Full wwPDB EM Validation Report ⓘ

Dec 7, 2022 – 11:39 AM JST

PDB ID	:	6K72
EMDB ID	:	EMD-9841
Title	:	eIF2(aP) - eIF2B complex
Authors	:	Kashiwagi, K.; Yokoyama, T.; Ito, T.
Deposited on	:	2019-06-05
Resolution	:	4.60 Å(reported)

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

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

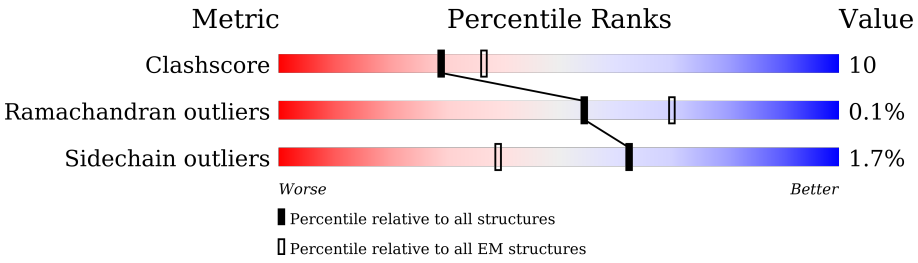
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 4.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
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	305	65% 28% 7%
1	B	305	69% 23% 7%
2	C	351	66% 24% 9%
2	D	351	68% 22% 9%
3	E	452	62% 12% 26%
3	F	452	61% 12% 27%
4	G	523	50% 18% 32%
4	H	523	51% 17% 32%

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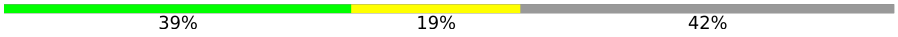
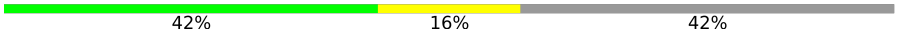
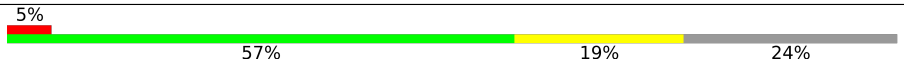
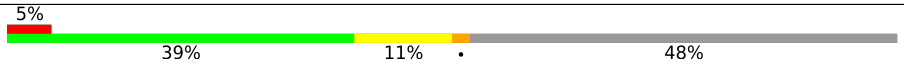
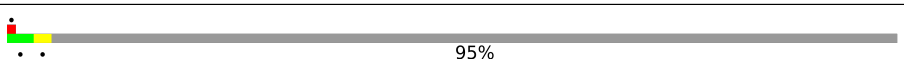
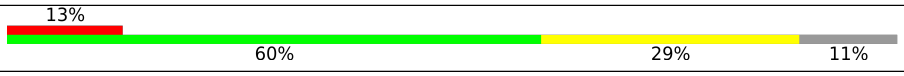
Mol	Chain	Length	Quality of chain
5	I	721	
5	J	721	
6	K	315	
6	L	315	
7	M	333	
8	P	472	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 32731 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 Translation initiation factor eIF-2B subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	285	Total	C	N	O	S	0	0
			2213	1425	368	409	11		
1	B	284	Total	C	N	O	S	0	0
			2204	1419	366	408	11		

- Molecule 2 is a protein called Translation initiation factor eIF-2B subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	318	Total	C	N	O	S	0	0
			2486	1571	438	462	15		
2	D	318	Total	C	N	O	S	0	0
			2486	1571	438	462	15		

- Molecule 3 is a protein called Translation initiation factor eIF-2B subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	333	Total	C	N	O	S	0	0
			2286	1452	394	427	13		
3	F	329	Total	C	N	O	S	0	0
			2255	1432	389	421	13		

- Molecule 4 is a protein called Translation initiation factor eIF-2B subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	357	Total	C	N	O	S	0	0
			2779	1756	495	514	14		
4	H	357	Total	C	N	O	S	0	0
			2779	1756	495	514	14		

- Molecule 5 is a protein called Translation initiation factor eIF-2B subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	421	Total	C	N	O	S	0	0
			3312	2087	585	625	15		
5	J	421	Total	C	N	O	S	0	0
			3312	2087	585	625	15		

- Molecule 6 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	239	Total	C	N	O	S	0	0
			1914	1211	328	365	10		
6	L	165	Total	C	N	O	S	0	0
			1356	860	232	259	5		

- Molecule 7 is a protein called Eukaryotic translation initiation factor 2 subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	16	Total	C	N	O	S	0	0
			145	93	24	27	1		

- Molecule 8 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

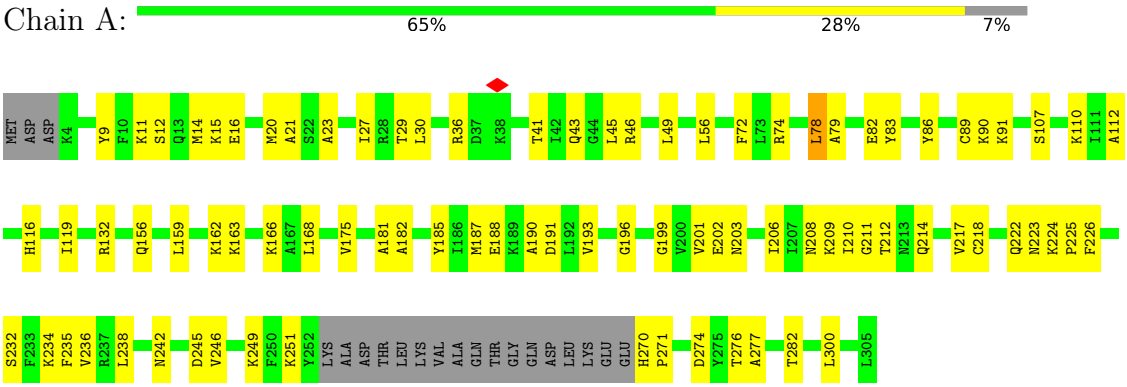
Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	421	Total	C	N	O	S	0	0
			3204	2039	559	589	17		

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.

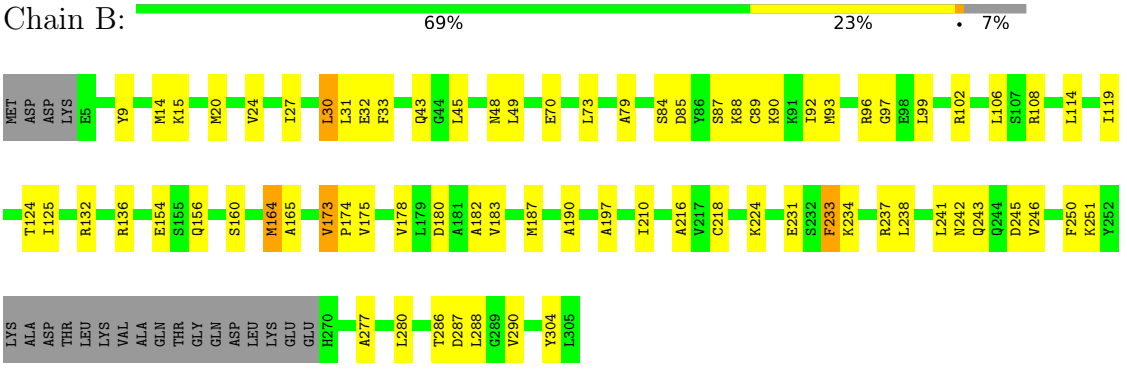
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain A:



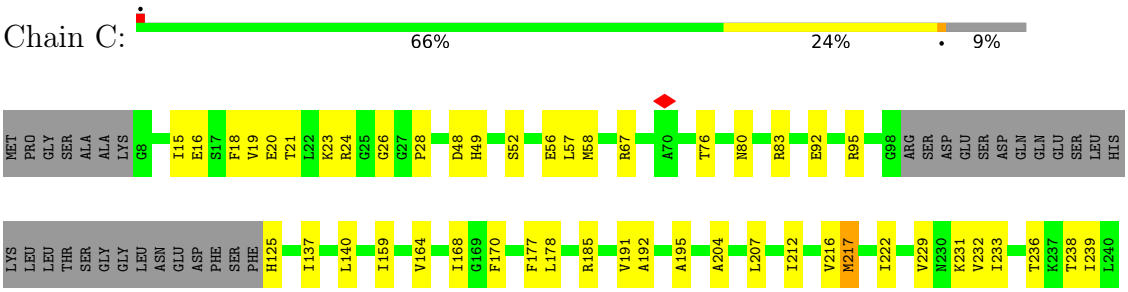
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

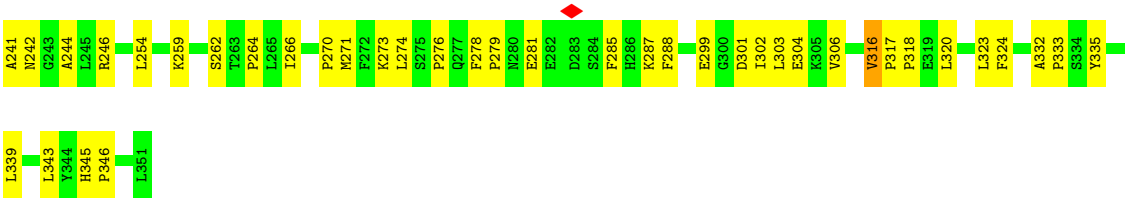
Chain B:



• Molecule 2: Translation initiation factor eIF-2B subunit beta

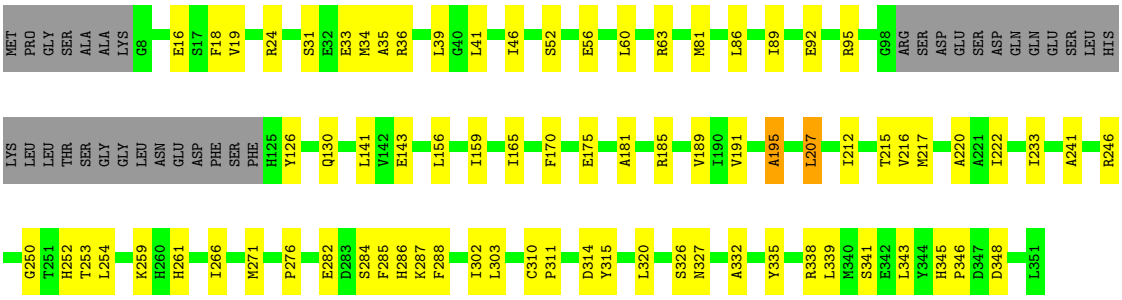
Chain C:





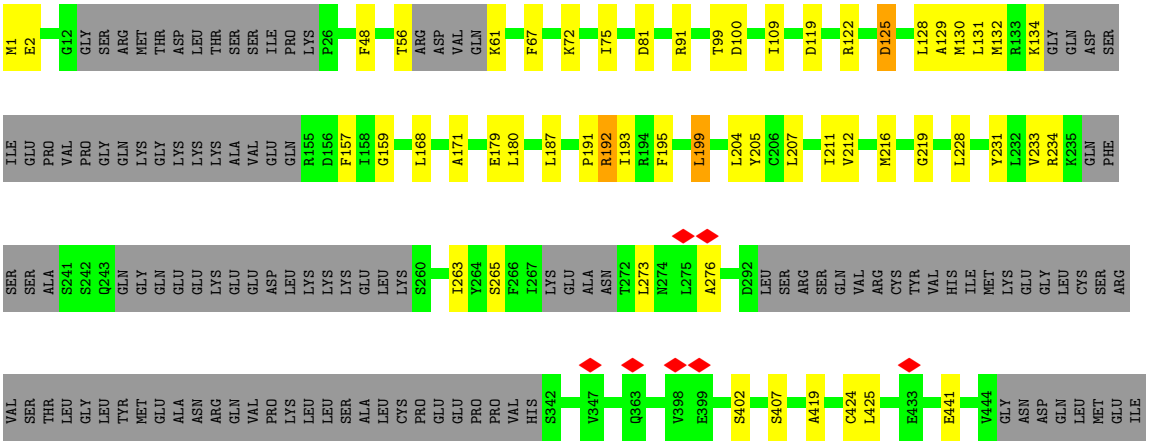
• Molecule 2: Translation initiation factor eIF-2B subunit beta

Chain D:



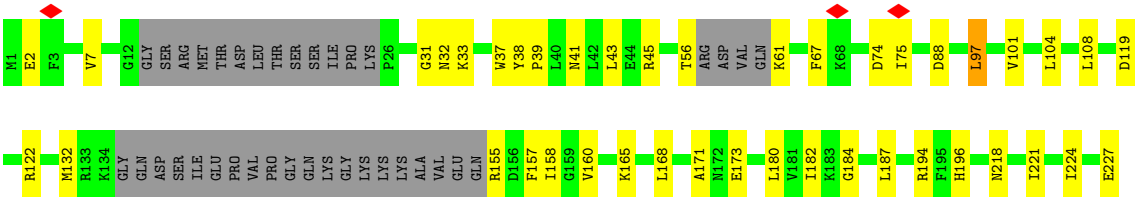
• Molecule 3: Translation initiation factor eIF-2B subunit gamma

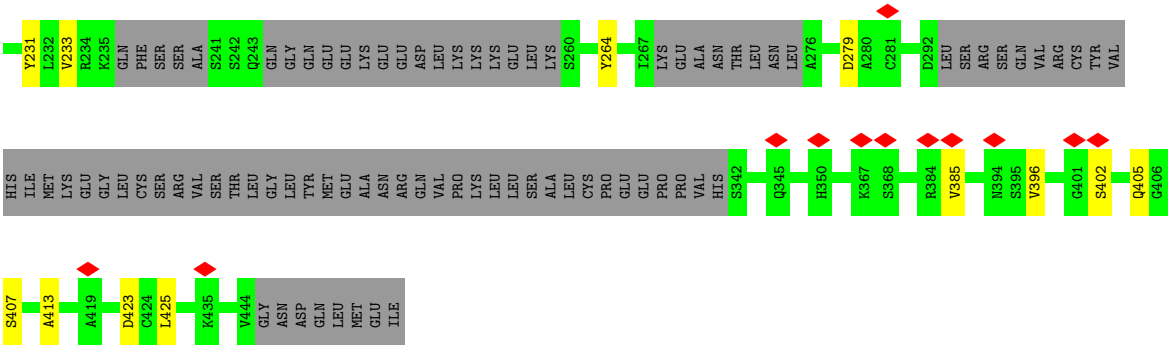
Chain E:



