:ARG:HB2	4:N:374:VAL:HG23	1.86	0.55
1:A:1091:PHE:O	1:A:1095:LEU:CB	2.55	0.55
1:A:240:GLN:NE2	1:A:241:LEU:O	2.40	0.55
1:A:1064:GLY:N	3:E:67:A:N1	2.55	0.55
2:D:113:TRP:HE1	2:D:153:LEU:HD11	1.72	0.55
1:A:104:LEU:HD12	1:A:147:LEU:HD12	1.88	0.55
1:A:281:PHE:HB3	1:A:291:THR:HB	1.88	0.54
2:D:46:GLU:HB3	2:D:49:VAL:HG23	1.89	0.54
3:E:5:A:H62	2:H:362:LYS:HG2	1.72	0.54
4:N:586:ASN:OD1	4:N:613:TYR:OH	2.25	0.54
1:A:69:HIS:ND1	1:A:89:SER:OG	2.39	0.54
1:A:108:SER:HB2	1:A:112:ALA:HA	1.88	0.54
1:A:198:HIS:ND1	1:A:227:ASP:OD2	2.40	0.54
4:N:574:GLU:OE1	4:N:577:ARG:NH2	2.41	0.54
1:A:358:VAL:HG21	5:O:584:LYS:HG3	1.90	0.54
1:A:658:CYS:HA	1:A:722:ILE:HB	1.90	0.54
2:D:348:ILE:HG12	2:D:368:CYS:H	1.71	0.54
1:A:775:ALA:HB1	1:A:779:LYS:HG2	1.89	0.54
5:O:621:ASP:OD1	5:O:625:LYS:N	2.41	0.54
1:A:124:PRO:HG3	1:A:186:PRO:HB2	1.90	0.53
1:A:141:GLY:CA	1:A:156:LEU:O	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:284:LEU:HB2	2:H:289:LEU:HD21	1.90	0.53
2:D:276:VAL:HG11	2:D:293:ARG:HD2	1.90	0.53
1:A:297:CYS:SG	1:A:298:GLN:N	2.79	0.53
2:D:355:ARG:HB2	2:D:358:ASN:HA	1.91	0.53
1:A:132:TYR:HD1	1:A:144:SER:HB2	1.73	0.53
1:A:45:TRP:HA	1:A:54:SER:O	2.09	0.53
1:A:180:THR:OG1	1:A:195:PHE:O	2.25	0.53
1:A:943:SER:HA	1:A:958:VAL:O	2.08	0.53
4:N:611:LEU:HB3	4:N:650:LEU:HD21	1.89	0.53
1:A:99:ARG:HB3	1:A:101:VAL:HG22	1.90	0.53
1:A:370:MET:O	4:N:226:HIS:ND1	2.36	0.53
2:H:414:ARG:NH1	2:H:417:MET:SD	2.82	0.53
4:N:311:PHE:HB2	4:N:324:LEU:HB3	1.90	0.53
4:N:645:GLN:HA	4:N:662:SER:HB2	1.91	0.53
1:A:248:LYS:HA	1:A:255:GLY:HA2	1.90	0.53
2:H:239:PHE:HB3	2:H:266:TYR:HE1	1.73	0.53
1:A:88:ILE:HD11	1:A:117:LEU:HD22	1.90	0.53
3:E:18:A:OP2	2:H:307:GLN:NE2	2.38	0.53
2:H:40:LEU:HD22	2:H:96:ILE:HD11	1.91	0.52
2:D:113:TRP:NE1	2:D:174:GLU:OE1	2.42	0.52
1:A:84:GLY:HA2	1:A:98:ARG:HG2	1.91	0.52
2:H:139:ASN:HD21	2:H:156:LYS:HA	1.73	0.52
4:N:413:ILE:O	4:N:417:HIS:ND1	2.35	0.52
5:O:408:GLN:NE2	5:O:439:GLY:O	2.34	0.52
1:A:433:ARG:NH2	5:O:654:ASP:O	2.42	0.52
1:A:577:LEU:O	1:A:581:ARG:NH1	2.42	0.52
1:A:857:GLU:HA	1:A:860:LYS:HG2	1.91	0.52
2:H:127:ASN:HB3	2:H:170:PHE:HB3	1.92	0.52
2:H:221:LEU:HD11	2:H:272:ALA:HA	1.91	0.52
2:H:341:GLU:OE1	2:H:382:LYS:NZ	2.42	0.52
1:A:513:ASN:OD1	1:A:514:HIS:N	2.42	0.52
1:A:655:ARG:HB2	1:A:725:GLU:HG2	1.92	0.52
2:D:112:MET:SD	3:E:60:A:N6	2.76	0.52
1:A:708:GLN:HA	1:A:723:THR:HA	1.92	0.52
4:N:573:LEU:HD11	5:O:263:ARG:HG3	1.90	0.52
1:A:104:LEU:HD11	1:A:150:GLY:HA2	1.91	0.51
1:A:569:ASN:ND2	1:A:1025:ASN:O	2.43	0.51
2:H:133:LEU:H	2:H:168:PHE:HA	1.74	0.51
1:A:459:LEU:HG	1:A:464:ILE:HB	1.92	0.51
1:A:520:ILE:HG23	1:A:554:PHE:HE1	1.75	0.51
2:D:100:ASN:HA	2:D:111:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:369:PHE:HB3	2:H:371:THR:H	1.75	0.51
1:A:909:ILE:HG13	1:A:944:ILE:HG12	1.92	0.51
2:D:39:SER:OG	2:D:85:ASN:ND2	2.41	0.51
5:O:422:SER:OG	5:O:423:ILE:N	2.43	0.51
1:A:112:ALA:O	1:A:138:THR:OG1	2.22	0.51
1:A:513:ASN:ND2	1:A:516:THR:OG1	2.35	0.51
1:A:643:THR:O	1:A:647:CYS:CB	2.59	0.51
4:N:315:SER:HB3	4:N:320:LYS:H	1.74	0.51
4:N:475:ASP:O	4:N:479:LEU:HB2	2.11	0.51
1:A:232:VAL:O	1:A:240:GLN:NE2	2.44	0.51
1:A:272:VAL:O	1:A:279:PHE:HA	2.10	0.51
2:F:71:ARG:NH2	2:F:75:THR:O	2.44	0.51
5:O:385:TYR:HA	5:O:389:PHE:HD2	1.76	0.51
1:A:239:ARG:NH1	1:A:240:GLN:O	2.44	0.50
4:N:364:THR:HG22	4:N:369:LEU:HG	1.93	0.50
2:D:49:VAL:HG22	2:D:105:LYS:HD3	1.93	0.50
2:D:374:GLU:HA	2:D:377:LYS:HG2	1.91	0.50
1:A:737:LEU:HB2	1:A:850:ILE:HB	1.92	0.50
2:D:333:VAL:HG21	2:D:392:LEU:HD11	1.92	0.50
3:E:14:A:C6	2:H:352:LYS:HB2	2.46	0.50
1:A:525:PHE:HA	1:A:862:PHE:HZ	1.76	0.50
4:N:614:ASP:HA	4:N:617:PHE:HB2	1.94	0.50
5:O:386:ASP:HA	5:O:390:VAL:HB	1.93	0.50
1:A:365:LEU:HD11	4:N:575:ASN:HB3	1.93	0.50
1:A:76:LYS:N	1:A:88:ILE:O	2.45	0.50
1:A:163:LYS:N	1:A:175:GLY:O	2.44	0.50
2:F:47:PRO:HB3	2:F:77:THR:HA	1.93	0.50
2:H:101:TYR:HD2	2:H:138:ASP:HB2	1.76	0.50
1:A:355:PRO:HA	4:N:629:ASP:HA	1.93	0.50
2:D:39:SER:HA	2:D:85:ASN:HA	1.92	0.50
2:F:142:LEU:O	2:F:146:PHE:HB2	2.12	0.50
5:O:440:ARG:HB3	5:O:442:LYS:HG2	1.93	0.50
1:A:516:THR:HG22	1:A:519:ILE:HD12	1.94	0.50
1:A:900:ALA:O	1:A:902:LYS:NZ	2.40	0.50
4:N:360:ILE:HD12	4:N:373:LEU:HD12	1.94	0.50
1:A:704:LYS:HA	1:A:726:CYS:O	2.12	0.50
2:D:215:LYS:HA	2:D:305:LYS:HZ3	1.76	0.50
2:H:72:ASP:N	2:H:77:THR:O	2.41	0.49
3:E:25:A:O2'	2:H:220:ASN:OD1	2.24	0.49
2:H:350:SER:HB2	2:H:368:CYS:HB2	1.93	0.49
1:A:234:ASP:HB3	1:A:241:LEU:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:ASP:O	1:A:1000:ARG:NH1	2.45	0.49
2:D:85:ASN:HD21	2:D:116:ARG:HH11	1.61	0.49
3:E:37:A:N6	2:H:39:SER:O	2.42	0.49
1:A:809:VAL:O	1:A:821:TRP:HA	2.13	0.49
1:A:923:ILE:HD13	2:D:74:ILE:HG21	1.95	0.49
2:D:61:ILE:HG21	2:D:95:ALA:HB2	1.94	0.49
4:N:652:THR:OG1	4:N:654:ASP:OD1	2.23	0.49
5:O:252:SER:O	5:O:256:LEU:N	2.44	0.49
2:F:101:TYR:HA	2:F:108:LEU:HD22	1.94	0.49
1:A:429:LEU:HA	5:O:657:ASN:HA	1.95	0.49
2:D:333:VAL:O	2:D:355:ARG:NH1	2.45	0.49
2:H:183:ILE:HG12	2:H:198:VAL:HG11	1.93	0.49
1:A:220:ARG:HG3	1:A:221:PHE:HD1	1.77	0.49
1:A:389:GLU:HG3	5:O:635:ARG:HD3	1.94	0.49
1:A:431:TYR:HB2	5:O:658:CYS:HB2	1.95	0.49
1:A:81:HIS:O	1:A:98:ARG:NH2	2.46	0.49
1:A:1045:ARG:HD2	3:E:63:A:C4	2.48	0.49
4:N:520:ASP:O	4:N:524:ASP:N	2.40	0.49
5:O:486:LEU:HA	5:O:489:ASN:HB2	1.94	0.49
1:A:132:TYR:HA	1:A:144:SER:HA	1.94	0.49
4:N:614:ASP:HB3	4:N:618:HIS:HD2	1.78	0.49
5:O:649:MET:HA	5:O:659:ILE:O	2.13	0.49
1:A:210:ASN:HA	1:A:235:LEU:HD12	1.95	0.49
1:A:366:SER:HA	4:N:574:GLU:HB2	1.95	0.49
2:D:414:ARG:O	2:D:418:ARG:HB2	2.13	0.48
3:E:12:A:H1'	3:E:13:A:C8	2.47	0.48
2:H:102:THR:HG1	2:H:109:CYS:HG	1.60	0.48
2:H:223:VAL:HG13	2:H:289:LEU:HA	1.95	0.48
5:O:343:TYR:O	5:O:347:SER:N	2.46	0.48
1:A:765:ILE:HG13	1:A:781:THR:HG23	1.94	0.48
2:H:276:VAL:HG21	2:H:293:ARG:HG2	1.95	0.48
1:A:76:LYS:H	1:A:89:SER:HA	1.78	0.48
1:A:765:ILE:HD12	1:A:778:LEU:HD21	1.95	0.48
1:A:847:PRO:HB2	1:A:850:ILE:HD11	1.95	0.48
1:A:998:VAL:HG12	1:A:1001:LYS:HD2	1.94	0.48
2:D:304:LEU:O	2:D:308:TYR:CB	2.61	0.48
4:N:309:THR:HA	4:N:326:ARG:HG3	1.95	0.48
1:A:359:ASP:HA	5:O:580:ARG:HD3	1.96	0.48
1:A:649:GLY:HA2	1:A:671:PRO:HA	1.96	0.48
4:N:648:LEU:HD11	4:N:663:TYR:HE1	1.78	0.48
5:O:389:PHE:HE1	5:O:493:SER:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASP:O	1:A:189:ASN:ND2	2.47	0.48
3:E:21:A:H5'	3:E:22:A:H2'	1.96	0.48
4:N:466:SER:OG	4:N:467:THR:N	2.46	0.48
1:A:83:ASP:OD1	1:A:83:ASP:N	2.42	0.48
4:N:407:VAL:HG11	4:N:554:VAL:HG11	1.96	0.48
1:A:36:SER:OG	1:A:78:ILE:O	2.30	0.48
1:A:439:ARG:HD2	5:O:655:GLU:HG3	1.95	0.48
1:A:258:ASP:OD1	1:A:258:ASP:N	2.47	0.48
1:A:854:ASP:O	1:A:858:LEU:N	2.40	0.48
1:A:261:GLN:HG2	1:A:305:LEU:HD21	1.95	0.47
4:N:527:LYS:HA	4:N:530:ILE:HG22	1.96	0.47
4:N:610:ILE:O	4:N:613:TYR:CB	2.60	0.47
5:O:546:HIS:HB2	5:O:547:PHE:HD1	1.79	0.47
1:A:306:SER:OG	1:A:308:ASN:OD1	2.28	0.47
1:A:1045:ARG:HG2	3:E:64:A:C8	2.49	0.47
1:A:122:TYR:HA	1:A:131:ILE:HA	1.96	0.47
1:A:312:LEU:H	1:A:323:THR:HG23	1.78	0.47
1:A:312:LEU:HB3	1:A:323:THR:HA	1.96	0.47
1:A:896:THR:OG1	1:A:898:ASP:OD1	2.25	0.47
4:N:580:ARG:HA	4:N:583:ASN:HD22	1.79	0.47
1:A:534:VAL:HG22	1:A:865:VAL:HB	1.96	0.47
1:A:951:GLU:HG2	1:A:952:LEU:HG	1.96	0.47
5:O:611:LEU:HD21	5:O:659:ILE:HG12	1.96	0.47
1:A:693:GLN:O	1:A:755:TRP:NE1	2.45	0.47
2:D:120:LEU:HD13	3:E:60:A:H61	1.78	0.47
2:D:251:GLU:HG3	3:E:54:A:H62	1.79	0.47
2:H:41:TYR:OH	2:H:110:ARG:NH1	2.47	0.47
2:H:269:HIS:CE1	2:H:293:ARG:HH11	2.32	0.47
2:H:333:VAL:HA	2:H:337:LYS:HB3	1.96	0.47
2:H:130:ILE:HG22	2:H:133:LEU:HD21	1.96	0.47
4:N:282:LYS:HG3	4:N:284:ILE:H	1.79	0.47
1:A:531:ASN:HA	1:A:534:VAL:HG12	1.96	0.47
1:A:622:PHE:O	1:A:626:LEU:CB	2.62	0.47
2:F:79:LEU:HD22	2:H:391:PRO:HD3	1.96	0.47
2:H:328:ASN:N	2:H:363:GLY:O	2.38	0.47
2:D:385:GLN:NE2	2:D:386:ILE:O	2.48	0.47
2:H:113:TRP:HB2	2:H:153:LEU:HG	1.96	0.47
4:N:531:SER:OG	4:N:533:ASN:OD1	2.30	0.47
5:O:559:GLN:HA	5:O:562:THR:HG22	1.97	0.47
1:A:207:LEU:HD21	1:A:212:LEU:HD12	1.97	0.47
1:A:369:GLY:HA3	4:N:638:ASN:HD22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:LEU:HD11	1:A:828:LEU:HB2	1.96	0.47
1:A:904:GLY:N	1:A:1009:GLY:O	2.48	0.47
5:O:606:LYS:HA	5:O:609:ILE:HD12	1.95	0.47
1:A:312:LEU:HB3	1:A:324:TRP:H	1.80	0.47
2:D:139:ASN:O	2:D:143:TYR:CB	2.63	0.46
3:E:19:A:C8	2:H:293:ARG:HB2	2.50	0.46
5:O:399:ASN:ND2	5:O:519:ASP:OD2	2.46	0.46
2:H:158:ALA:HB3	2:H:166:LYS:H	1.79	0.46
2:D:135:PRO:O	2:D:165:SER:OG	2.33	0.46
5:O:409:LEU:HD13	5:O:479:LEU:HD11	1.97	0.46
1:A:348:ASN:O	4:N:635:ARG:NH1	2.49	0.46
1:A:672:SER:HA	1:A:736:SER:HB3	1.96	0.46
1:A:945:ILE:HD12	1:A:954:GLY:HA2	1.98	0.46
2:D:334:ASP:H	2:D:337:LYS:HB3	1.80	0.46
2:D:252:LYS:HZ1	2:D:260:GLY:H	1.63	0.46
1:A:649:GLY:HA3	1:A:669:LEU:HG	1.96	0.46
1:A:700:GLU:OE2	1:A:772:ARG:NH1	2.49	0.46
2:D:173:PHE:HB3	2:D:179:ALA:HB2	1.97	0.46
2:H:119:SER:O	2:H:123:LYS:CB	2.64	0.46
2:H:274:LYS:O	2:H:278:ALA:CB	2.59	0.46
5:O:295:VAL:HG13	5:O:312:LYS:HB3	1.98	0.46
1:A:31:GLU:HB3	1:A:49:SER:HB2	1.97	0.46
1:A:643:THR:O	1:A:647:CYS:HB2	2.16	0.46
1:A:972:LEU:O	1:A:976:SER:N	2.45	0.46
2:D:67:ILE:HG12	2:D:84:VAL:HG22	1.98	0.46
2:H:157:ILE:HB	2:H:159:THR:HG23	1.97	0.46
5:O:384:LEU:HG	5:O:434:ILE:HD11	1.97	0.46
3:E:7:A:H5"	2:H:328:ASN:ND2	2.31	0.46
2:H:273:VAL:HA	2:H:293:ARG:HH22	1.80	0.46
4:N:577:ARG:NH1	4:N:641:ASP:OD2	2.44	0.46
1:A:1016:GLY:N	1:A:1035:ASP:OD1	2.48	0.46
4:N:619:GLN:NE2	4:N:628:MET:O	2.48	0.46
2:H:67:ILE:HG12	2:H:84:VAL:HG13	1.97	0.46
2:H:223:VAL:HB	2:H:226:ILE:HD11	1.98	0.46
2:H:333:VAL:HG22	2:H:337:LYS:HG2	1.98	0.46
2:D:247:SER:H	2:D:265:ASN:HB2	1.81	0.45
3:E:2:A:H62	2:F:198:VAL:HG13	1.81	0.45
5:O:637:LEU:O	5:O:641:ASP:HB2	2.16	0.45
2:D:252:LYS:O	3:E:54:A:N6	2.49	0.45
2:H:314:GLU:OE2	2:H:318:LYS:NZ	2.49	0.45
2:H:356:THR:N	2:H:360:LYS:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:323:ASN:OD1	2:H:324:LEU:N	2.50	0.45
5:O:404:ILE:HG12	5:O:554:VAL:HG13	1.98	0.45
1:A:126:SER:HB2	1:A:129:ASN:HD22	1.82	0.45
1:A:168:ASN:HD22	1:A:210:ASN:H	1.64	0.45
1:A:1036:THR:HA	1:A:1039:TYR:HD2	1.81	0.45
1:A:435:LYS:HE2	1:A:435:LYS:HB3	1.81	0.45
1:A:627:LEU:HD23	1:A:630:LEU:HD12	1.97	0.45
1:A:677:GLY:HA3	1:A:741:LEU:HD13	1.98	0.45
2:D:43:GLY:O	2:D:109:CYS:HA	2.17	0.45
2:H:315:LYS:HE3	2:H:399:ARG:HH21	1.82	0.45
1:A:340:MET:HA	4:N:647:LYS:HZ3	1.81	0.45
1:A:893:LYS:O	1:A:946:ARG:NH2	2.39	0.45
2:D:326:VAL:HG21	2:D:338:LEU:HD21	1.98	0.45
4:N:270:ASN:HA	4:N:273:ILE:HD12	1.99	0.45
1:A:125:HIS:HE1	1:A:130:ASN:HB2	1.82	0.45
1:A:226:ALA:HB3	1:A:256:GLY:HA2	1.99	0.45
1:A:655:ARG:HG2	1:A:665:THR:HG22	1.99	0.45
2:H:137:ILE:HG23	2:H:141:ALA:HB3	1.99	0.45
1:A:68:GLY:HA3	1:A:94:HIS:CG	2.53	0.45
1:A:80:SER:O	1:A:122:TYR:OH	2.34	0.45
2:H:307:GLN:NE2	2:H:311:TYR:OH	2.41	0.45
1:A:176:ARG:NH1	1:A:182:ASP:OD2	2.49	0.44
1:A:764:ILE:HB	1:A:782:SER:HB3	1.99	0.44
1:A:414:ILE:HG12	1:A:427:PRO:HB2	2.00	0.44
2:H:189:MET:HG2	2:H:190:LEU:H	1.82	0.44
1:A:675:ILE:HD11	1:A:737:LEU:HD22	1.98	0.44
1:A:820:LYS:HE3	1:A:822:LEU:HD11	1.98	0.44
1:A:917:GLN:N	1:A:969:GLU:OE1	2.51	0.44
2:D:324:LEU:HD13	2:D:395:ALA:HA	1.99	0.44
2:H:355:ARG:HG2	2:H:361:SER:HB3	1.98	0.44
5:O:409:LEU:HA	5:O:412:VAL:HG12	1.99	0.44
1:A:295:HIS:NE2	1:A:298:GLN:O	2.51	0.44
1:A:593:GLU:O	1:A:597:GLU:N	2.48	0.44
1:A:825:ASN:HB3	1:A:828:LEU:HB3	2.00	0.44
2:H:128:ILE:H	2:H:172:HIS:HB2	1.82	0.44
4:N:614:ASP:O	4:N:618:HIS:N	2.49	0.44
1:A:745:GLU:HA	1:A:748:ASN:HD22	1.82	0.44
2:H:333:VAL:HG13	2:H:337:LYS:HB3	2.00	0.44
5:O:296:PRO:HA	5:O:311:PHE:HA	1.99	0.44
1:A:68:GLY:O	1:A:105:ASN:ND2	2.39	0.44
2:D:316:MET:HA	2:D:319:TYR:HD2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:CYS:HA	1:A:67:ARG:HG2	2.00	0.44
2:D:281:ASP:HA	2:D:291:VAL:HB	1.99	0.44
2:H:273:VAL:HG23	2:H:293:ARG:HH12	1.83	0.43
5:O:580:ARG:HA	5:O:583:ASN:HD22	1.82	0.43
3:E:8:A:N7	2:F:68:ARG:HB3	2.33	0.43
1:A:55:SER:OG	1:A:64:THR:OG1	2.27	0.43
2:D:299:GLU:HA	2:D:305:LYS:HE3	2.00	0.43
2:D:348:ILE:HA	2:D:368:CYS:HB2	2.00	0.43
3:E:37:A:H5"	2:H:118:PRO:HG3	2.00	0.43
2:F:164:LYS:NZ	2:F:165:SER:O	2.50	0.43
4:N:266:LEU:HD23	4:N:269:LYS:HD3	2.01	0.43
2:D:304:LEU:O	2:D:308:TYR:HB2	2.18	0.43
5:O:338:LYS:HA	5:O:341:LYS:HE3	2.01	0.43
2:H:131:LYS:NZ	2:H:202:LEU:O	2.40	0.43
1:A:945:ILE:HA	1:A:956:PRO:HA	1.99	0.43
3:E:9:A:OP1	2:H:393:TYR:OH	2.37	0.43
3:E:37:A:H1'	3:E:38:A:H2'	2.01	0.43
4:N:485:ASN:O	4:N:489:ASN:HB2	2.19	0.43
1:A:760:PHE:HE2	1:A:771:LEU:HD22	1.83	0.43
1:A:977:GLY:HA3	1:A:1066:HIS:HB2	2.01	0.43
1:A:992:LEU:HD22	1:A:998:VAL:HG13	2.00	0.43
2:F:43:GLY:H	2:F:110:ARG:HD2	1.82	0.43
2:H:133:LEU:O	2:H:194:GLN:NE2	2.52	0.43
4:N:343:TYR:O	4:N:347:SER:CB	2.66	0.43
5:O:611:LEU:HD12	5:O:652:THR:HB	2.00	0.43
1:A:657:GLU:HB3	1:A:723:THR:HG23	2.00	0.43
3:E:65:A:H1'	3:E:66:A:H5"	2.01	0.43
4:N:297:LEU:N	4:N:310:LEU:O	2.52	0.43
4:N:600:TRP:HE3	4:N:610:ILE:HD11	1.84	0.43
2:H:153:LEU:HD13	2:H:174:GLU:HA	1.99	0.43
4:N:426:THR:HG21	4:N:446:CYS:H	1.84	0.43
1:A:388:SER:O	5:O:635:ARG:NH2	2.52	0.42
1:A:757:THR:HG21	1:A:760:PHE:HB3	2.00	0.42
1:A:824:PHE:HE1	1:A:829:VAL:HG13	1.84	0.42
2:D:71:ARG:HA	2:D:78:SER:HA	2.01	0.42
2:D:112:MET:HG2	2:D:153:LEU:HD23	2.00	0.42
3:E:4:A:N6	2:H:331:ASP:OD2	2.50	0.42
2:H:101:TYR:HE1	2:H:110:ARG:HB2	1.84	0.42
2:H:324:LEU:O	2:H:366:PHE:HA	2.19	0.42
4:N:291:TYR:HB3	4:N:313:VAL:HG11	2.01	0.42
1:A:482:LEU:HD23	1:A:482:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:101:TYR:HB3	2:D:108:LEU:HB3	2.01	0.42
2:F:186:LEU:HD13	2:F:189:MET:HB3	2.01	0.42
1:A:166:CYS:N	1:A:173:SER:OG	2.49	0.42
1:A:344:PRO:HA	4:N:647:LYS:HE3	2.00	0.42
1:A:835:GLU:O	1:A:839:LYS:N	2.52	0.42
1:A:952:LEU:HD22	1:A:955:VAL:HG11	2.01	0.42
2:F:134:HIS:HD1	2:F:136:ASP:H	1.68	0.42
2:H:69:VAL:HA	2:H:82:ALA:HB1	2.01	0.42
2:H:210:GLN:HA	2:H:213:GLU:HB2	2.00	0.42
4:N:325:LYS:O	4:N:372:CYS:HA	2.18	0.42
2:D:293:ARG:NH2	3:E:49:A:H5"	2.34	0.42
5:O:549:ASP:N	5:O:549:ASP:OD1	2.53	0.42
1:A:274:SER:OG	1:A:275:SER:N	2.52	0.42
2:D:112:MET:HB3	2:D:113:TRP:H	1.72	0.42
5:O:679:GLN:OE1	5:O:682:HIS:N	2.44	0.42
1:A:47:GLY:HA3	1:A:75:VAL:HG11	2.02	0.42
1:A:577:LEU:HG	1:A:581:ARG:HH22	1.85	0.42
5:O:398:THR:OG1	5:O:399:ASN:N	2.50	0.42
1:A:834:GLU:O	1:A:838:LEU:N	2.49	0.42
1:A:914:VAL:HG22	1:A:940:ALA:HB2	2.01	0.42
2:D:134:HIS:HB2	2:D:194:GLN:HB3	2.02	0.42
3:E:23:A:N1	2:H:261:PHE:HB2	2.34	0.42
3:E:37:A:H62	2:H:114:SER:HB2	1.84	0.42
2:H:242:PHE:HD2	2:H:279:LEU:HD11	1.85	0.42
2:H:308:TYR:O	2:H:311:TYR:HB2	2.20	0.42
1:A:207:LEU:HD22	1:A:235:LEU:HD11	2.01	0.42
1:A:853:CYS:SG	1:A:854:ASP:N	2.93	0.42
5:O:394:LYS:HZ2	5:O:496:ASN:HA	1.85	0.41
5:O:475:ASP:OD1	5:O:476:TYR:N	2.53	0.41
1:A:440:ASN:HA	5:O:615:TYR:HD1	1.84	0.41
1:A:854:ASP:HB3	1:A:857:GLU:HB2	2.01	0.41
1:A:1099:TYR:HB3	1:A:1103:ARG:HH12	1.84	0.41
4:N:473:GLN:HE22	4:N:538:LYS:H	1.67	0.41
5:O:400:ASN:OD1	5:O:401:TYR:N	2.47	0.41
1:A:916:LEU:HG	1:A:968:ILE:HA	2.02	0.41
1:A:1019:ASN:HD22	1:A:1022:LYS:HD2	1.85	0.41
2:F:134:HIS:HB3	2:F:137:ILE:HG13	2.02	0.41
4:N:608:PRO:HA	4:N:611:LEU:HD13	2.02	0.41
2:F:128:ILE:HG13	2:F:130:ILE:HD11	2.01	0.41
1:A:556:MET:SD	1:A:1027:ASN:ND2	2.94	0.41
3:E:5:A:H1'	2:F:41:TYR:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:40:LEU:O	2:H:83:TYR:HA	2.21	0.41
2:H:354:MET:HB3	2:H:364:PHE:CZ	2.56	0.41
4:N:343:TYR:O	4:N:347:SER:HB3	2.20	0.41
1:A:201:SER:HB3	1:A:217:LYS:HG2	2.02	0.41
3:E:12:A:N1	2:F:114:SER:OG	2.50	0.41
2:H:61:ILE:HG22	2:H:91:ALA:HB1	2.01	0.41
4:N:311:PHE:O	4:N:323:VAL:HA	2.21	0.41
4:N:575:ASN:O	4:N:579:PHE:N	2.48	0.41
5:O:421:LEU:O	5:O:472:GLN:NE2	2.34	0.41
1:A:171:VAL:HG21	1:A:235:LEU:HD22	2.01	0.41
2:D:44:ASP:HB3	2:D:107:ARG:HB3	2.02	0.41
2:H:69:VAL:HG12	2:H:71:ARG:HG3	2.03	0.41
4:N:326:ARG:CZ	4:N:328:PRO:HG3	2.51	0.41
1:A:260:VAL:HG22	1:A:272:VAL:HG13	2.03	0.41
1:A:770:VAL:HG11	1:A:778:LEU:HD22	2.03	0.41
1:A:917:GLN:OE1	1:A:936:ARG:N	2.53	0.41
1:A:918:SER:O	1:A:932:ILE:N	2.54	0.41
2:H:135:PRO:HA	2:H:165:SER:HB3	2.03	0.41
2:H:225:ASN:N	2:H:260:GLY:O	2.54	0.41
2:H:356:THR:HB	2:H:360:LYS:H	1.86	0.41
5:O:294:LEU:HD23	5:O:311:PHE:HD2	1.85	0.41
5:O:529:LEU:HD12	5:O:529:LEU:HA	1.92	0.41
5:O:588:ILE:HD11	5:O:674:PHE:HA	2.02	0.41
1:A:556:MET:O	1:A:560:SER:OG	2.27	0.41
1:A:1042:GLN:OE1	1:A:1103:ARG:NH1	2.52	0.41
3:E:8:A:H2'	2:F:83:TYR:CZ	2.56	0.41
2:F:51:GLU:HB3	2:F:54:LEU:HD22	2.02	0.41
1:A:907:VAL:HA	1:A:947:GLY:H	1.86	0.40
2:D:134:HIS:CE1	2:D:136:ASP:HB2	2.56	0.40
2:H:229:GLU:OE1	2:H:285:ASN:ND2	2.54	0.40
1:A:813:ASN:O	1:A:817:ASN:HA	2.21	0.40
1:A:893:LYS:HD2	1:A:955:VAL:HG11	2.04	0.40
2:D:64:VAL:HG22	2:D:86:PHE:HE1	1.86	0.40
2:F:96:ILE:HA	2:F:100:ASN:HB2	2.02	0.40
1:A:198:HIS:CD2	1:A:216:GLY:H	2.39	0.40
2:D:234:GLN:HG2	2:D:284:LEU:HD22	2.03	0.40
2:H:304:LEU:O	2:H:307:GLN:CB	2.61	0.40
1:A:282:ILE:HD11	1:A:287:PRO:HA	2.04	0.40
1:A:439:ARG:HH21	5:O:652:THR:HA	1.87	0.40
2:D:309:GLU:OE2	3:E:47:A:N6	2.55	0.40
4:N:409:LEU:HD13	4:N:479:LEU:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ASN:HD21	1:A:638:VAL:HG22	1.87	0.40
2:D:400:LYS:HD2	2:D:400:LYS:HA	1.91	0.40
4:N:323:VAL:HG13	4:N:377:TYR:HA	2.04	0.40
5:O:603:SER:OG	5:O:604:GLY:N	2.52	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	1030/1115 (92%)	882 (86%)	147 (14%)	1 (0%)	51	85
2	D	388/581 (67%)	332 (86%)	55 (14%)	1 (0%)	41	76
2	F	163/581 (28%)	125 (77%)	38 (23%)	0	100	100
2	H	392/581 (68%)	333 (85%)	58 (15%)	1 (0%)	41	76
4	N	421/458 (92%)	362 (86%)	59 (14%)	0	100	100
5	O	443/689 (64%)	373 (84%)	70 (16%)	0	100	100
All	All	2837/4005 (71%)	2407 (85%)	427 (15%)	3 (0%)	54	85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	199	ALA
2	H	200	PRO
1	A	338	PRO