• Molecule 3: Translation initiation factor eIF-2B subunit gamma

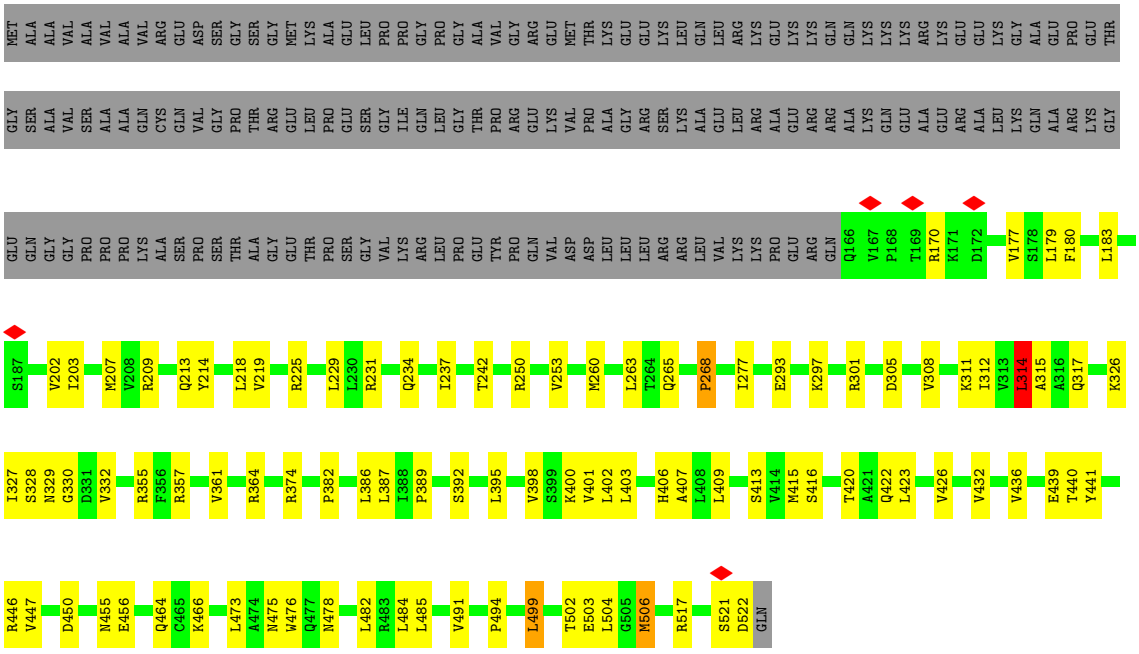
Chain F:





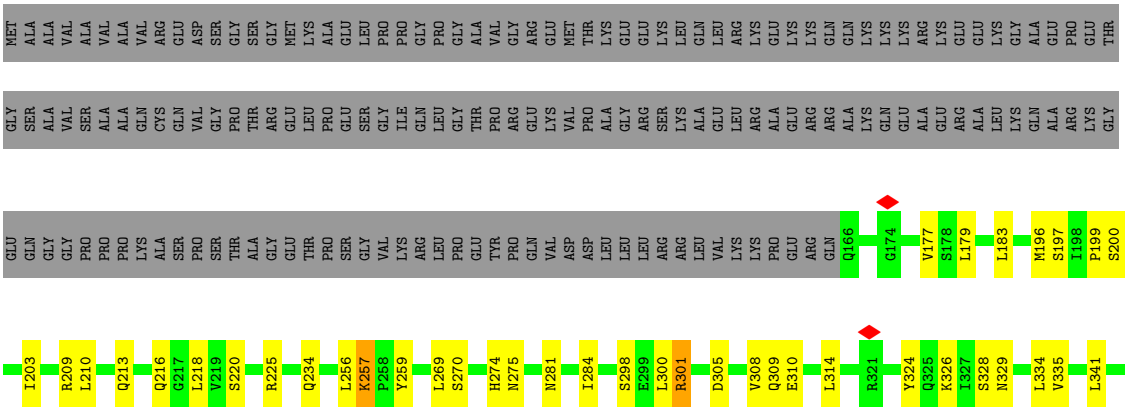
• Molecule 4: Translation initiation factor eIF-2B subunit delta

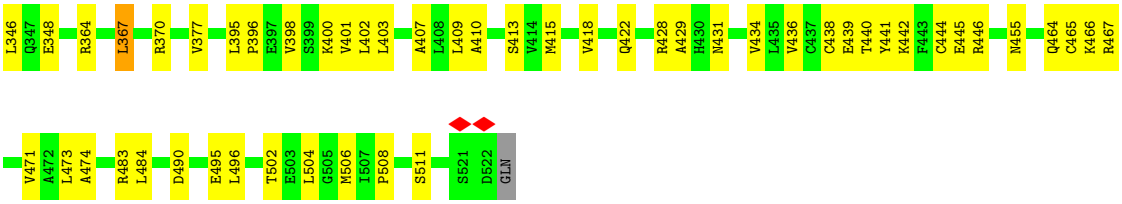
Chain G:



• Molecule 4: Translation initiation factor eIF-2B subunit delta

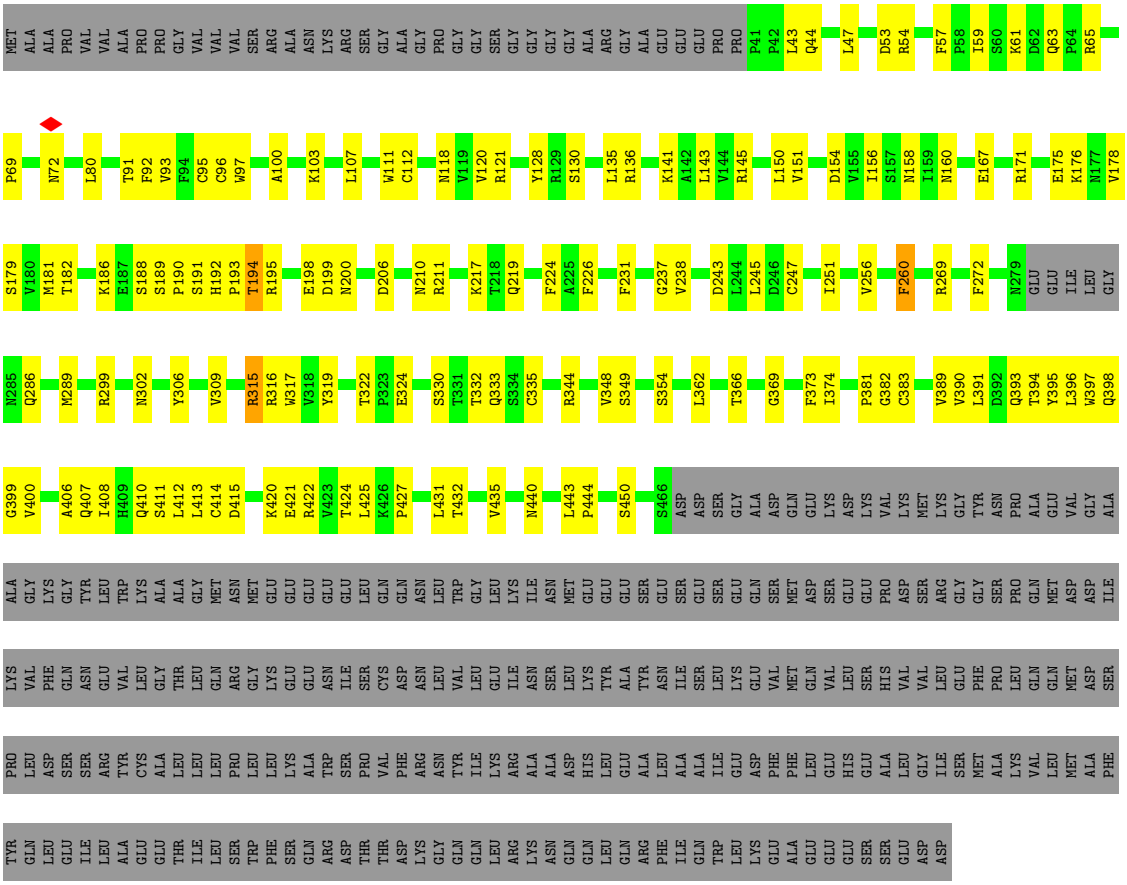
Chain H:





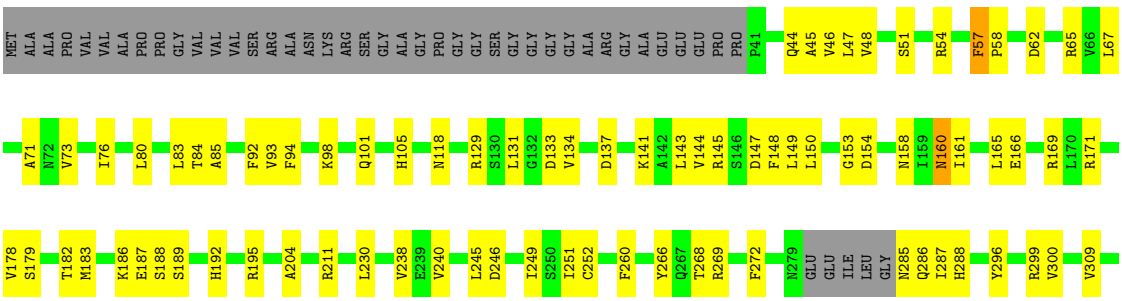
• Molecule 5: Translation initiation factor eIF-2B subunit epsilon

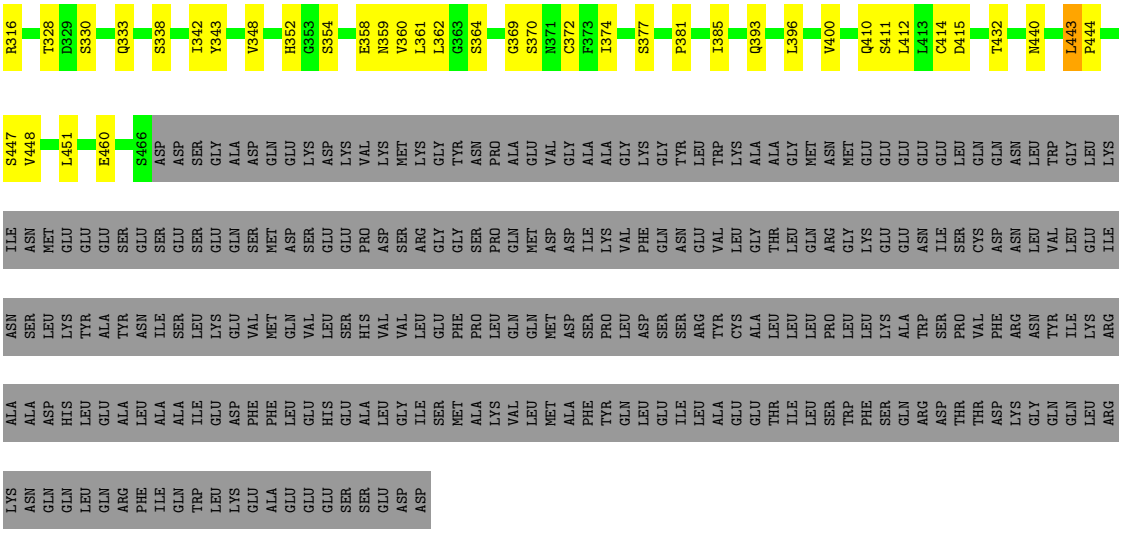
Chain I:



• Molecule 5: Translation initiation factor eIF-2B subunit epsilon

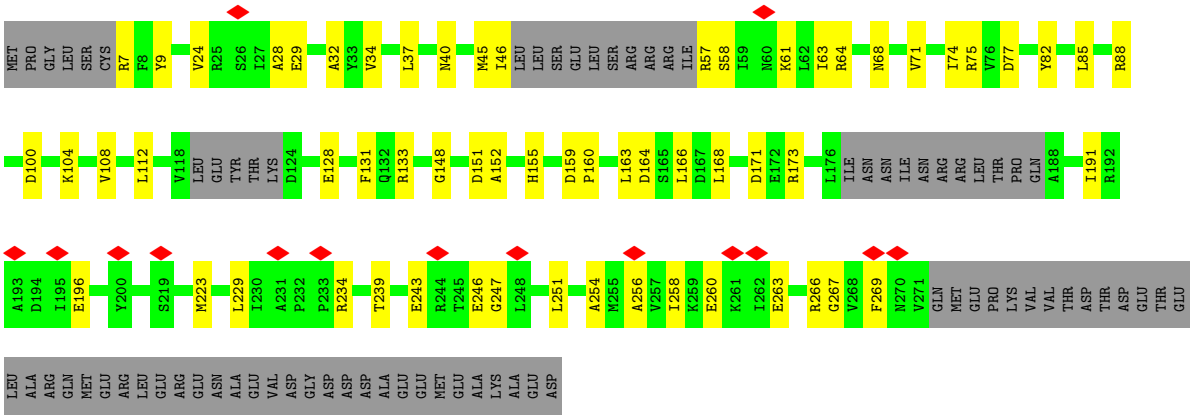
Chain J:





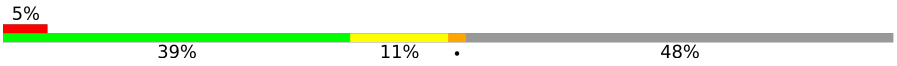
• Molecule 6: Eukaryotic translation initiation factor 2 subunit 1

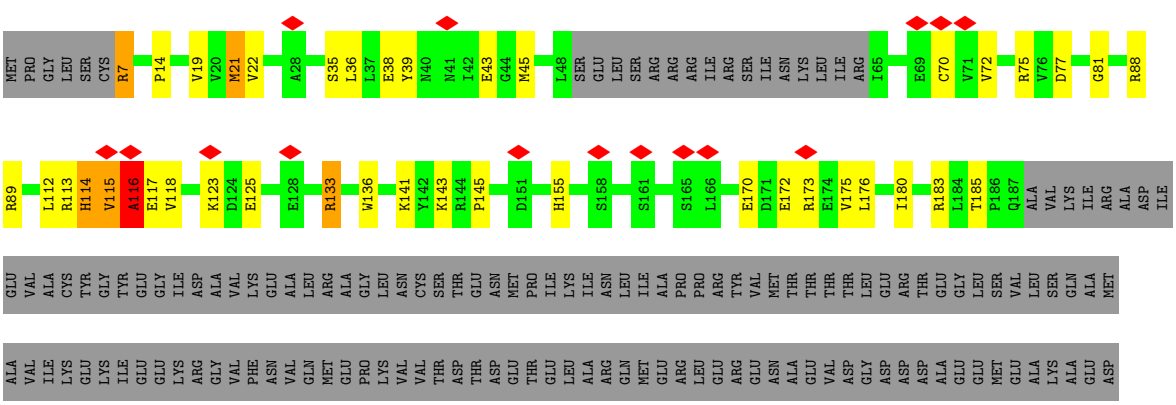
Chain K:



• Molecule 6: Eukaryotic translation initiation factor 2 subunit 1

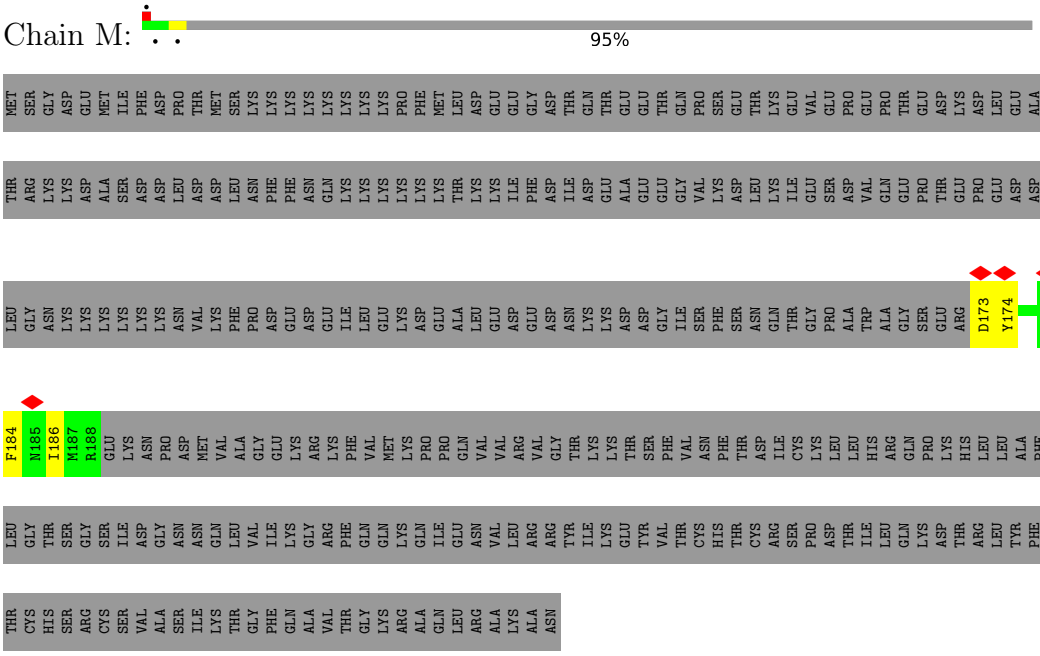
Chain L:





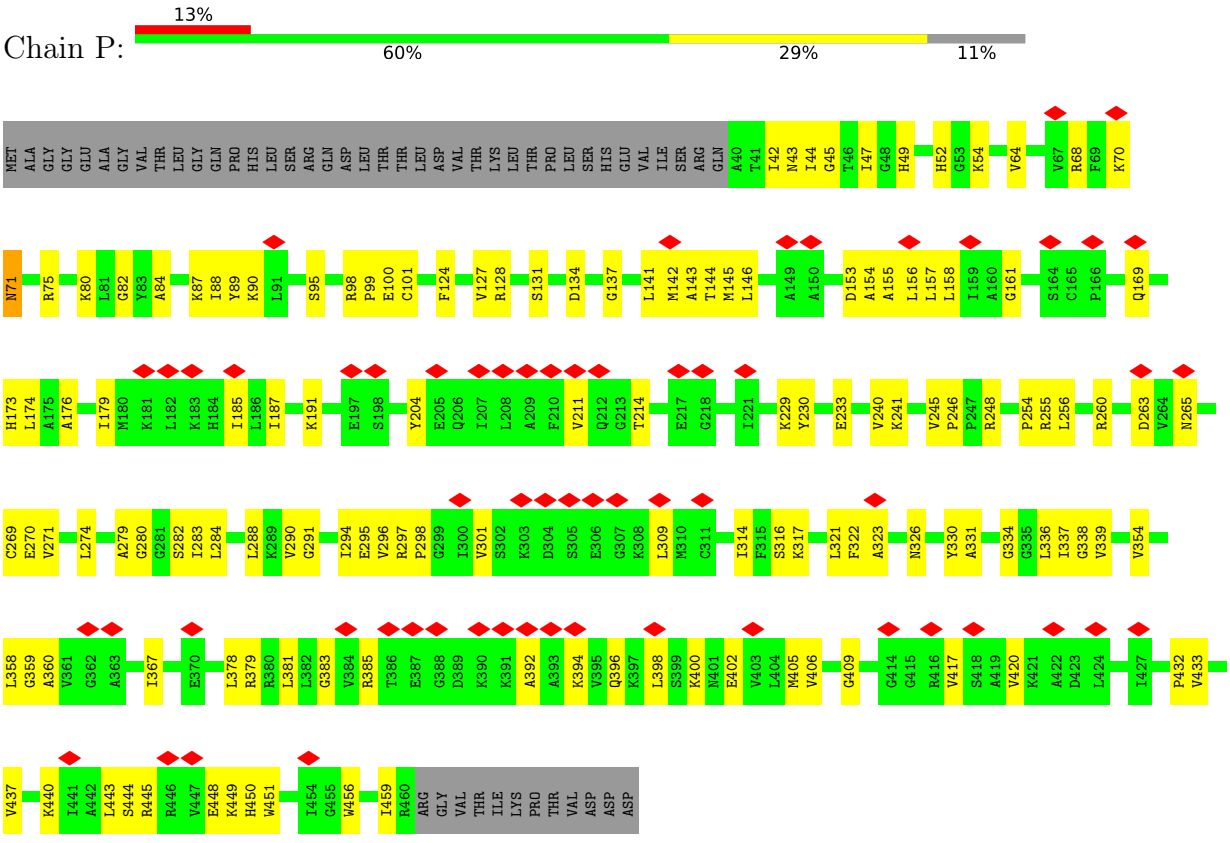
• Molecule 7: Eukaryotic translation initiation factor 2 subunit 2

Chain M:



• Molecule 8: Eukaryotic translation initiation factor 2 subunit 3

Chain P:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	719877	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	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	0.079	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0104	Depositor
Map size (Å)	367.5, 367.5, 367.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.47, 1.47, 1.47	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	0.34	0/2249	0.69	1/3038 (0.0%)
1	B	0.35	0/2240	0.69	3/3027 (0.1%)
2	C	0.34	0/2533	0.66	1/3426 (0.0%)
2	D	0.37	0/2533	0.67	1/3426 (0.0%)
3	E	0.32	0/2312	0.71	4/3139 (0.1%)
3	F	0.33	0/2281	0.72	3/3096 (0.1%)
4	G	0.36	0/2831	0.73	3/3847 (0.1%)
4	H	0.36	0/2831	0.70	1/3847 (0.0%)
5	I	0.35	0/3380	0.70	1/4597 (0.0%)
5	J	0.35	0/3380	0.70	2/4597 (0.0%)
6	K	0.30	0/1940	0.59	0/2610
6	L	0.31	0/1379	0.71	0/1859
7	M	0.23	0/147	0.65	1/197 (0.5%)
8	P	0.29	0/3257	0.64	1/4403 (0.0%)
All	All	0.34	0/33293	0.69	22/45109 (0.0%)

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	5
1	B	0	2
2	C	0	4
2	D	0	4
3	E	0	2
3	F	0	3
4	G	0	1
4	H	0	2
5	I	0	3
5	J	0	2
6	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	L	0	5
All	All	0	34

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	314	LEU	CA-CB-CG	8.47	134.77	115.30
3	F	119	ASP	CB-CG-OD1	7.92	125.43	118.30
4	H	367	LEU	CA-CB-CG	6.87	131.11	115.30
1	B	30	LEU	CA-CB-CG	6.22	129.60	115.30
5	J	443	LEU	CA-CB-CG	6.04	129.19	115.30
3	F	168	LEU	CA-CB-CG	6.01	129.11	115.30
3	E	119	ASP	CB-CG-OD1	5.93	123.64	118.30
4	G	485	LEU	CA-CB-CG	5.90	128.87	115.30
3	E	187	LEU	CA-CB-CG	5.87	128.79	115.30
3	E	180	LEU	CA-CB-CG	5.85	128.76	115.30
1	B	106	LEU	CA-CB-CG	5.75	128.52	115.30
3	E	125	ASP	CB-CG-OD1	5.64	123.38	118.30
5	J	57	PHE	C-N-CD	-5.58	108.34	120.60
8	P	274	LEU	CA-CB-CG	5.49	127.92	115.30
2	D	207	LEU	CA-CB-CG	5.47	127.89	115.30
2	C	212	ILE	CG1-CB-CG2	-5.35	99.62	111.40
1	A	56	LEU	CA-CB-CG	5.30	127.50	115.30
3	F	97	LEU	CA-CB-CG	5.30	127.49	115.30
7	M	173	ASP	CB-CG-OD2	5.26	123.04	118.30
1	B	45	LEU	CA-CB-CG	5.25	127.37	115.30
4	G	402	LEU	CA-CB-CG	5.20	127.26	115.30
5	I	43	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	GLN	Peptide
1	A	209	LYS	Peptide
1	A	242	ASN	Peptide
1	A	277	ALA	Peptide
1	A	83	TYR	Peptide
1	B	156	GLN	Peptide
1	B	233	PHE	Peptide

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Mol	Chain	Res	Type	Group
2	C	125	HIS	Peptide
2	C	170	PHE	Peptide
2	C	195	ALA	Peptide
2	C	28	PRO	Peptide
2	D	126	TYR	Peptide
2	D	170	PHE	Peptide
2	D	195	ALA	Peptide
2	D	287	LYS	Peptide
3	E	179	GLU	Peptide
3	E	2	GLU	Peptide
3	F	108	LEU	Peptide
3	F	2	GLU	Peptide
3	F	279	ASP	Peptide
4	G	268	PRO	Peptide
4	H	270	SER	Peptide
4	H	495	GLU	Peptide
5	I	175	GLU	Peptide
5	I	260	PHE	Peptide
5	I	315	ARG	Peptide
5	J	260	PHE	Peptide
5	J	358	GLU	Peptide
6	K	223	MET	Peptide
6	L	114	HIS	Peptide
6	L	116	ALA	Peptide
6	L	117	GLU	Peptide
6	L	155	HIS	Peptide
6	L	170	GLU	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	2213	0	2293	58	0
1	B	2204	0	2280	45	0
2	C	2486	0	2500	56	0
2	D	2486	0	2500	46	0
3	E	2286	0	2031	34	0
3	F	2255	0	1996	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	2779	0	2838	61	0
4	H	2779	0	2838	61	0
5	I	3312	0	3283	106	0
5	J	3312	0	3283	73	0
6	K	1914	0	1933	40	0
6	L	1356	0	1349	22	0
7	M	145	0	138	17	0
8	P	3204	0	3346	88	0
All	All	32731	0	32608	675	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 10.

All (675) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:192:HIS:CE1	5:I:194:THR:HB	1.43	1.53
2:C:304:GLU:CD	5:I:193:PRO:HG2	1.43	1.36
5:I:192:HIS:ND1	5:I:194:THR:HG22	1.48	1.26
5:I:192:HIS:CE1	5:I:194:THR:CB	2.19	1.26
5:I:192:HIS:ND1	5:I:194:THR:CG2	2.17	1.06
2:C:304:GLU:CD	5:I:193:PRO:CG	2.29	0.99
2:D:339:LEU:O	2:D:343:LEU:HB2	1.59	0.99
7:M:179:LEU:HD11	8:P:230:TYR:CZ	1.97	0.99
2:C:304:GLU:OE1	5:I:193:PRO:HG2	1.64	0.98
2:C:339:LEU:O	2:C:343:LEU:HB2	1.68	0.94
5:I:192:HIS:CE1	5:I:194:THR:H	1.87	0.93
7:M:179:LEU:HD11	8:P:230:TYR:CE1	2.05	0.91
2:C:304:GLU:OE2	5:I:193:PRO:HB2	1.80	0.81
5:I:192:HIS:ND1	5:I:194:THR:N	2.27	0.81
1:A:45:LEU:O	1:A:49:LEU:HB2	1.81	0.80
5:I:192:HIS:ND1	5:I:194:THR:CB	2.39	0.79
7:M:179:LEU:HD11	8:P:230:TYR:CE2	2.19	0.77
5:I:192:HIS:CE1	5:I:194:THR:CG2	2.64	0.77
5:I:192:HIS:HE1	5:I:194:THR:CB	1.77	0.76
5:I:193:PRO:O	5:I:195:ARG:N	2.21	0.74
5:I:192:HIS:HE1	5:I:194:THR:HB	0.89	0.73
4:H:310:GLU:O	4:H:314:LEU:HB2	1.89	0.73
5:I:192:HIS:CE1	5:I:194:THR:N	2.57	0.72
1:B:164:MET:SD	1:B:164:MET:N	2.63	0.70
1:A:199:GLY:HA2	1:A:234:LYS:HB3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:179:LEU:CD1	8:P:230:TYR:CZ	2.73	0.70
4:G:170:ARG:HE	4:G:265:GLN:HG2	1.57	0.68
2:C:304:GLU:CG	5:I:193:PRO:HG2	2.24	0.67
6:L:133:ARG:HH22	6:L:175:VAL:HG11	1.60	0.67
5:J:46:VAL:HG23	5:J:92:PHE:HB2	1.76	0.67
2:C:304:GLU:OE1	5:I:193:PRO:CG	2.41	0.67
3:F:157:PHE:HB2	3:F:171:ALA:HB3	1.78	0.66
2:C:304:GLU:OE2	5:I:193:PRO:CG	2.44	0.66
1:A:159:LEU:HD21	1:A:162:LYS:HD2	1.77	0.65
6:L:22:VAL:HG21	6:L:36:LEU:HA	1.79	0.65
6:K:28:ALA:H	6:K:32:ALA:HA	1.61	0.65
2:C:304:GLU:OE2	5:I:193:PRO:CB	2.45	0.64
7:M:179:LEU:HD11	8:P:230:TYR:CD1	2.32	0.64
3:E:48:PHE:H	4:H:199:PRO:HG3	1.63	0.64
5:I:382:GLY:HA3	5:I:399:GLY:H	1.64	0.63
5:J:47:LEU:HD12	5:J:93:VAL:HG23	1.80	0.63
2:C:266:ILE:HG22	2:C:323:LEU:HB3	1.81	0.63
5:I:47:LEU:HD12	5:I:93:VAL:HG13	1.81	0.62
3:F:194:ARG:HH21	5:I:237:GLY:HA3	1.64	0.62
3:F:7:VAL:HG22	3:F:104:LEU:HB2	1.80	0.62
5:I:192:HIS:CG	5:I:194:THR:HG22	2.31	0.62
5:I:408:ILE:HG13	5:I:425:LEU:HD22	1.82	0.62
2:C:302:ILE:HD11	4:G:374:ARG:HE	1.64	0.62
8:P:87:LYS:H	8:P:99:PRO:HD3	1.62	0.62
2:C:301:ASP:HA	5:I:191:SER:O	1.99	0.62
3:E:402:SER:HA	3:E:419:ALA:HB3	1.82	0.62
5:I:344:ARG:HE	5:I:348:VAL:HG11	1.65	0.62
4:H:310:GLU:HA	4:H:314:LEU:HD13	1.82	0.61
4:H:326:LYS:O	4:H:400:LYS:NZ	2.32	0.61
5:I:394:THR:HG22	5:I:411:SER:HB3	1.82	0.61
8:P:248:ARG:NH1	8:P:284:LEU:O	2.33	0.61
5:J:44:GLN:HE22	5:J:145:ARG:H	1.48	0.61
6:K:160:PRO:O	6:K:173:ARG:NH2	2.34	0.61
2:D:233:ILE:HG13	2:D:266:ILE:HB	1.83	0.61
4:G:407:ALA:HB3	4:G:415:MET:HB3	1.81	0.61
3:F:165:LYS:HB3	3:F:264:TYR:HE1	1.65	0.61
4:G:364:ARG:NH2	4:G:464:GLN:O	2.34	0.61
4:G:473:LEU:HD21	4:G:484:LEU:HD21	1.81	0.61
2:D:302:ILE:HG23	4:H:377:VAL:HG11	1.83	0.60
4:G:314:LEU:HA	4:G:317:GLN:HG2	1.83	0.60
6:K:243:GLU:HB2	6:K:246:GLU:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:409:LEU:HB3	4:H:413:SER:HB3	1.83	0.60
1:B:14:MET:HG3	1:B:15:LYS:HG2	1.82	0.60
2:C:92:GLU:OE2	2:C:95:ARG:NH2	2.34	0.60
4:H:444:CYS:SG	4:H:445:GLU:N	2.72	0.60
3:F:39:PRO:O	3:F:43:LEU:HB2	2.02	0.60
4:H:177:VAL:HG12	4:H:179:LEU:H	1.65	0.60
2:D:332:ALA:HB3	2:D:335:TYR:HB2	1.83	0.60
5:I:192:HIS:CE1	5:I:194:THR:CA	2.84	0.59
5:I:95:CYS:SG	5:I:96:CYS:N	2.74	0.59
6:K:7:ARG:NH1	6:K:9:TYR:O	2.35	0.59
1:A:12:SER:O	1:A:16:GLU:HB2	2.02	0.59
1:A:20:MET:O	1:A:132:ARG:NH1	2.35	0.59
1:B:241:LEU:N	1:B:245:ASP:OD2	2.34	0.59
1:B:114:LEU:HD11	1:B:290:VAL:HG22	1.84	0.59
5:I:154:ASP:HB3	5:I:299:ARG:HG3	1.83	0.59
2:C:159:ILE:O	2:C:185:ARG:NH1	2.35	0.59
5:J:48:VAL:HA	5:J:94:PHE:HB2	1.83	0.59
4:H:464:GLN:HE21	4:H:471:VAL:HG22	1.67	0.59
8:P:211:VAL:HB	8:P:214:THR:HB	1.84	0.59
1:B:30:LEU:HA	1:B:33:PHE:HB3	1.84	0.59
6:L:143:LYS:HB3	6:L:145:PRO:HD2	1.85	0.59
7:M:186:ILE:O	7:M:186:ILE:HG22	2.03	0.59
3:E:205:TYR:HB3	3:E:207:LEU:HD23	1.85	0.58
4:G:403:LEU:HD21	4:G:420:THR:HG23	1.84	0.58
4:G:403:LEU:HB3	4:G:436:VAL:HG12	1.85	0.58
3:E:407:SER:HA	3:E:425:LEU:HA	1.84	0.58
4:H:210:LEU:HD13	4:H:213:GLN:HG3	1.85	0.58
5:J:354:SER:OG	5:J:372:CYS:SG	2.61	0.58
6:L:114:HIS:HB3	6:L:125:GLU:HB2	1.84	0.58
2:D:39:LEU:HD13	2:D:141:LEU:HD21	1.85	0.58
2:D:143:GLU:OE2	2:D:327:ASN:ND2	2.32	0.58
2:D:303:LEU:HD11	5:J:192:HIS:HE2	1.68	0.58
4:H:234:GLN:HE22	4:H:301:ARG:HB2	1.67	0.58
1:A:188:GLU:OE1	1:A:222:GLN:NE2	2.36	0.58
5:I:193:PRO:C	5:I:195:ARG:H	2.07	0.58
5:J:58:PRO:HD2	5:J:448:VAL:HG11	1.85	0.58
2:C:299:GLU:HG3	2:C:303:LEU:HB2	1.85	0.58
4:G:326:LYS:O	4:G:400:LYS:NZ	2.37	0.58
4:G:464:GLN:HE22	4:G:466:LYS:HD3	1.69	0.58
4:G:311:LYS:O	4:G:315:ALA:CB	2.52	0.58
4:H:216:GLN:HE22	4:H:218:LEU:HB2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:44:GLN:HE22	5:I:145:ARG:H	1.52	0.57
5:I:366:THR:HA	5:I:383:CYS:HB2	1.86	0.57
2:D:86:LEU:HD13	2:D:89:ILE:HD11	1.85	0.57
3:E:134:LYS:HD3	3:E:273:LEU:HD23	1.86	0.57
1:A:74:ARG:NH1	6:K:29:GLU:O	2.37	0.57
1:B:187:MET:HG2	1:B:218:CYS:HB3	1.86	0.57
5:J:46:VAL:HG13	5:J:150:LEU:HD23	1.85	0.57
5:J:51:SER:OG	5:J:65:ARG:NH1	2.37	0.57
2:C:24:ARG:NH1	2:C:26:GLY:O	2.38	0.57
4:G:202:VAL:HG13	4:G:203:ILE:HD12	1.85	0.57
8:P:153:ASP:OD1	8:P:248:ARG:NH2	2.38	0.57
1:A:89:CYS:SG	6:K:75:ARG:NH2	2.74	0.57
3:E:125:ASP:HA	4:H:209:ARG:HH22	1.70	0.57
4:G:311:LYS:O	4:G:315:ALA:HB2	2.05	0.57
6:K:58:SER:O	6:K:61:LYS:NZ	2.36	0.57
8:P:142:MET:O	8:P:146:LEU:HB2	2.05	0.57
1:A:223:ASN:ND2	4:H:429:ALA:O	2.37	0.57
6:L:36:LEU:HD13	6:L:38:GLU:HB3	1.86	0.57
2:C:270:PRO:HD2	2:C:273:LYS:HE2	1.87	0.57
6:L:35:SER:HA	6:L:43:GLU:HA	1.86	0.56
1:B:20:MET:O	1:B:132:ARG:NH1	2.38	0.56
5:J:443:LEU:HD22	5:J:444:PRO:HD2	1.86	0.56
5:I:206:ASP:HB3	5:I:210:ASN:H	1.70	0.56
5:J:330:SER:H	5:J:333:GLN:HE22	1.53	0.56
5:J:414:CYS:SG	5:J:415:ASP:N	2.74	0.56
2:D:288:PHE:O	5:J:316:ARG:NH2	2.38	0.56
3:E:207:LEU:HD12	3:E:211:ILE:HG12	1.87	0.56
2:D:31:SER:O	2:D:35:ALA:HB2	2.05	0.56
6:K:24:VAL:HA	6:K:34:VAL:HA	1.88	0.56
3:F:184:GLY:HA2	5:I:224:PHE:HE2	1.70	0.56
5:I:136:ARG:HH21	5:I:260:PHE:HB2	1.71	0.56
1:B:246:VAL:O	1:B:251:LYS:NZ	2.38	0.56
1:A:9:TYR:HD2	1:A:29:THR:HG23	1.71	0.56
5:I:63:GLN:NE2	5:I:415:ASP:OD2	2.38	0.56
5:I:167:GLU:OE1	5:I:171:ARG:NH1	2.39	0.56
5:J:186:LYS:NZ	5:J:187:GLU:O	2.38	0.56
5:J:189:SER:HB3	5:J:192:HIS:HB2	1.87	0.56
3:E:122:ARG:O	4:H:209:ARG:NH1	2.39	0.55
4:H:438:CYS:SG	4:H:439:GLU:N	2.77	0.55
1:B:70:GLU:OE1	1:B:237:ARG:NH1	2.40	0.55
2:D:31:SER:HA	2:D:34:MET:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:414:CYS:SG	5:I:415:ASP:N	2.78	0.55
4:G:387:LEU:HG	4:G:389:PRO:HD2	1.88	0.55
1:A:46:ARG:HH21	1:A:90:LYS:HB3	1.72	0.55
5:I:190:PRO:HG3	5:I:243:ASP:OD2	2.07	0.55
4:H:428:ARG:HH22	4:H:496:LEU:HA	1.71	0.55
2:D:92:GLU:OE2	2:D:95:ARG:NH2	2.40	0.55
3:E:157:PHE:HB2	3:E:171:ALA:HB3	1.88	0.55
4:H:275:ASN:ND2	4:H:441:TYR:O	2.39	0.55
5:J:195:ARG:HH11	5:J:245:LEU:HD23	1.72	0.55
6:K:63:ILE:HG13	6:K:64:ARG:HG3	1.87	0.55
4:G:439:GLU:OE1	4:G:441:TYR:N	2.36	0.55
5:I:322:THR:HG22	5:I:324:GLU:H	1.71	0.55
6:K:163:LEU:HA	6:K:166:LEU:HD23	1.89	0.55
6:K:196:GLU:HB2	6:K:234:ARG:HG3	1.89	0.55
4:H:464:GLN:HE22	4:H:466:LYS:HD3	1.72	0.55
5:I:158:ASN:ND2	5:I:319:TYR:O	2.40	0.55
2:C:16:GLU:HA	2:C:19:VAL:HG22	1.87	0.54
2:C:239:ILE:HG13	2:C:274:LEU:HA	1.89	0.54
4:G:260:MET:HG2	4:G:277:ILE:HG21	1.89	0.54
5:I:362:LEU:HB3	5:I:366:THR:HG21	1.89	0.54
8:P:49:HIS:HA	8:P:137:GLY:HA3	1.89	0.54
3:E:128:LEU:HD21	3:E:263:ILE:HG23	1.88	0.54
5:I:421:GLU:HG3	5:I:422:ARG:HG3	1.89	0.54
8:P:71:ASN:O	8:P:80:LYS:NZ	2.39	0.54
8:P:409:GLY:HA2	8:P:440:LYS:HG3	1.88	0.54
8:P:143:ALA:HB1	8:P:354:VAL:HG11	1.89	0.54
5:I:389:VAL:HG13	5:I:406:ALA:HB3	1.89	0.54
8:P:260:ARG:NH1	8:P:280:GLY:O	2.37	0.54
8:P:263:ASP:OD2	8:P:265:ASN:ND2	2.41	0.54
6:L:136:TRP:O	6:L:141:LYS:NZ	2.35	0.54
8:P:169:GLN:NE2	8:P:383:GLY:O	2.39	0.54
5:J:71:ALA:H	5:J:73:VAL:HG22	1.72	0.54
5:J:360:VAL:HG11	5:J:374:ILE:HG22	1.89	0.54
6:L:116:ALA:HB3	6:L:118:VAL:HA	1.88	0.54
3:E:91:ARG:NH1	3:E:219:GLY:O	2.41	0.54
4:G:234:GLN:HE22	4:G:301:ARG:HA	1.73	0.54
4:G:517:ARG:NH2	4:G:522:ASP:OD2	2.41	0.54
6:K:77:ASP:HB2	6:K:82:TYR:HB3	1.89	0.54
8:P:256:LEU:N	8:P:358:LEU:O	2.40	0.53
3:F:218:ASN:HB3	3:F:221:ILE:HD13	1.90	0.53
4:G:328:SER:OG	4:G:329:ASN:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:141:LEU:HB2	8:P:144:THR:HB	1.90	0.53
5:J:166:GLU:OE1	5:J:169:ARG:NH1	2.41	0.53
2:D:241:ALA:HB2	2:D:276:PRO:HA	1.90	0.53
2:D:259:LYS:HB2	2:D:320:LEU:HD11	1.91	0.53
5:J:62:ASP:HA	5:J:98:LYS:HE3	1.90	0.53
4:G:268:PRO:HG2	4:G:456:GLU:HG2	1.90	0.53
6:K:151:ASP:O	6:K:155:HIS:ND1	2.41	0.53
5:J:246:ASP:OD1	5:J:269:ARG:NH2	2.42	0.53
7:M:179:LEU:HD11	8:P:230:TYR:CD2	2.44	0.53
8:P:43:ASN:ND2	8:P:334:GLY:O	2.42	0.53
4:H:395:LEU:HD12	4:H:396:PRO:HD3	1.91	0.53
5:I:432:THR:HB	5:I:450:SER:HB3	1.91	0.53
5:J:83:LEU:HD12	5:J:118:ASN:HD21	1.73	0.53
8:P:84:ALA:O	8:P:131:SER:OG	2.26	0.53
1:A:12:SER:O	1:A:16:GLU:CB	2.57	0.53
2:D:215:THR:HG22	4:H:483:ARG:HB3	1.91	0.53
5:I:193:PRO:C	5:I:195:ARG:N	2.61	0.53
1:A:182:ALA:HB2	1:B:210:ILE:HB	1.90	0.52
2:D:191:VAL:O	2:D:217:MET:N	2.38	0.52
4:G:499:LEU:HD13	4:G:506:MET:HE2	1.90	0.52
5:I:135:LEU:HD22	5:I:260:PHE:HZ	1.73	0.52
5:J:178:VAL:O	5:J:285:ASN:N	2.42	0.52
8:P:450:HIS:ND1	8:P:451:TRP:O	2.42	0.52
3:F:41:ASN:O	3:F:45:ARG:N	2.37	0.52
4:H:401:VAL:HG13	4:H:434:VAL:HA	1.90	0.52
5:I:53:ASP:OD2	5:I:302:ASN:ND2	2.42	0.52
5:I:59:ILE:HD11	5:I:65:ARG:HH21	1.75	0.52
6:K:32:ALA:H	6:K:46:ILE:HG23	1.74	0.52
1:B:85:ASP:O	6:L:75:ARG:NH2	2.42	0.52
2:D:195:ALA:HB1	4:H:364:ARG:HH11	1.75	0.52
8:P:101:CYS:HB3	8:P:124:PHE:HB3	1.91	0.52
1:A:45:LEU:HA	1:A:49:LEU:HD12	1.91	0.52
1:B:190:ALA:O	1:B:224:LYS:NZ	2.32	0.52
7:M:179:LEU:CD1	8:P:230:TYR:CE1	2.85	0.52
2:D:165:ILE:HG23	2:D:189:VAL:HG23	1.91	0.52
8:P:323:ALA:N	8:P:326:ASN:O	2.42	0.52
8:P:402:GLU:OE2	8:P:445:ARG:NH1	2.43	0.52
2:C:177:PHE:HD2	2:C:178:LEU:HD12	1.73	0.52
2:C:236:THR:O	2:C:273:LYS:NZ	2.33	0.52
3:F:385:VAL:HA	3:F:402:SER:H	1.74	0.52
4:H:407:ALA:HA	4:H:442:LYS:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:211:ARG:HA	5:J:288:HIS:HA	1.90	0.52
8:P:406:VAL:HB	8:P:443:LEU:HD13	1.92	0.52
2:D:159:ILE:O	2:D:185:ARG:NH1	2.43	0.52
5:J:84:THR:HG22	5:J:118:ASN:HD22	1.74	0.52
5:J:348:VAL:HG12	5:J:362:LEU:HD11	1.92	0.52
1:A:107:SER:HA	1:A:110:LYS:HG2	1.92	0.52
5:I:411:SER:OG	5:I:412:LEU:N	2.42	0.52
2:D:271:MET:HG3	2:D:326:SER:HB2	1.92	0.51
2:D:345:HIS:ND1	2:D:348:ASP:OD2	2.43	0.51
4:G:450:ASP:HA	4:G:491:VAL:HG11	1.90	0.51
8:P:448:GLU:HG3	8:P:450:HIS:H	1.75	0.51
1:A:30:LEU:HD12	1:A:72:PHE:HZ	1.75	0.51
1:A:196:GLY:O	1:A:208:ASN:ND2	2.43	0.51
1:A:208:ASN:O	1:A:274:ASP:N	2.41	0.51
1:B:27:ILE:HA	1:B:30:LEU:HD23	1.92	0.51
2:D:16:GLU:HA	2:D:19:VAL:HG22	1.92	0.51
5:J:369:GLY:H	5:J:385:ILE:HB	1.75	0.51
3:F:33:LYS:HB2	3:F:37:TRP:CD1	2.44	0.51
4:G:170:ARG:HG2	4:G:265:GLN:HE21	1.75	0.51
5:J:352:HIS:O	5:J:370:SER:OG	2.27	0.51
6:K:7:ARG:HH21	6:K:128:GLU:HB3	1.75	0.51
8:P:301:VAL:HG21	8:P:432:PRO:HD2	1.92	0.51
8:P:288:LEU:HB3	8:P:331:ALA:HB3	1.92	0.51
2:C:57:LEU:HB3	2:C:58:MET:HE2	1.93	0.51
3:E:56:THR:O	3:E:61:LYS:N	2.43	0.51
4:H:465:CYS:HB2	4:H:467:ARG:HD3	1.91	0.51
5:I:181:MET:HE2	5:I:256:VAL:HG21	1.92	0.51
1:B:242:ASN:N	1:B:245:ASP:OD2	2.44	0.51
2:C:204:ALA:HB1	4:G:482:LEU:HD21	1.91	0.51
6:K:74:ILE:HG22	6:K:75:ARG:HG2	1.93	0.51
6:K:191:ILE:HB	6:K:239:THR:HB	1.92	0.51
1:A:214:GLN:HA	1:A:217:VAL:HG12	1.93	0.51
5:I:217:LYS:HZ2	5:I:219:GLN:HB3	1.76	0.51
8:P:45:GLY:O	8:P:156:LEU:N	2.42	0.51
8:P:291:GLY:HA2	8:P:317:LYS:HG3	1.93	0.51
6:K:263:GLU:HG3	6:K:267:GLY:HA3	1.92	0.51
2:C:244:ALA:HB2	2:C:318:PRO:HD3	1.92	0.50
4:G:392:SER:HA	4:G:395:LEU:HB2	1.94	0.50
1:B:286:THR:HG23	1:B:288:LEU:H	1.76	0.50
2:D:220:ALA:HB3	4:H:418:VAL:HG12	1.92	0.50
5:I:381:PRO:HG2	5:I:398:GLN:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:405:MET:HG3	8:P:444:SER:HB2	1.93	0.50
1:B:154:GLU:O	1:B:160:SER:OG	2.29	0.50
1:B:99:LEU:HA	1:B:102:ARG:HG2	1.93	0.50
2:C:259:LYS:HB2	2:C:320:LEU:HD11	1.92	0.50
2:D:253:THR:OG1	4:H:422:GLN:NE2	2.37	0.50
4:G:476:TRP:NE1	4:G:482:LEU:O	2.40	0.50
8:P:153:ASP:HB3	8:P:246:PRO:HG3	1.94	0.50
8:P:398:LEU:HD22	8:P:420:VAL:HG11	1.94	0.50
1:A:21:ALA:HA	1:A:132:ARG:HH11	1.76	0.50
1:B:231:GLU:HG2	1:B:233:PHE:H	1.77	0.50
4:G:502:THR:HG23	4:G:504:LEU:H	1.76	0.50
8:P:68:ARG:N	8:P:71:ASN:OD1	2.44	0.50
8:P:146:LEU:HD21	8:P:176:ALA:HB1	1.92	0.50
2:D:46:ILE:O	2:D:130:GLN:NE2	2.45	0.50
5:I:54:ARG:HD3	5:I:57:PHE:HD2	1.76	0.50
5:J:48:VAL:O	5:J:153:GLY:N	2.44	0.50
8:P:191:LYS:O	8:P:204:TYR:OH	2.30	0.50
2:D:33:GLU:HA	2:D:36:ARG:HG2	1.94	0.50
3:E:134:LYS:HB2	3:E:273:LEU:HB3	1.92	0.49
1:A:222:GLN:HA	4:H:431:ASN:HD22	1.77	0.49
3:F:132:MET:HG2	3:F:158:ILE:HG21	1.94	0.49
6:L:180:ILE:HG12	6:L:185:THR:HG22	1.94	0.49
4:H:256:LEU:HD13	4:H:259:TYR:HD2	1.76	0.49
5:I:373:PHE:HB3	5:I:390:VAL:HG12	1.93	0.49
5:J:147:ASP:OD2	5:J:169:ARG:NE	2.40	0.49
5:J:364:SER:H	5:J:381:PRO:HB3	1.77	0.49
5:J:396:LEU:HB3	5:J:400:VAL:HG21	1.93	0.49
6:K:247:GLY:O	6:K:251:LEU:HB2	2.12	0.49
3:E:131:LEU:HD23	3:E:204:LEU:HG	1.93	0.49
3:F:155:ARG:HE	3:F:173:GLU:HB3	1.77	0.49
5:J:411:SER:OG	5:J:412:LEU:N	2.45	0.49
2:C:80:ASN:ND2	2:C:274:LEU:O	2.41	0.49
3:E:159:GLY:O	3:E:168:LEU:N	2.44	0.49
5:J:141:LYS:HD2	5:J:143:LEU:HD23	1.94	0.49
5:J:393:GLN:OE1	5:J:410:GLN:NE2	2.33	0.49
2:C:168:ILE:HD11	2:C:254:LEU:HD13	1.95	0.49
5:I:443:LEU:HD22	5:I:444:PRO:HD2	1.95	0.49
8:P:176:ALA:HA	8:P:456:TRP:HE1	1.77	0.49
1:A:45:LEU:HD12	1:A:46:ARG:HD2	1.94	0.49
4:G:409:LEU:HB2	4:G:413:SER:HB3	1.94	0.49
8:P:269:CYS:SG	8:P:270:GLU:N	2.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:CYS:SG	6:L:75:ARG:NH2	2.70	0.49
5:J:343:TYR:HD2	5:J:361:LEU:HB3	1.78	0.49
6:L:19:VAL:HG22	6:L:72:VAL:HG12	1.95	0.49
7:M:180:LEU:HA	7:M:184:PHE:CD2	2.48	0.49
1:A:206:ILE:HG22	1:A:276:THR:HG22	1.95	0.49
2:C:76:THR:HG22	2:C:238:THR:HG22	1.95	0.49
2:C:304:GLU:CD	5:I:193:PRO:CB	2.80	0.49
2:D:282:GLU:OE2	2:D:285:PHE:N	2.46	0.49
4:H:403:LEU:HB2	4:H:436:VAL:HG12	1.94	0.49
4:G:409:LEU:HD12	4:G:447:VAL:HA	1.94	0.49
5:J:204:ALA:HA	5:J:240:VAL:HA	1.95	0.49
3:E:129:ALA:HA	3:E:265:SER:HA	1.95	0.48
7:M:179:LEU:O	7:M:184:PHE:HD2	1.95	0.48
7:M:180:LEU:HA	7:M:184:PHE:HD2	1.77	0.48
3:F:56:THR:O	3:F:61:LYS:N	2.45	0.48
6:L:14:PRO:HD3	6:L:39:TYR:HE2	1.78	0.48
2:D:60:LEU:HD22	2:D:63:ARG:HH12	1.78	0.48
4:H:305:ASP:HA	4:H:308:VAL:HG12	1.93	0.48
5:I:349:SER:OG	5:I:366:THR:O	2.31	0.48
8:P:282:SER:HA	8:P:336:LEU:HA	1.94	0.48
4:H:502:THR:HG23	4:H:504:LEU:H	1.78	0.48
4:H:324:TYR:HE1	4:H:348:GLU:HG2	1.79	0.48
8:P:42:ILE:HD11	8:P:245:VAL:HG12	1.96	0.48
8:P:157:LEU:HD11	8:P:187:ILE:HG12	1.94	0.48
4:G:406:HIS:HB2	4:G:416:SER:HA	1.95	0.48
4:G:475:ASN:HB3	4:G:478:ASN:HD21	1.79	0.48
4:G:502:THR:OG1	4:G:503:GLU:OE1	2.31	0.48
1:A:82:GLU:OE2	6:K:88:ARG:NH1	2.46	0.48
4:G:357:ARG:HG2	4:G:382:PRO:HB2	1.96	0.48
5:I:69:PRO:O	5:I:306:TYR:OH	2.27	0.48
5:J:182:THR:HB	5:J:251:ILE:HD11	1.94	0.48
8:P:255:ARG:HA	8:P:359:GLY:HA2	1.95	0.48
3:F:74:ASP:OD1	3:F:74:ASP:N	2.47	0.48
4:G:521:SER:OG	6:K:57:ARG:NH1	2.47	0.48