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	865/1016 (85%)	864 (100%)	1 (0%)	93 96
2	D	300/484 (62%)	300 (100%)	0	100 100
2	F	125/484 (26%)	124 (99%)	1 (1%)	81 89
2	H	312/484 (64%)	312 (100%)	0	100 100
4	N	334/436 (77%)	334 (100%)	0	100 100
5	O	352/641 (55%)	351 (100%)	1 (0%)	92 95
All	All	2288/3545 (64%)	2285 (100%)	3 (0%)	93 96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	421	LEU
2	F	75	THR
5	O	310	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	HIS
1	A	129	ASN
1	A	189	ASN
1	A	196	ASN
1	A	210	ASN
1	A	240	GLN
1	A	541	ASN
1	A	569	ASN
1	A	724	GLN
1	A	748	ASN
1	A	1019	ASN
1	A	1027	ASN
2	D	85	ASN
2	H	85	ASN
2	H	127	ASN
2	H	234	GLN
2	H	285	ASN
2	H	328	ASN

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Mol	Chain	Res	Type
4	N	289	GLN
4	N	353	ASN
4	N	380	ASN
4	N	391	ASN
4	N	445	HIS
4	N	473	GLN
4	N	583	ASN
4	N	638	ASN
5	O	489	ASN
5	O	559	GLN
5	O	575	ASN
5	O	583	ASN
5	O	618	HIS
5	O	638	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	E	66/90 (73%)	58 (87%)	5 (7%)