4:H:220:SER:O	4:H:225:ARG:NH2	2.45	0.48
5:I:198:GLU:O	5:I:217:LYS:NZ	2.38	0.48
7:M:186:ILE:O	7:M:186:ILE:CG2	2.61	0.48
1:A:187:MET:HG2	1:A:218:CYS:HB3	1.96	0.48
1:A:193:VAL:HG23	1:A:226:PHE:HA	1.96	0.48
3:E:67:PHE:O	3:E:72:LYS:NZ	2.45	0.48
8:P:298:PRO:HG3	8:P:433:VAL:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:191:PRO:HG2	3:E:192:ARG:HD2	1.96	0.48
3:F:155:ARG:HA	3:F:173:GLU:HB3	1.95	0.48
5:I:92:PHE:HE1	5:I:121:ARG:HD2	1.79	0.48
1:B:286:THR:OG1	1:B:287:ASP:N	2.45	0.47
5:J:342:ILE:HG22	5:J:359:ASN:H	1.78	0.47
1:B:9:TYR:OH	1:B:32:GLU:OE1	2.32	0.47
2:C:345:HIS:HD2	2:C:346:PRO:HD2	1.79	0.47
4:G:332:VAL:HG11	4:G:357:ARG:HH21	1.78	0.47
4:G:398:VAL:HG13	4:G:432:VAL:HG11	1.94	0.47
5:J:188:SER:OG	5:J:189:SER:N	2.47	0.47
1:A:41:THR:HG23	1:A:45:LEU:HB2	1.97	0.47
1:B:31:LEU:HD21	1:B:97:GLY:HA3	1.96	0.47
2:D:156:LEU:O	2:D:185:ARG:NH2	2.47	0.47
3:E:99:THR:OG1	3:E:100:ASP:N	2.45	0.47
8:P:90:LYS:HZ3	8:P:241:LYS:HE3	1.78	0.47
2:C:242:ASN:HD21	2:C:278:PHE:HD1	1.61	0.47
2:D:175:GLU:HB2	2:D:207:LEU:HD23	1.96	0.47
3:E:109:ILE:H	3:E:109:ILE:HG13	1.49	0.47
4:G:327:ILE:HD13	4:G:400:LYS:HZ1	1.79	0.47
4:G:361:VAL:HG23	4:G:386:LEU:HG	1.97	0.47
5:I:344:ARG:HB3	5:I:348:VAL:HG21	1.97	0.47
5:J:171:ARG:NH2	5:J:182:THR:OG1	2.47	0.47
6:L:172:GLU:O	6:L:176:LEU:N	2.47	0.47
1:A:232:SER:HA	1:A:235:PHE:HE2	1.79	0.47
2:C:137:ILE:HA	2:C:140:LEU:HB2	1.96	0.47
2:D:250:GLY:N	2:D:314:ASP:OD2	2.47	0.47
5:I:188:SER:OG	5:I:189:SER:N	2.47	0.47
5:I:393:GLN:HB3	5:I:410:GLN:HA	1.95	0.47
6:K:71:VAL:HG21	6:K:85:LEU:HB2	1.95	0.47
8:P:47:ILE:N	8:P:156:LEU:O	2.43	0.47
2:C:52:SER:N	2:C:56:GLU:OE2	2.47	0.47
4:G:305:ASP:HA	4:G:308:VAL:HG22	1.97	0.47
6:K:155:HIS:O	6:K:159:ASP:N	2.48	0.47
1:A:190:ALA:O	1:A:224:LYS:NZ	2.34	0.47
1:B:84:SER:OG	6:L:88:ARG:NH2	2.43	0.47
1:B:216:ALA:HB1	1:B:280:LEU:HD21	1.96	0.47
5:I:176:LYS:HG3	5:I:178:VAL:HG12	1.96	0.47
6:K:108:VAL:O	6:K:112:LEU:HB2	2.15	0.47
8:P:297:ARG:HA	8:P:314:ILE:HD13	1.97	0.47
1:A:181:ALA:HB2	1:B:180:ASP:HB3	1.97	0.47
2:D:252:HIS:ND1	2:D:315:TYR:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:407:SER:HA	3:F:425:LEU:HA	1.97	0.47
4:H:439:GLU:OE1	4:H:440:THR:N	2.48	0.47
5:I:176:LYS:HD3	5:I:179:SER:HB2	1.96	0.47
5:I:199:ASP:HA	5:I:217:LYS:HZ3	1.80	0.47
8:P:378:LEU:HD13	8:P:456:TRP:HH2	1.81	0.47
2:C:231:LYS:HG3	2:C:264:PRO:HG2	1.96	0.46
2:C:222:ILE:HG13	4:G:422:GLN:NE2	2.30	0.46
5:J:161:ILE:HG22	5:J:165:LEU:HB2	1.97	0.46
5:I:61:LYS:HA	5:I:97:TRP:HH2	1.79	0.46
5:I:156:ILE:HD13	5:I:309:VAL:HG21	1.97	0.46
1:B:24:VAL:HA	1:B:27:ILE:HG22	1.97	0.46
3:E:205:TYR:HE1	3:E:228:LEU:HD21	1.79	0.46
5:I:100:ALA:HA	5:I:103:LYS:HE2	1.96	0.46
8:P:95:SER:HA	8:P:233:GLU:HA	1.97	0.46
5:I:396:LEU:HB3	5:I:400:VAL:HG21	1.97	0.46
2:C:304:GLU:HA	5:I:315:ARG:HH22	1.80	0.46
2:D:216:VAL:HG11	4:H:473:LEU:HD11	1.98	0.46
4:G:218:LEU:HD12	4:G:219:VAL:HG23	1.98	0.46
4:H:328:SER:OG	4:H:329:ASN:N	2.47	0.46
8:P:54:LYS:NZ	8:P:134:ASP:OD1	2.40	0.46
4:G:423:LEU:HA	4:G:426:VAL:HG22	1.98	0.46
4:H:183:LEU:HD22	4:H:455:ASN:H	1.81	0.46
4:H:284:ILE:HG22	4:H:300:LEU:HD11	1.98	0.46
5:J:414:CYS:HB3	5:J:432:THR:HA	1.98	0.46
8:P:45:GLY:N	8:P:154:ALA:O	2.43	0.46
1:A:41:THR:O	1:A:46:ARG:NH1	2.49	0.46
5:I:407:GLN:HB2	5:I:424:THR:HG23	1.97	0.46
1:B:183:VAL:O	1:B:187:MET:N	2.49	0.46
2:D:52:SER:N	2:D:56:GLU:OE2	2.49	0.46
6:K:7:ARG:HA	6:K:40:ASN:HB2	1.96	0.46
7:M:174:TYR:O	7:M:178:GLU:HB2	2.16	0.46
2:C:233:ILE:HG22	2:C:266:ILE:HD11	1.98	0.45
2:D:207:LEU:HB2	2:D:212:ILE:HD13	1.98	0.45
4:H:298:SER:O	4:H:301:ARG:NH1	2.49	0.45
5:I:354:SER:OG	5:I:369:GLY:O	2.30	0.45
3:E:195:PHE:HB2	5:J:238:VAL:HB	1.97	0.45
5:J:158:ASN:N	5:J:158:ASN:OD1	2.48	0.45
5:J:338:SER:HB3	5:J:342:ILE:HG13	1.97	0.45
6:K:164:ASP:OD1	6:K:173:ARG:NH2	2.49	0.45
1:A:191:ASP:HA	1:A:224:LYS:HD3	1.98	0.45
1:A:201:VAL:HG13	1:A:203:ASN:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:405:GLN:O	3:F:423:ASP:N	2.43	0.45
5:I:91:THR:HG23	5:I:120:VAL:HG23	1.98	0.45
5:J:148:PHE:N	5:J:252:CYS:O	2.49	0.45
3:E:199:LEU:HD22	3:E:199:LEU:HA	1.82	0.45
3:F:122:ARG:HB3	4:G:209:ARG:HB2	1.99	0.45
4:H:471:VAL:HB	4:H:474:ALA:HB2	1.98	0.45
4:H:483:ARG:HH11	4:H:484:LEU:H	1.64	0.45
5:I:413:LEU:HG	5:I:431:LEU:HB2	1.98	0.45
6:K:24:VAL:HG11	6:K:64:ARG:HB3	1.97	0.45
8:P:254:PRO:HD2	8:P:360:ALA:HB2	1.98	0.45
1:A:14:MET:HG3	1:A:15:LYS:HG3	1.97	0.45
1:A:211:GLY:HA2	1:A:214:GLN:HE22	1.81	0.45
5:I:192:HIS:ND1	5:I:194:THR:CA	2.80	0.45
5:I:211:ARG:HG2	5:I:286:GLN:HE21	1.81	0.45
5:I:395:TYR:HD2	5:I:412:LEU:HD13	1.81	0.45
7:M:180:LEU:HD12	7:M:184:PHE:CE2	2.51	0.45
2:C:15:ILE:HD12	2:C:67:ARG:HH22	1.80	0.45
2:C:164:VAL:HG22	2:C:229:VAL:HG23	1.97	0.45
4:G:237:ILE:O	4:G:297:LYS:NZ	2.47	0.45
5:I:135:LEU:HD21	5:I:150:LEU:HD21	1.98	0.45
5:J:328:THR:O	5:J:333:GLN:NE2	2.48	0.45
6:K:256:ALA:O	6:K:260:GLU:HB2	2.17	0.45
4:G:183:LEU:HD22	4:G:455:ASN:H	1.82	0.45
5:J:296:TYR:HE2	5:J:309:VAL:HG23	1.82	0.45
2:C:301:ASP:CA	5:I:191:SER:O	2.63	0.45
3:F:122:ARG:O	4:G:213:GLN:NE2	2.49	0.45
8:P:280:GLY:HA2	8:P:338:GLY:HA2	1.98	0.45
1:B:119:ILE:HG21	1:B:125:ILE:HD11	1.98	0.45
3:E:56:THR:OG1	3:E:81:ASP:O	2.34	0.45
4:G:330:GLY:N	4:G:355:ARG:O	2.46	0.45
1:A:202:GLU:HA	1:A:300:LEU:HD21	1.98	0.45
2:C:262:SER:HB3	2:D:261:HIS:HA	1.99	0.45
8:P:179:ILE:HG13	8:P:456:TRP:HB3	1.98	0.45
8:P:279:ALA:O	8:P:339:VAL:N	2.50	0.45
1:B:277:ALA:HB3	1:B:280:LEU:HD22	1.99	0.44
2:C:232:VAL:HG21	2:C:254:LEU:HD21	1.99	0.44
3:E:193:ILE:HG22	5:J:240:VAL:HB	1.99	0.44
3:F:160:VAL:HG12	3:F:196:HIS:HE1	1.82	0.44
5:J:129:ARG:N	5:J:133:ASP:OD2	2.50	0.44
5:J:451:LEU:HD13	5:J:460:GLU:HA	1.98	0.44
6:K:37:LEU:HD21	6:K:68:ASN:HD21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ALA:H	1:B:96:ARG:NH1	2.15	0.44
4:H:335:VAL:HG12	4:H:402:LEU:HD12	1.99	0.44
4:H:483:ARG:NH1	4:H:484:LEU:O	2.51	0.44
1:A:236:VAL:HG13	1:A:238:LEU:H	1.82	0.44
1:B:197:ALA:O	1:B:234:LYS:NZ	2.43	0.44
2:C:324:PHE:HE2	2:C:333:PRO:HA	1.80	0.44
3:E:122:ARG:HA	4:H:209:ARG:HD2	2.00	0.44
5:I:69:PRO:HG2	5:I:397:TRP:CE2	2.52	0.44
1:A:210:ILE:HD13	1:A:271:PRO:HG2	2.00	0.44
2:C:48:ASP:OD1	2:C:49:HIS:N	2.50	0.44
2:D:18:PHE:CG	2:D:41:LEU:HD11	2.51	0.44
8:P:44:ILE:HA	8:P:154:ALA:HB3	1.99	0.44
8:P:282:SER:HB2	8:P:336:LEU:HD12	2.00	0.44
1:A:112:ALA:O	1:A:116:HIS:ND1	2.51	0.44
8:P:321:LEU:HD23	8:P:339:VAL:HA	2.00	0.44
1:A:11:LYS:HA	1:A:14:MET:HG2	1.99	0.44
2:C:278:PHE:HB2	2:C:281:GLU:HB3	1.98	0.44
3:E:132:MET:HG3	3:E:199:LEU:HD12	1.98	0.44
4:G:177:VAL:HG12	4:G:179:LEU:H	1.82	0.44
5:J:154:ASP:OD2	5:J:300:VAL:N	2.51	0.44
5:J:286:GLN:NE2	5:J:287:ILE:O	2.51	0.44
1:A:238:LEU:HD11	1:A:246:VAL:HA	1.99	0.44
2:D:284:SER:OG	2:D:286:HIS:O	2.31	0.44
5:J:179:SER:HA	5:J:286:GLN:HB3	2.00	0.44
1:A:246:VAL:O	1:A:251:LYS:NZ	2.41	0.44
2:C:316:VAL:HA	2:C:317:PRO:HD3	1.80	0.44
2:D:222:ILE:HG12	2:D:254:LEU:HD12	2.00	0.44
3:F:155:ARG:HH21	3:F:173:GLU:HG2	1.83	0.44
4:H:326:LYS:NZ	4:H:506:MET:SD	2.77	0.44
5:J:76:ILE:HD11	5:J:105:HIS:CD2	2.53	0.44
3:E:1:MET:HG3	3:E:99:THR:HG21	2.00	0.44
4:G:214:TYR:OH	4:G:225:ARG:NH2	2.47	0.44
1:A:208:ASN:HB3	1:A:212:THR:HG21	1.98	0.43
2:D:31:SER:O	2:D:35:ALA:CB	2.65	0.43
4:H:257:LYS:NZ	4:H:281:ASN:HD21	2.15	0.43
5:J:47:LEU:HB3	5:J:93:VAL:HA	2.00	0.43
3:F:38:TYR:HA	3:F:41:ASN:HB2	2.00	0.43
4:H:269:LEU:HD11	4:H:274:HIS:HB2	2.00	0.43
4:H:407:ALA:HB3	4:H:415:MET:HB3	2.01	0.43
5:I:141:LYS:HD3	5:I:143:LEU:HD23	1.99	0.43
5:I:243:ASP:OD1	5:I:243:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:89:TYR:HA	8:P:127:VAL:HG23	1.99	0.43
8:P:309:LEU:HD13	8:P:367:ILE:HG12	2.01	0.43
5:J:141:LYS:HE3	5:J:143:LEU:HB2	1.99	0.43
5:J:195:ARG:HD3	5:J:245:LEU:HB3	1.99	0.43
6:K:229:LEU:HB3	8:P:271:VAL:HG23	1.99	0.43
8:P:437:VAL:HG13	8:P:459:ILE:HB	1.99	0.43
2:C:332:ALA:HB3	2:C:335:TYR:HB2	2.00	0.43
4:G:440:THR:OG1	4:G:503:GLU:OE2	2.36	0.43
5:I:128:TYR:HD2	5:I:130:SER:H	1.66	0.43
8:P:322:PHE:HB3	8:P:338:GLY:HA3	1.99	0.43
2:C:18:PHE:HA	2:C:21:THR:HG22	2.00	0.43
2:C:191:VAL:HG13	2:C:216:VAL:HG12	2.01	0.43
4:G:502:THR:OG1	4:G:503:GLU:N	2.51	0.43
5:J:266:TYR:HB3	5:J:272:PHE:HE1	1.84	0.43
8:P:127:VAL:HG12	8:P:128:ARG:HG3	2.01	0.43
1:A:36:ARG:HD3	1:A:45:LEU:HD21	2.01	0.43
1:A:270:HIS:HE1	1:B:178:VAL:HA	1.84	0.43
6:K:133:ARG:HE	6:K:168:LEU:HD21	1.83	0.43
8:P:169:GLN:HB3	8:P:173:HIS:CD2	2.54	0.43
1:A:43:GLN:HG2	6:K:45:MET:HG2	1.99	0.43
4:G:312:ILE:HD13	4:G:312:ILE:HA	1.86	0.43
5:I:269:ARG:HD2	5:I:272:PHE:HD2	1.83	0.43
8:P:294:ILE:HG12	8:P:358:LEU:HB3	2.01	0.43
6:K:171:ASP:N	6:K:171:ASP:OD1	2.50	0.43
6:L:112:LEU:HA	6:L:115:VAL:HG22	2.01	0.43
1:A:245:ASP:OD1	1:A:245:ASP:N	2.47	0.43
2:C:288:PHE:O	5:I:316:ARG:NH2	2.52	0.43
3:F:231:TYR:HD2	3:F:233:VAL:HG23	1.84	0.43
4:G:229:LEU:HD13	4:G:229:LEU:HA	1.91	0.43
5:J:54:ARG:HD3	5:J:57:PHE:HD2	1.84	0.43
6:K:258:ILE:HG23	6:K:269:PHE:HE2	1.83	0.43
5:J:76:ILE:O	5:J:80:LEU:HB2	2.18	0.43
1:A:119:ILE:H	1:A:119:ILE:HG13	1.56	0.42
1:A:210:ILE:HD11	1:B:182:ALA:HA	2.01	0.42
3:E:72:LYS:HE3	3:E:75:ILE:HG12	2.01	0.42
4:H:508:PRO:O	4:H:511:SER:OG	2.35	0.42
5:I:107:LEU:HA	5:I:112:CYS:HB3	2.01	0.42
6:K:254:ALA:O	6:K:258:ILE:HG12	2.19	0.42
3:E:231:TYR:HD2	3:E:233:VAL:HG23	1.84	0.42
4:H:334:LEU:HD23	4:H:398:VAL:HG21	2.00	0.42
4:H:346:LEU:HD13	4:H:346:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:44:GLN:HE22	5:J:144:VAL:HA	1.85	0.42
8:P:141:LEU:HG	8:P:145:MET:HB2	2.01	0.42
5:I:431:LEU:HB3	5:I:435:VAL:HG21	2.00	0.42
5:J:149:LEU:HD23	5:J:251:ILE:HG23	2.01	0.42
1:B:173:VAL:HG22	1:B:174:PRO:HD2	2.01	0.42
1:B:238:LEU:HD11	1:B:250:PHE:HE2	1.84	0.42
6:K:100:ASP:OD1	6:K:104:LYS:NZ	2.48	0.42
1:A:23:ALA:O	1:A:27:ILE:HG12	2.19	0.42
1:A:86:TYR:HB2	6:K:75:ARG:HD2	2.01	0.42
2:C:241:ALA:HB2	2:C:276:PRO:HA	2.01	0.42
3:E:130:MET:HB2	3:E:265:SER:HB2	2.02	0.42
4:G:250:ARG:HA	4:G:253:VAL:HG12	2.01	0.42
6:K:247:GLY:O	6:K:251:LEU:CB	2.66	0.42
8:P:400:LYS:HA	8:P:417:VAL:HG23	2.01	0.42
1:A:45:LEU:HD22	1:A:49:LEU:HD12	2.01	0.42
1:A:185:TYR:HA	1:B:243:GLN:HE21	1.83	0.42
1:B:108:ARG:HG2	1:B:136:ARG:HD3	2.01	0.42
1:B:124:THR:HG23	1:B:190:ALA:HA	2.02	0.42
2:C:20:GLU:HA	2:C:23:LYS:HG2	2.01	0.42
2:D:36:ARG:HA	2:D:39:LEU:HG	2.02	0.42
8:P:47:ILE:O	8:P:158:LEU:N	2.49	0.42
8:P:381:LEU:HD13	8:P:392:ALA:HA	2.01	0.42
2:C:192:ALA:HB2	2:C:217:MET:HE2	2.00	0.42
4:G:209:ARG:O	4:G:213:GLN:HG2	2.19	0.42
4:G:242:THR:N	4:G:293:GLU:OE2	2.45	0.42
4:H:197:SER:OG	4:H:199:PRO:O	2.33	0.42
1:A:78:LEU:H	1:A:78:LEU:HG	1.58	0.42
3:F:396:VAL:HA	3:F:413:ALA:HB3	2.02	0.42
4:G:409:LEU:HB3	4:G:447:VAL:HG23	2.01	0.42
4:H:409:LEU:HD22	4:H:410:ALA:H	1.84	0.42
1:B:43:GLN:HB2	6:L:45:MET:HG3	2.02	0.42
1:B:73:LEU:HD13	1:B:73:LEU:HA	1.93	0.42
1:B:90:LYS:HA	1:B:93:MET:HB2	2.01	0.42
2:C:246:ARG:HE	2:C:285:PHE:HD2	1.68	0.42
5:I:47:LEU:HD23	5:I:151:VAL:HG13	2.01	0.42
5:I:324:GLU:HG3	5:I:335:CYS:SG	2.59	0.42
2:D:310:CYS:HA	2:D:311:PRO:HD3	1.86	0.42
2:D:320:LEU:HD12	2:D:320:LEU:HA	1.88	0.42
4:G:260:MET:HA	4:G:263:LEU:HB2	2.02	0.42
4:H:490:ASP:OD1	4:H:490:ASP:N	2.53	0.42
5:I:182:THR:HB	5:I:251:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:410:GLN:HB3	5:I:427:PRO:HB3	2.02	0.42
6:K:112:LEU:HB3	6:K:131:PHE:CE1	2.55	0.42
7:M:179:LEU:HD11	8:P:230:TYR:CG	2.54	0.42
8:P:98:ARG:HB2	8:P:100:GLU:HG3	2.01	0.41
1:A:78:LEU:HD12	1:A:79:ALA:H	1.85	0.41
3:F:180:LEU:HD11	5:I:226:PHE:HB2	2.01	0.41
5:I:111:TRP:CD1	5:I:118:ASN:HB3	2.55	0.41
7:M:179:LEU:O	7:M:184:PHE:CD2	2.72	0.41
1:B:87:SER:O	1:B:92:ILE:N	2.54	0.41
3:F:31:GLY:N	3:F:33:LYS:O	2.53	0.41
7:M:179:LEU:CD1	8:P:230:TYR:CE2	2.98	0.41
8:P:88:ILE:HD13	8:P:240:VAL:HG11	2.02	0.41
8:P:256:LEU:HD13	8:P:283:ILE:HG22	2.02	0.41
3:E:109:ILE:HG12	3:E:276:ALA:HA	2.01	0.41
3:F:67:PHE:HD1	3:F:75:ILE:HD13	1.86	0.41
4:G:170:ARG:HH21	4:G:265:GLN:HA	1.86	0.41
4:H:213:GLN:O	4:H:216:GLN:NE2	2.52	0.41
4:H:367:LEU:HD13	4:H:370:ARG:HE	1.85	0.41
6:L:21:MET:HG3	6:L:70:CYS:HA	2.02	0.41
4:G:207:MET:HG2	4:G:263:LEU:HD21	2.02	0.41
5:I:330:SER:OG	5:I:332:THR:OG1	2.37	0.41
8:P:64:VAL:HB	8:P:84:ALA:HA	2.02	0.41
3:F:39:PRO:O	3:F:43:LEU:CB	2.68	0.41
3:F:182:ILE:HG21	3:F:187:LEU:HD22	2.03	0.41
4:G:180:PHE:HB3	4:G:183:LEU:HB2	2.02	0.41
8:P:82:GLY:H	8:P:134:ASP:HB3	1.85	0.41
8:P:290:VAL:HG12	8:P:330:TYR:HE1	1.84	0.41
8:P:296:VAL:HB	8:P:358:LEU:HG	2.01	0.41
1:B:48:ASN:OD1	1:B:49:LEU:N	2.54	0.41
2:C:303:LEU:HD21	5:I:317:TRP:HZ2	1.86	0.41
4:H:200:SER:OG	4:H:203:ILE:O	2.39	0.41
5:I:374:ILE:HG13	5:I:391:LEU:HD23	2.02	0.41
5:J:360:VAL:HG12	5:J:377:SER:H	1.84	0.41
3:F:88:ASP:N	3:F:88:ASP:OD1	2.53	0.41
5:J:443:LEU:HD11	5:J:447:SER:HB3	2.02	0.41
8:P:174:LEU:HD22	8:P:214:THR:HG23	2.02	0.41
8:P:295:GLU:HG3	8:P:314:ILE:O	2.20	0.41
1:A:163:LYS:HA	1:A:166:LYS:HG2	2.02	0.41
3:F:32:ASN:H	3:F:37:TRP:HZ2	1.69	0.41
5:J:45:ALA:HA	5:J:149:LEU:H	1.85	0.41
6:K:148:GLY:O	6:K:152:ALA:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:14:PRO:HD3	6:L:39:TYR:CE2	2.56	0.41
6:L:115:VAL:HB	6:L:116:ALA:H	1.61	0.41
8:P:294:ILE:O	8:P:316:SER:OG	2.38	0.41
2:C:306:VAL:O	5:I:315:ARG:NH1	2.54	0.41
2:D:159:ILE:HD11	2:D:181:ALA:HB1	2.02	0.41
3:F:97:LEU:HD12	3:F:101:VAL:HG11	2.03	0.41
5:I:231:PHE:HE1	5:I:238:VAL:HG11	1.86	0.41
3:F:33:LYS:H	3:F:37:TRP:HE1	1.69	0.40
4:H:483:ARG:HD2	4:H:483:ARG:HA	1.76	0.40
5:I:332:THR:OG1	5:I:333:GLN:OE1	2.31	0.40
5:J:85:ALA:O	5:J:160:ASN:ND2	2.54	0.40
5:J:149:LEU:HD21	5:J:249:ILE:HG22	2.02	0.40
5:J:183:MET:SD	5:J:269:ARG:NH1	2.90	0.40
8:P:43:ASN:HB2	8:P:153:ASP:H	1.85	0.40
1:A:168:LEU:HD23	1:A:175:VAL:HB	2.02	0.40
1:A:225:PRO:HA	1:A:282:THR:HG21	2.04	0.40
3:E:424:CYS:HA	3:E:441:GLU:HA	2.02	0.40
5:I:247:CYS:HB2	5:I:299:ARG:HB2	2.03	0.40
6:L:7:ARG:O	6:L:113:ARG:NE	2.54	0.40
1:B:165:ALA:HA	1:B:175:VAL:HG11	2.03	0.40
2:D:253:THR:HG1	4:H:422:GLN:HE21	1.60	0.40
3:E:212:VAL:O	3:E:216:MET:HG2	2.22	0.40
5:J:134:VAL:HA	5:J:137:ASP:HB2	2.03	0.40
8:P:52:HIS:HB3	8:P:161:GLY:H	1.86	0.40
8:P:155:ALA:HB3	8:P:185:ILE:HG12	2.02	0.40
1:B:237:ARG:HH12	1:B:304:TYR:HB3	1.87	0.40
3:F:224:ILE:HA	3:F:227:GLU:HG2	2.03	0.40
4:H:203:ILE:HA	4:H:259:TYR:CE1	2.56	0.40
5:I:186:LYS:HZ1	5:I:245:LEU:HD23	1.85	0.40
5:J:67:LEU:HD13	5:J:101:GLN:HG2	2.03	0.40
8:P:323:ALA:HA	8:P:337:ILE:HG13	2.02	0.40
2:D:341:SER:HA	2:D:346:PRO:HG3	2.04	0.40
5:I:195:ARG:HD2	5:I:200:ASN:HA	2.03	0.40
5:J:131:LEU:HD22	5:J:268:THR:HA	2.03	0.40
6:L:77:ASP:OD2	6:L:81:GLY:N	2.55	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	281/305 (92%)	247 (88%)	34 (12%)	0	100	100
1	B	280/305 (92%)	242 (86%)	38 (14%)	0	100	100
2	C	314/351 (90%)	292 (93%)	21 (7%)	1 (0%)	41	76
2	D	314/351 (90%)	285 (91%)	29 (9%)	0	100	100
3	E	317/452 (70%)	260 (82%)	57 (18%)	0	100	100
3	F	313/452 (69%)	257 (82%)	56 (18%)	0	100	100
4	G	355/523 (68%)	323 (91%)	31 (9%)	1 (0%)	41	76
4	H	355/523 (68%)	314 (88%)	41 (12%)	0	100	100
5	I	417/721 (58%)	352 (84%)	64 (15%)	1 (0%)	47	81
5	J	417/721 (58%)	357 (86%)	60 (14%)	0	100	100
6	K	231/315 (73%)	198 (86%)	33 (14%)	0	100	100
6	L	161/315 (51%)	120 (74%)	39 (24%)	2 (1%)	13	50
7	M	14/333 (4%)	14 (100%)	0	0	100	100
8	P	419/472 (89%)	337 (80%)	82 (20%)	0	100	100
All	All	4188/6139 (68%)	3598 (86%)	585 (14%)	5 (0%)	54	85