All (58) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	E	2	A
3	E	4	A
3	E	5	A
3	E	6	A
3	E	7	A
3	E	8	A
3	E	9	A
3	E	10	A
3	E	11	A
3	E	12	A
3	E	13	A
3	E	14	A
3	E	16	A
3	E	17	A
3	E	19	A
3	E	20	A
3	E	21	A
3	E	22	A

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Mol	Chain	Res	Type
3	E	23	A
3	E	24	A
3	E	25	A
3	E	26	A
3	E	28	A
3	E	29	A
3	E	30	A
3	E	31	A
3	E	32	A
3	E	33	A
3	E	34	A
3	E	35	A
3	E	36	A
3	E	37	A
3	E	38	A
3	E	40	A
3	E	41	A
3	E	42	A
3	E	43	A
3	E	44	A
3	E	45	A
3	E	47	A
3	E	48	A
3	E	49	A
3	E	50	A
3	E	51	A
3	E	52	A
3	E	53	A
3	E	54	A
3	E	55	A
3	E	56	A
3	E	57	A
3	E	58	A
3	E	59	A
3	E	61	A
3	E	62	A
3	E	63	A
3	E	65	A
3	E	66	A
3	E	67	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	E	7	A
3	E	48	A
3	E	49	A
3	E	57	A
3	E	64	A

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)

Of 2 ligands modelled in this entry, 2 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.

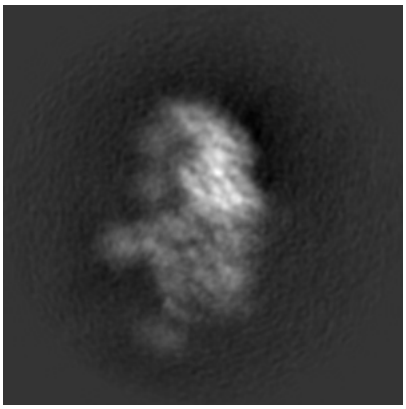
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4728. These allow visual inspection of the internal detail of the map and identification of artifacts.