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	I	194	THR
6	L	115	VAL
6	L	116	ALA
4	G	494	PRO
2	C	279	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	243/260 (94%)	240 (99%)	3 (1%)	71 84
1	B	242/260 (93%)	239 (99%)	3 (1%)	71 84
2	C	270/298 (91%)	264 (98%)	6 (2%)	52 71
2	D	270/298 (91%)	266 (98%)	4 (2%)	65 80
3	E	192/398 (48%)	189 (98%)	3 (2%)	62 79
3	F	188/398 (47%)	188 (100%)	0	100 100
4	G	313/444 (70%)	307 (98%)	6 (2%)	57 75
4	H	313/444 (70%)	307 (98%)	6 (2%)	57 75
5	I	376/626 (60%)	370 (98%)	6 (2%)	62 79
5	J	376/626 (60%)	372 (99%)	4 (1%)	73 85
6	K	211/280 (75%)	210 (100%)	1 (0%)	88 93
6	L	151/280 (54%)	144 (95%)	7 (5%)	27 53
7	M	16/304 (5%)	16 (100%)	0	100 100
8	P	353/397 (89%)	344 (98%)	9 (2%)	47 68
All	All	3514/5313 (66%)	3456 (98%)	58 (2%)	62 78

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LEU
1	A	91	LYS
1	A	249	LYS
1	B	88	LYS
1	B	164	MET
1	B	173	VAL
2	C	83	ARG
2	C	207	LEU
2	C	217	MET
2	C	271	MET
2	C	287	LYS