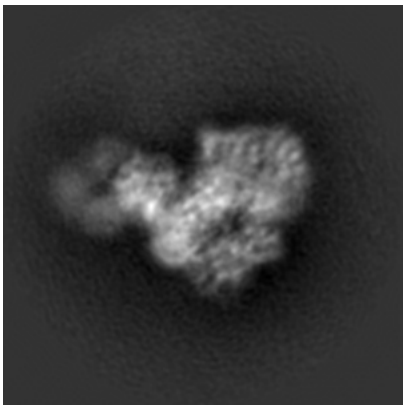
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

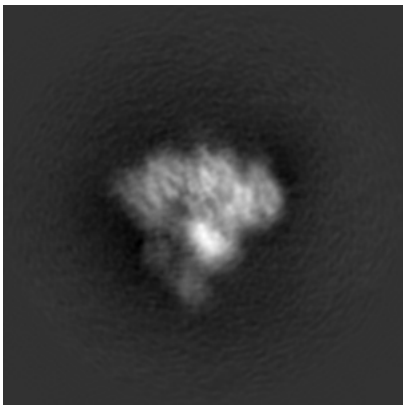
6.1.1 Primary map



X

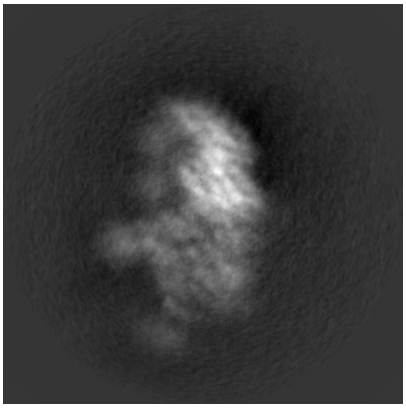


Y

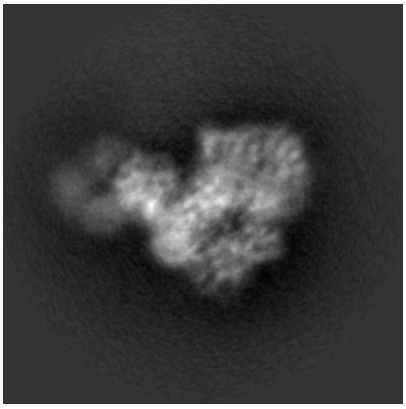


Z

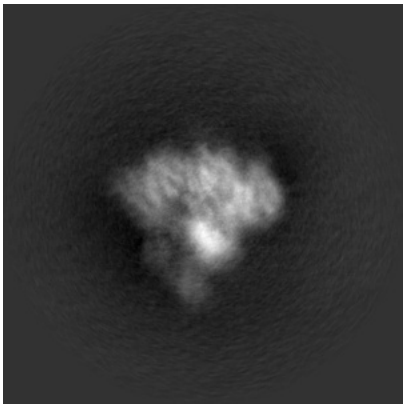
6.1.2 Raw map



X



Y

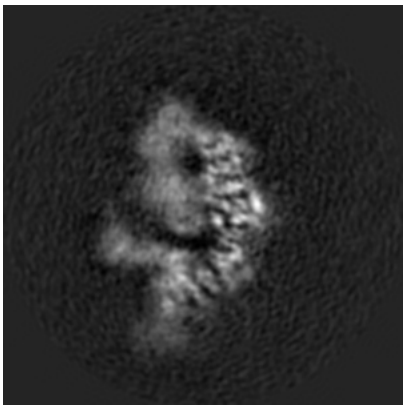


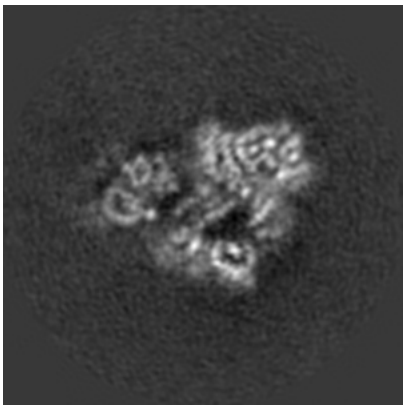
Z

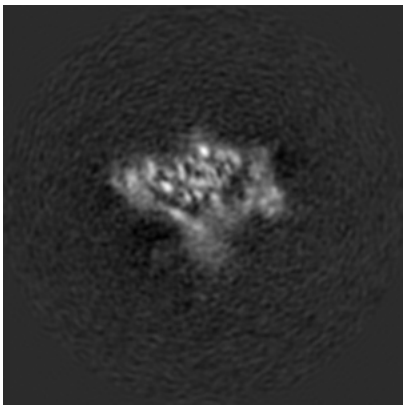
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

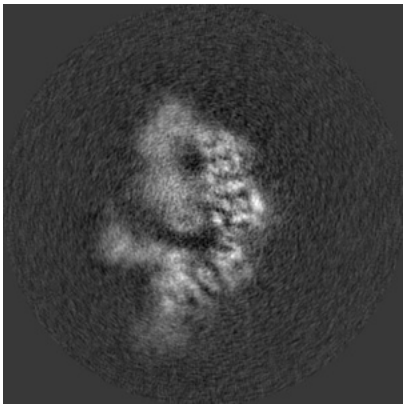
6.2.1 Primary map

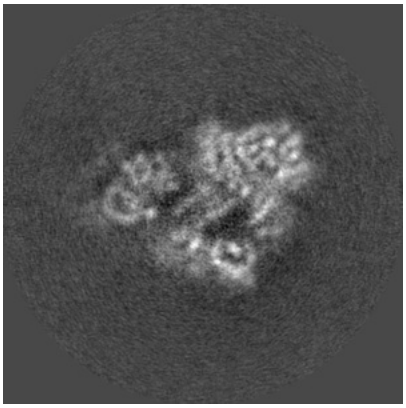

X Index: 144

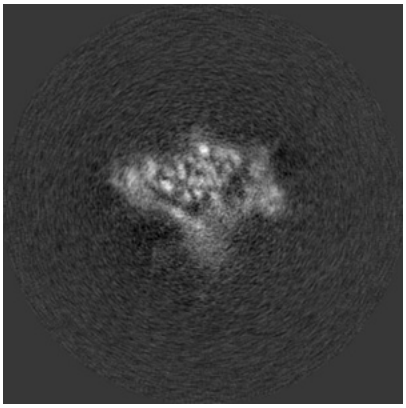

Y Index: 144


Z Index: 144

6.2.2 Raw map


X Index: 144

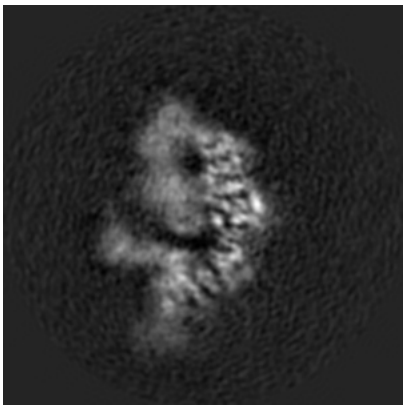

Y Index: 144

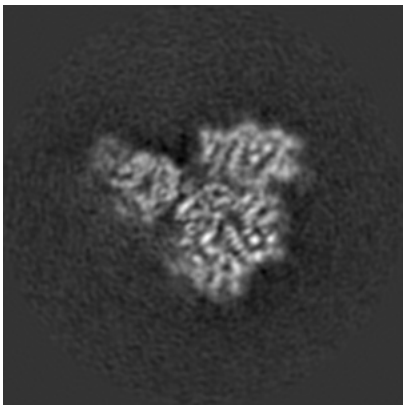

Z Index: 144

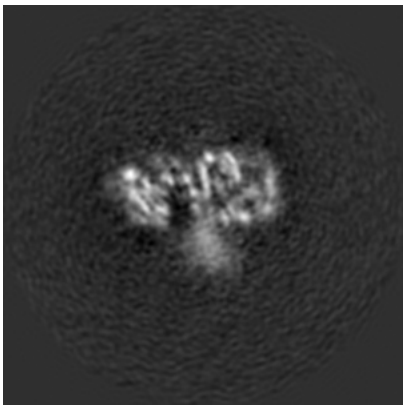
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

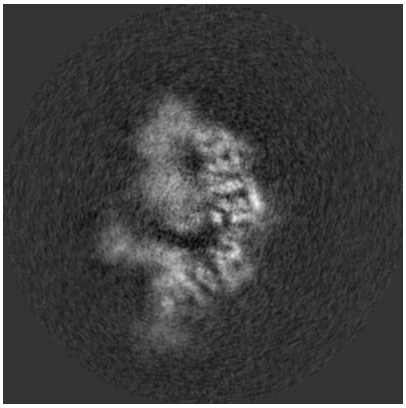
6.3.1 Primary map

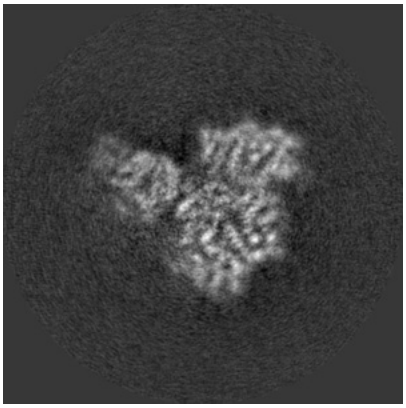

X Index: 144

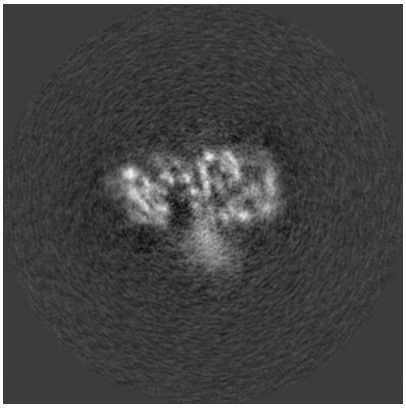

Y Index: 155


Z Index: 156

6.3.2 Raw map


X Index: 145

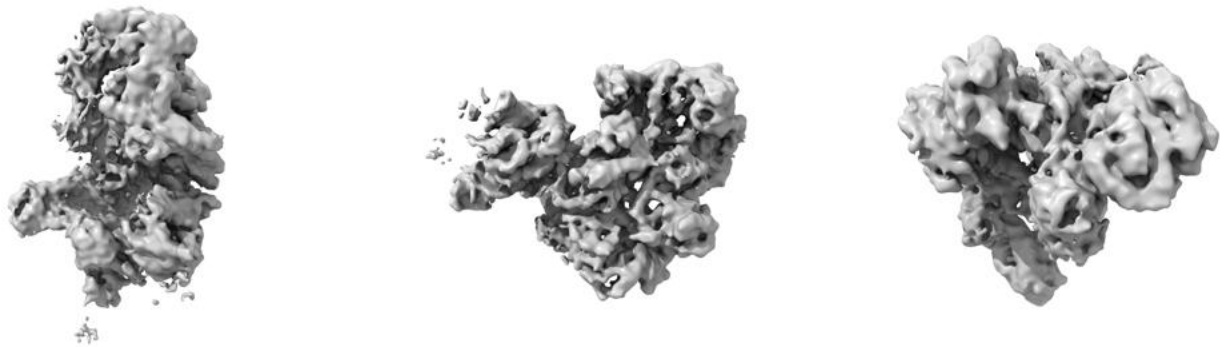

Y Index: 155


Z Index: 156

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

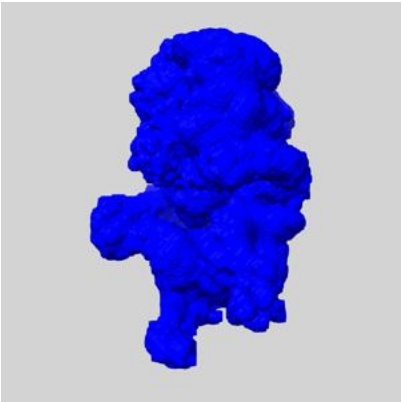
6.5 Mask visualisation (i)

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

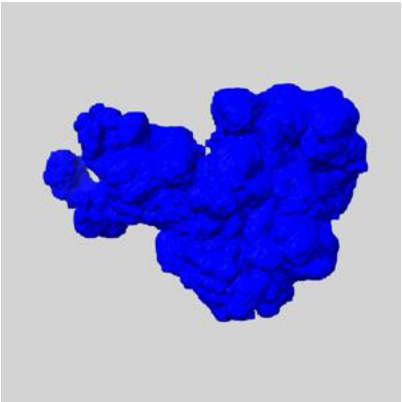
A mask typically either:

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

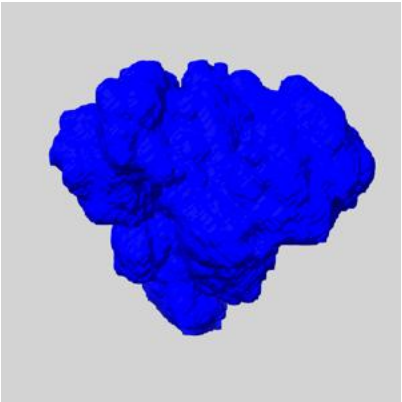
6.5.1 emd_4728_msk_1.map (i)



X



Y

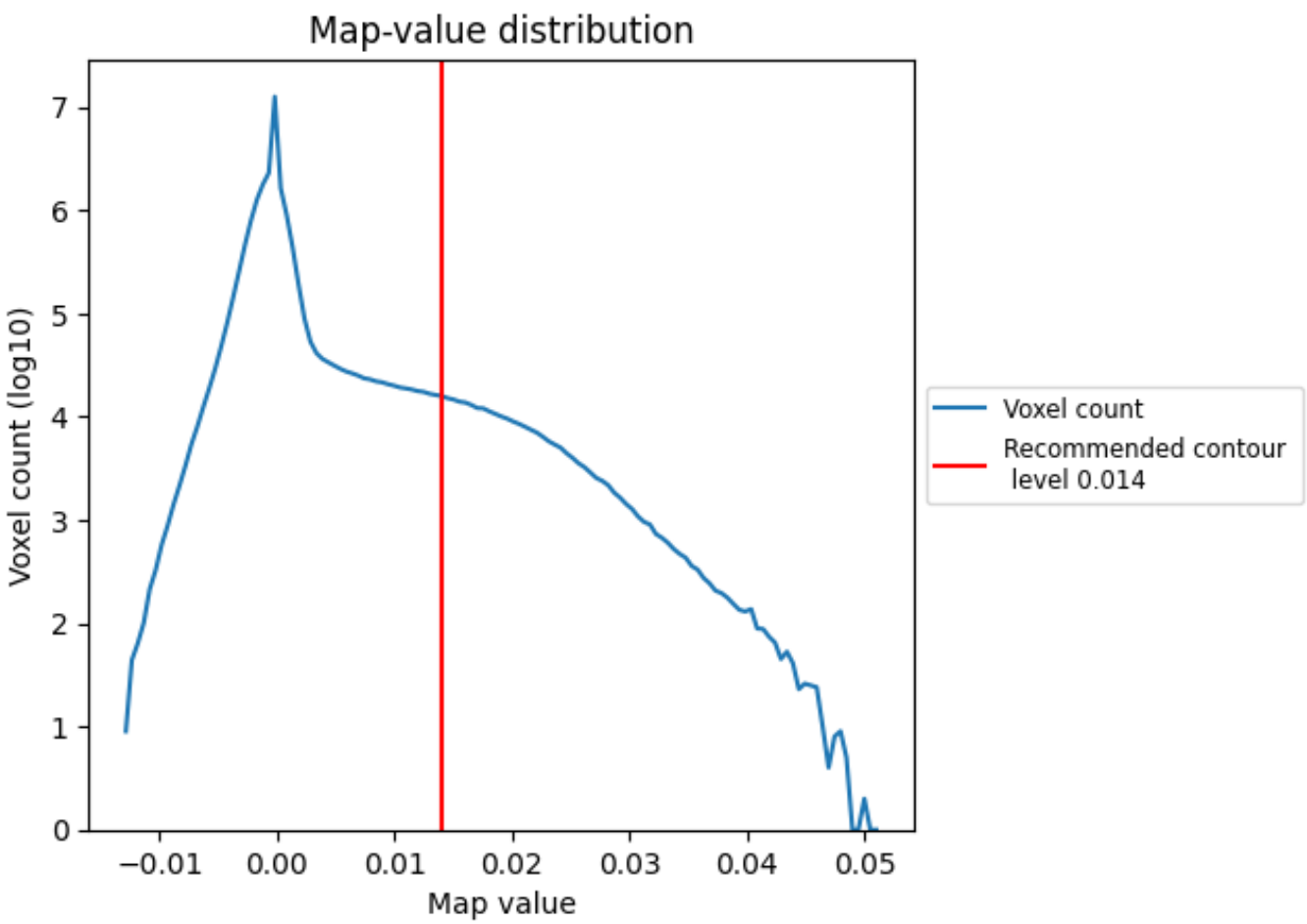


Z

7 Map analysis (i)

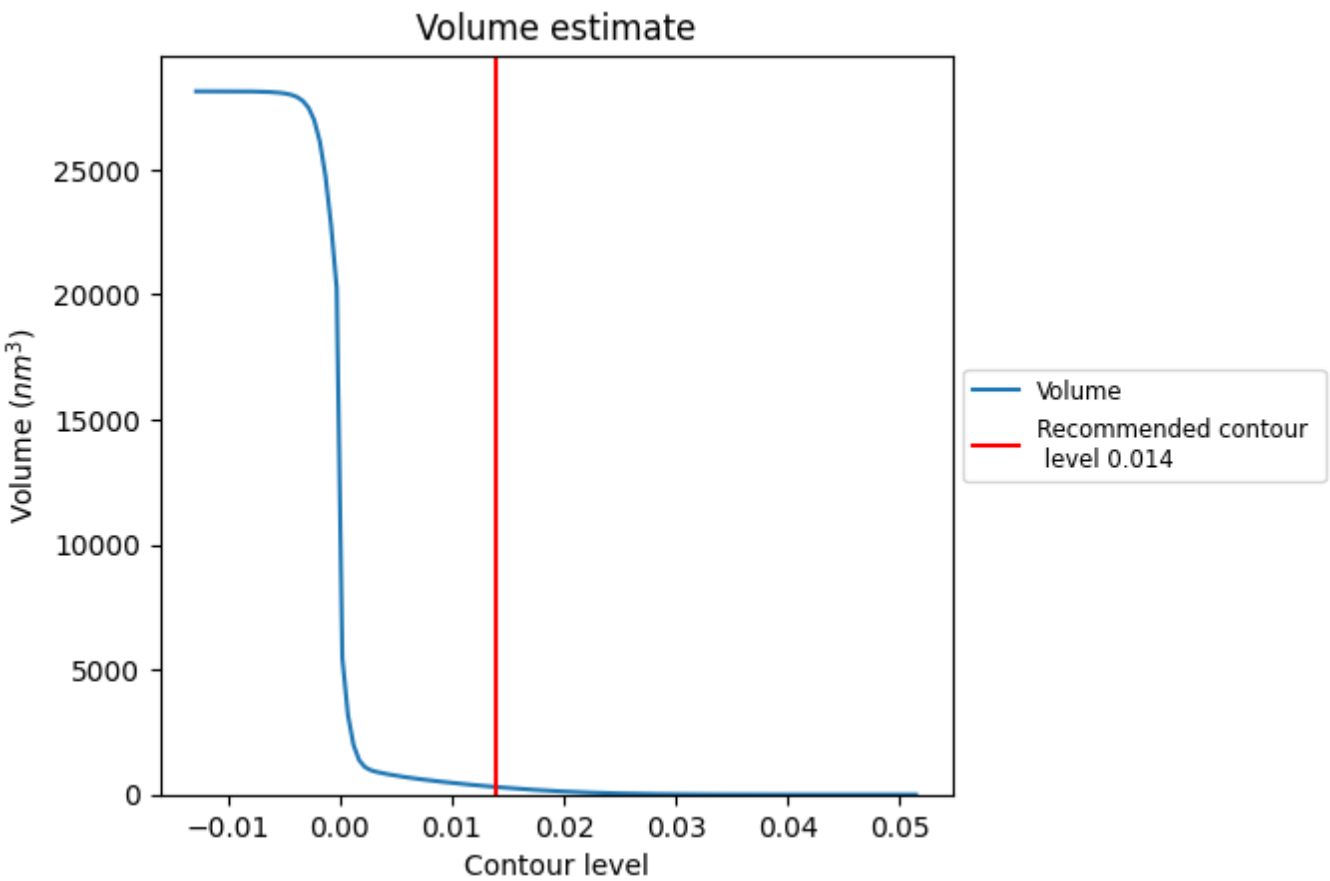
This section contains the results of statistical analysis of the map.