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Mol	Chain	Res	Type
2	C	316	VAL
2	D	24	ARG
2	D	81	MET
2	D	246	ARG
2	D	338	ARG
3	E	192	ARG
3	E	199	LEU
3	E	234	ARG
4	G	231	ARG
4	G	314	LEU
4	G	401	VAL
4	G	446	ARG
4	G	499	LEU
4	G	506	MET
4	H	196	MET
4	H	257	LYS
4	H	301	ARG
4	H	309	GLN
4	H	341	LEU
4	H	446	ARG
5	I	72	ASN
5	I	80	LEU
5	I	160	ASN
5	I	289	MET
5	I	420	LYS
5	I	440	ASN
5	J	160	ASN
5	J	230	LEU
5	J	299	ARG
5	J	440	ASN
6	K	266	ARG
6	L	7	ARG
6	L	21	MET
6	L	89	ARG
6	L	123	LYS
6	L	133	ARG
6	L	173	ARG
6	L	183	ARG
8	P	70	LYS
8	P	71	ASN
8	P	75	ARG
8	P	229	LYS

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Mol	Chain	Res	Type
8	P	379	ARG
8	P	385	ARG
8	P	394	LYS
8	P	396	GLN
8	P	449	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	A	270	HIS
2	C	242	ASN
2	C	277	GLN
2	C	345	HIS
2	D	130	GLN
2	D	132	ASN
2	D	138	ASN
2	D	154	GLN
2	D	201	HIS
3	E	274	ASN
3	F	41	ASN
3	F	196	HIS
4	G	234	GLN
4	G	265	GLN
4	G	329	ASN
4	G	347	GLN
4	G	422	GLN
4	H	234	GLN
4	H	238	GLN
4	H	281	ASN
4	H	422	GLN
4	H	431	ASN
4	H	479	HIS
5	I	72	ASN
5	I	160	ASN
5	I	286	GLN
5	I	288	HIS
5	I	440	ASN
5	J	105	HIS
5	J	118	ASN
5	J	160	ASN
5	J	168	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	J	286	GLN
5	J	288	HIS
5	J	434	GLN
5	J	440	ASN
6	K	68	ASN
8	P	138	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

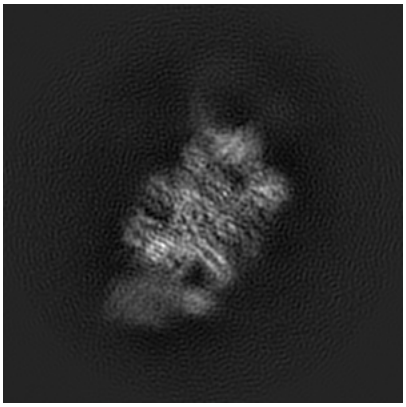
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9841. These allow visual inspection of the internal detail of the map and identification of artifacts.