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.

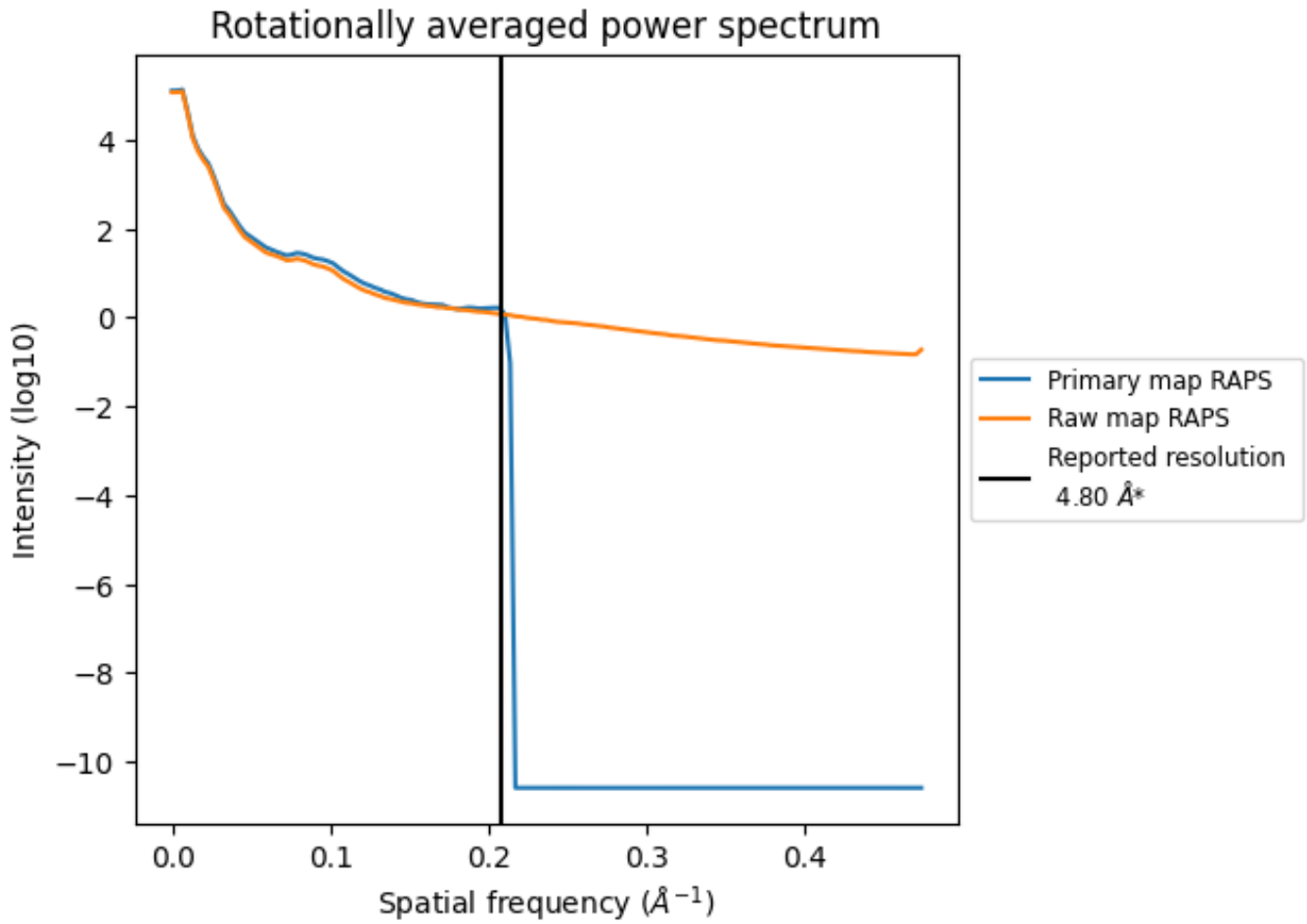
7.2 Volume estimate (i)



The volume at the recommended contour level is 301 nm^3; this corresponds to an approximate mass of 272 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)

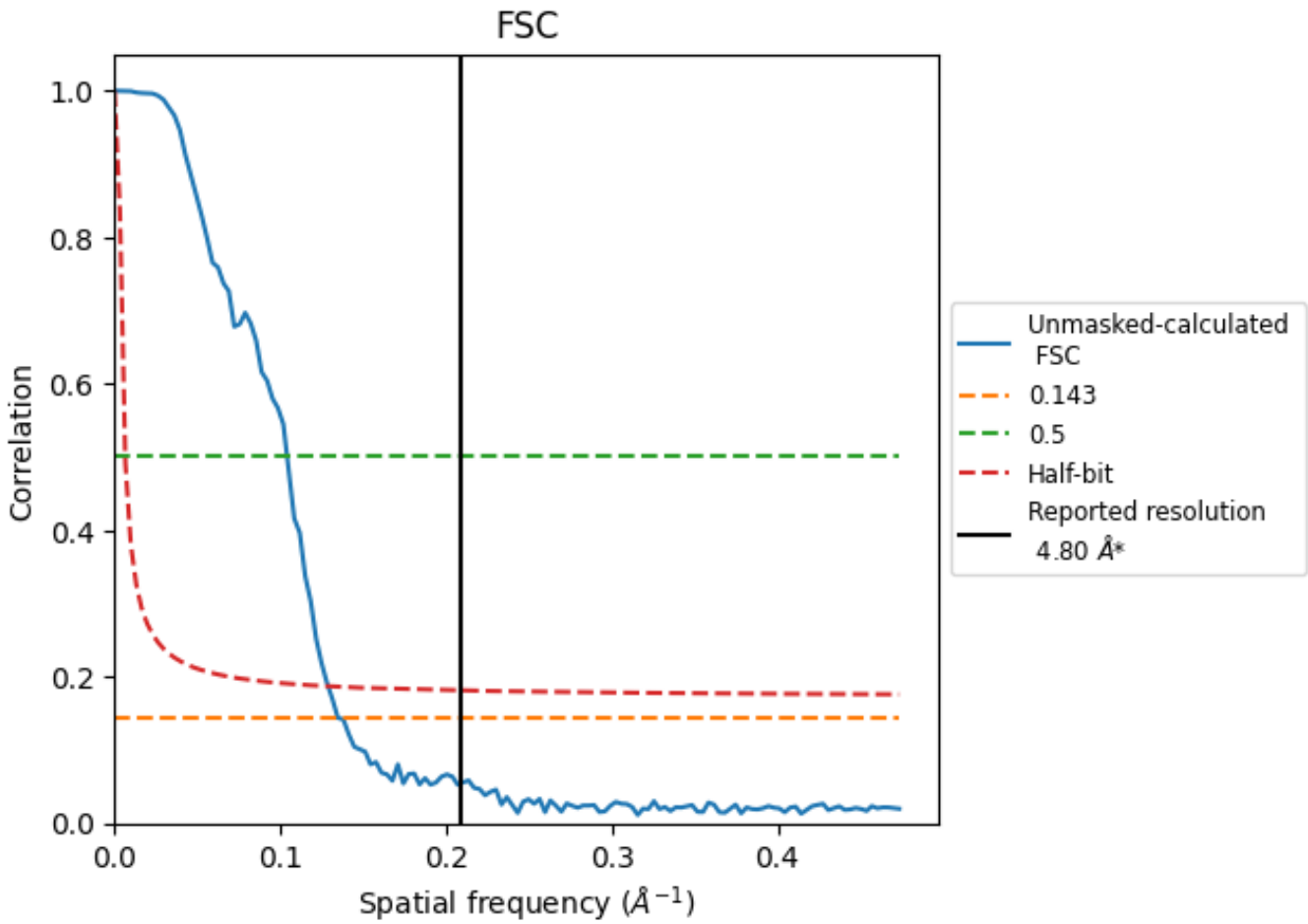


*Reported resolution corresponds to spatial frequency of 0.208 Å^{-1}

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 0.208 Å^{-1}

8.2 Resolution estimates (i)

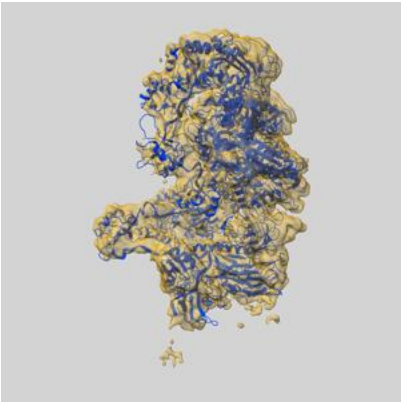
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.38	9.60	7.76

*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 7.38 differs from the reported value 4.8 by more than 10 %

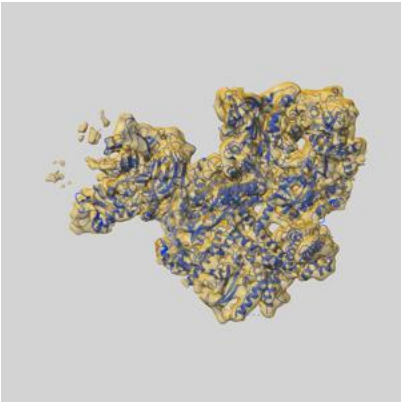
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4728 and PDB model 6R5K. Per-residue inclusion information can be found in section 3 on page 6.

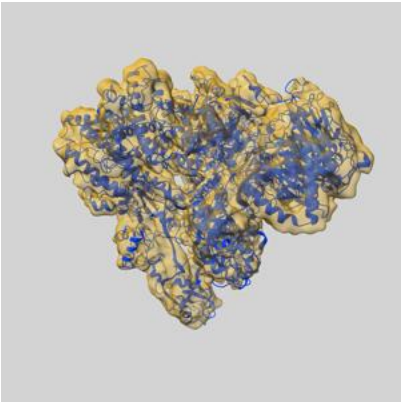
9.1 Map-model overlay (i)



X



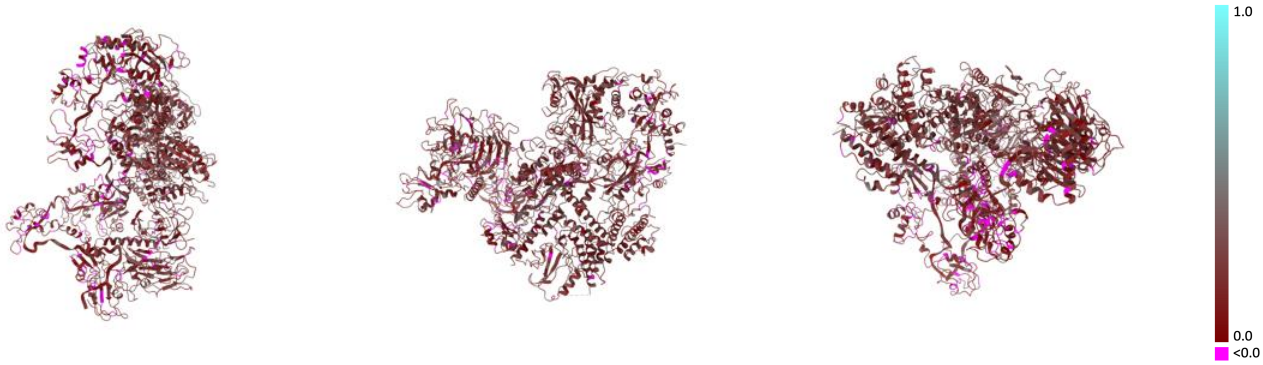
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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.

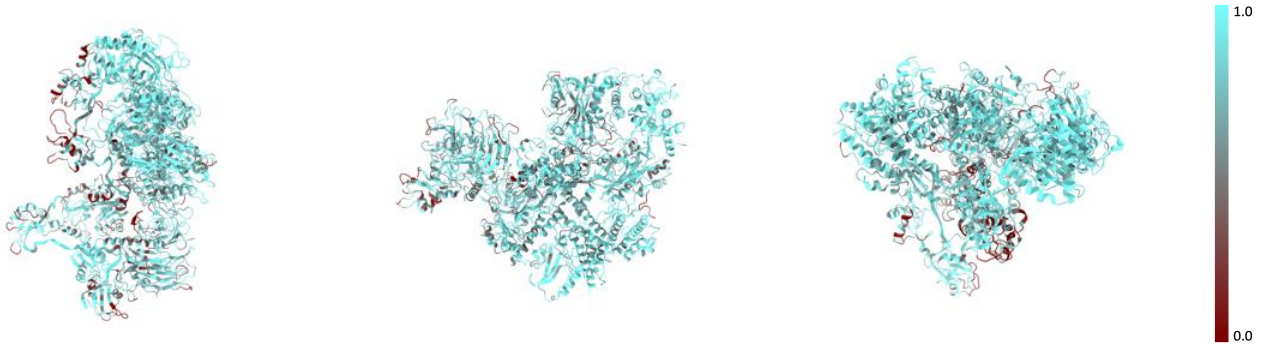
9.2 Q-score mapped to coordinate model (i)



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.

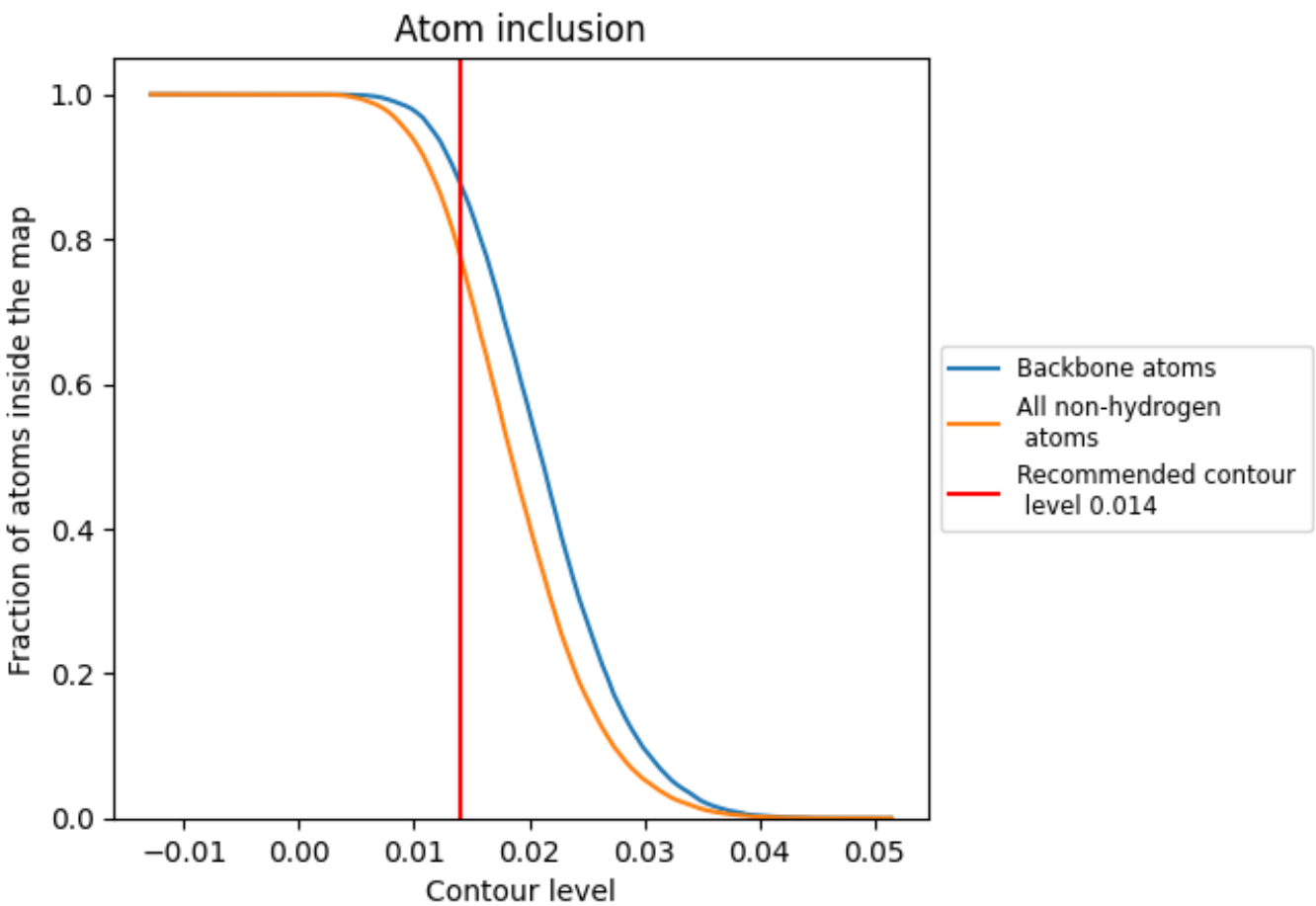
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 78% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7776	0.1970
A	0.8100	0.2180
D	0.6030	0.1240
E	0.8272	0.1770
F	0.6361	0.1800
H	0.7696	0.1440
N	0.8286	0.2420
O	0.8413	0.2330