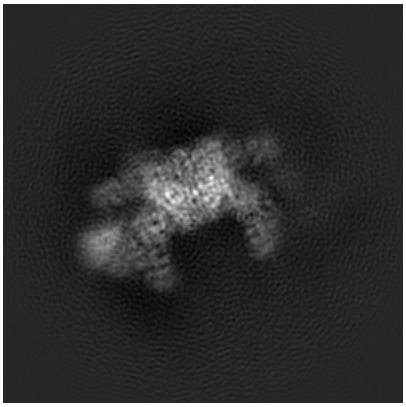
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

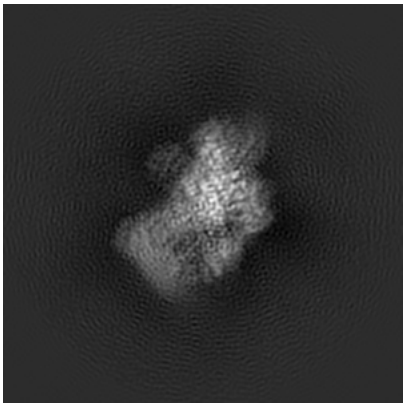
6.1.1 Primary map



X



Y

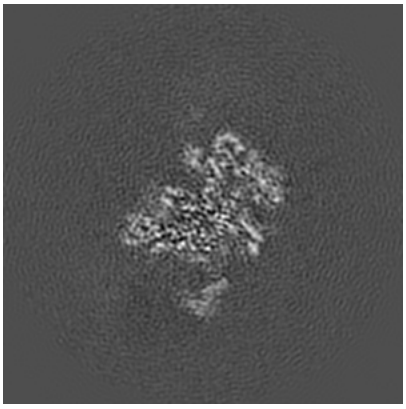


Z

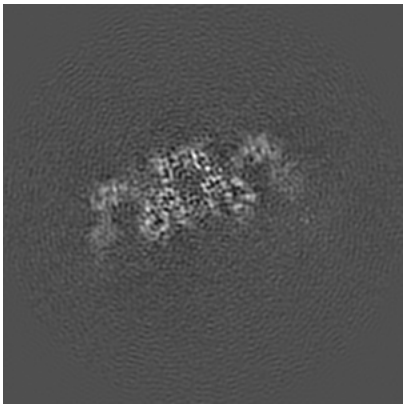
The images above show the map projected in three orthogonal directions.

6.2 Central slices

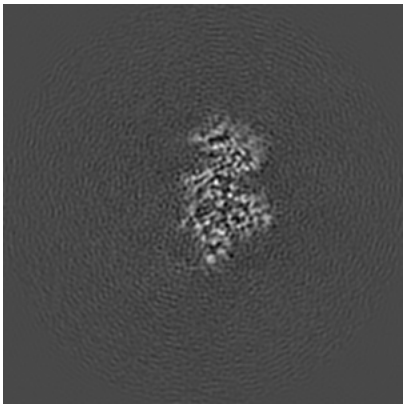
6.2.1 Primary map



X Index: 125



Y Index: 125

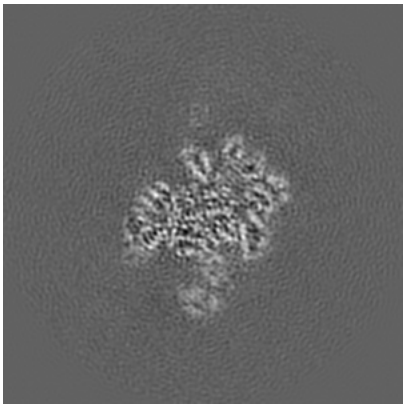


Z Index: 125

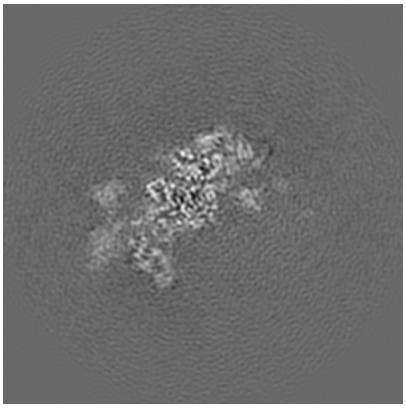
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

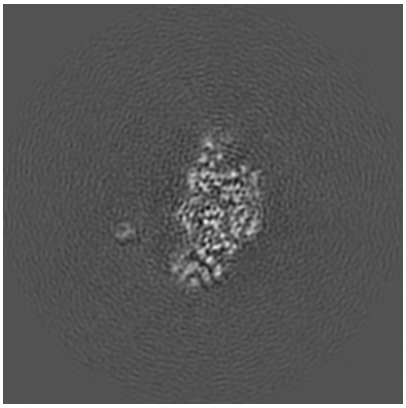
6.3.1 Primary map



X Index: 130



Y Index: 115

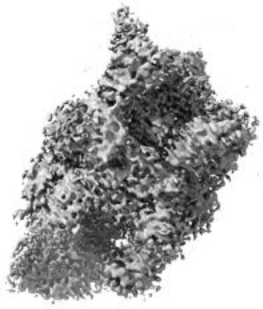


Z Index: 110

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 0.0104. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

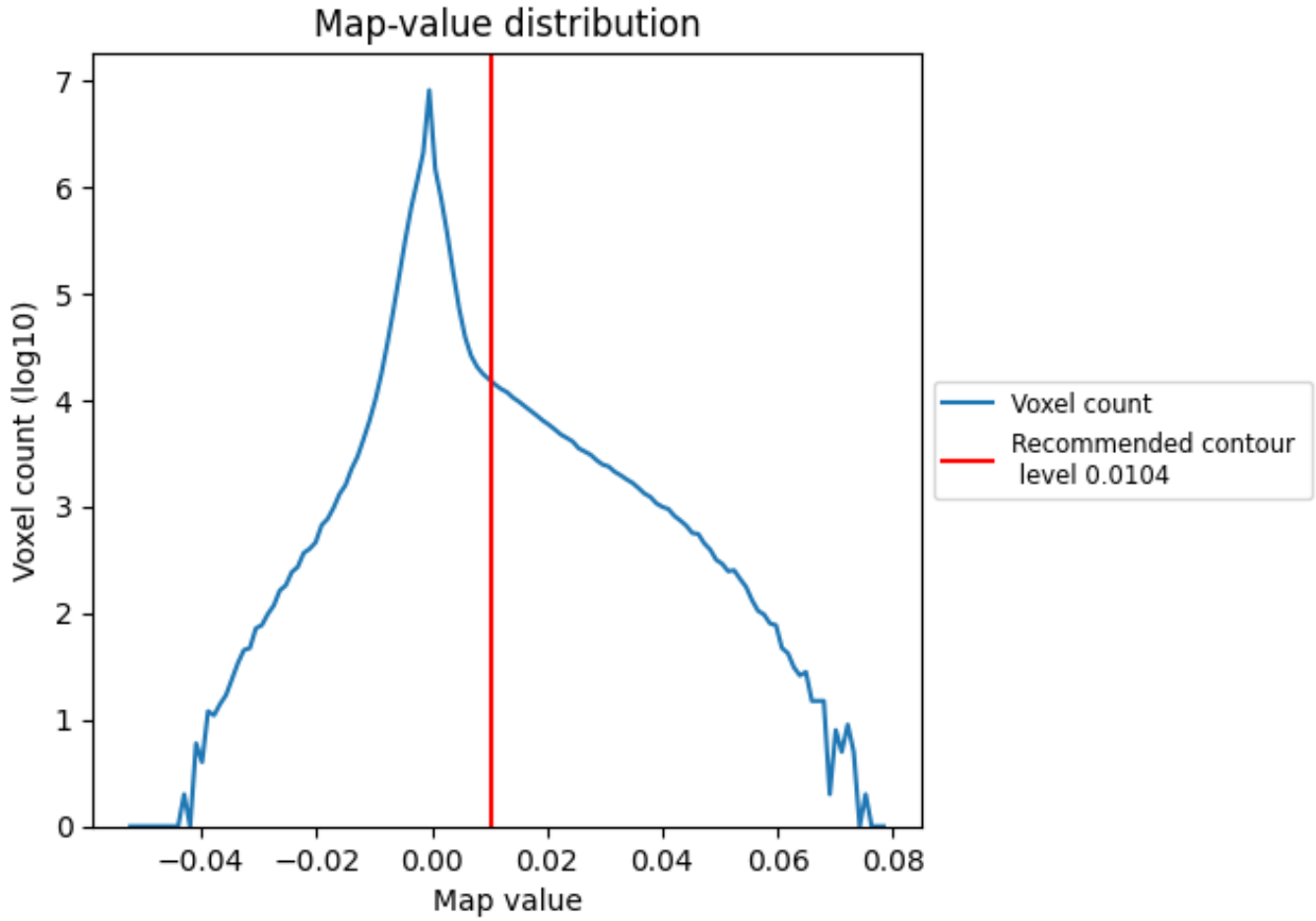
6.5 Mask visualisation (i)

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

7 Map analysis

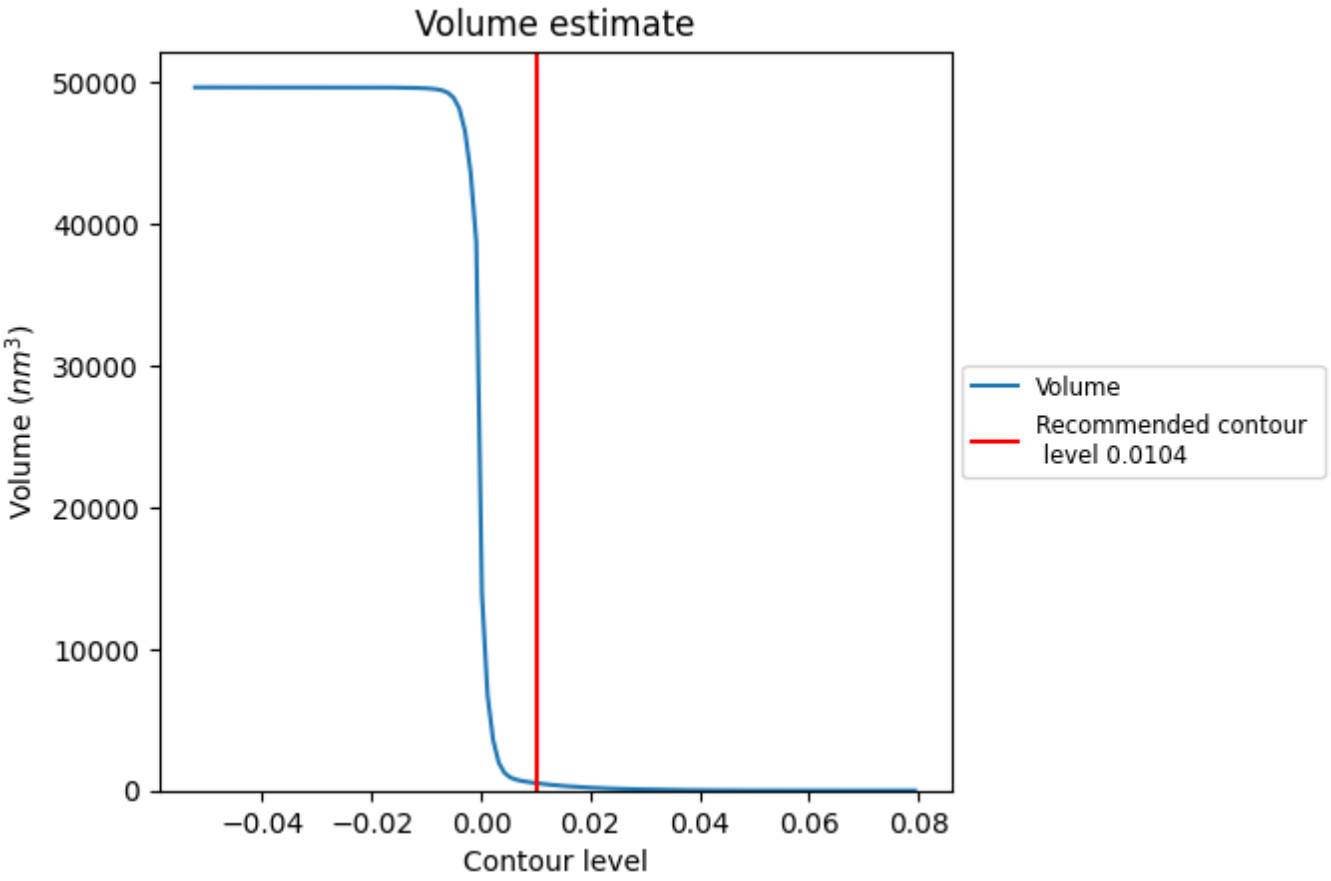
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

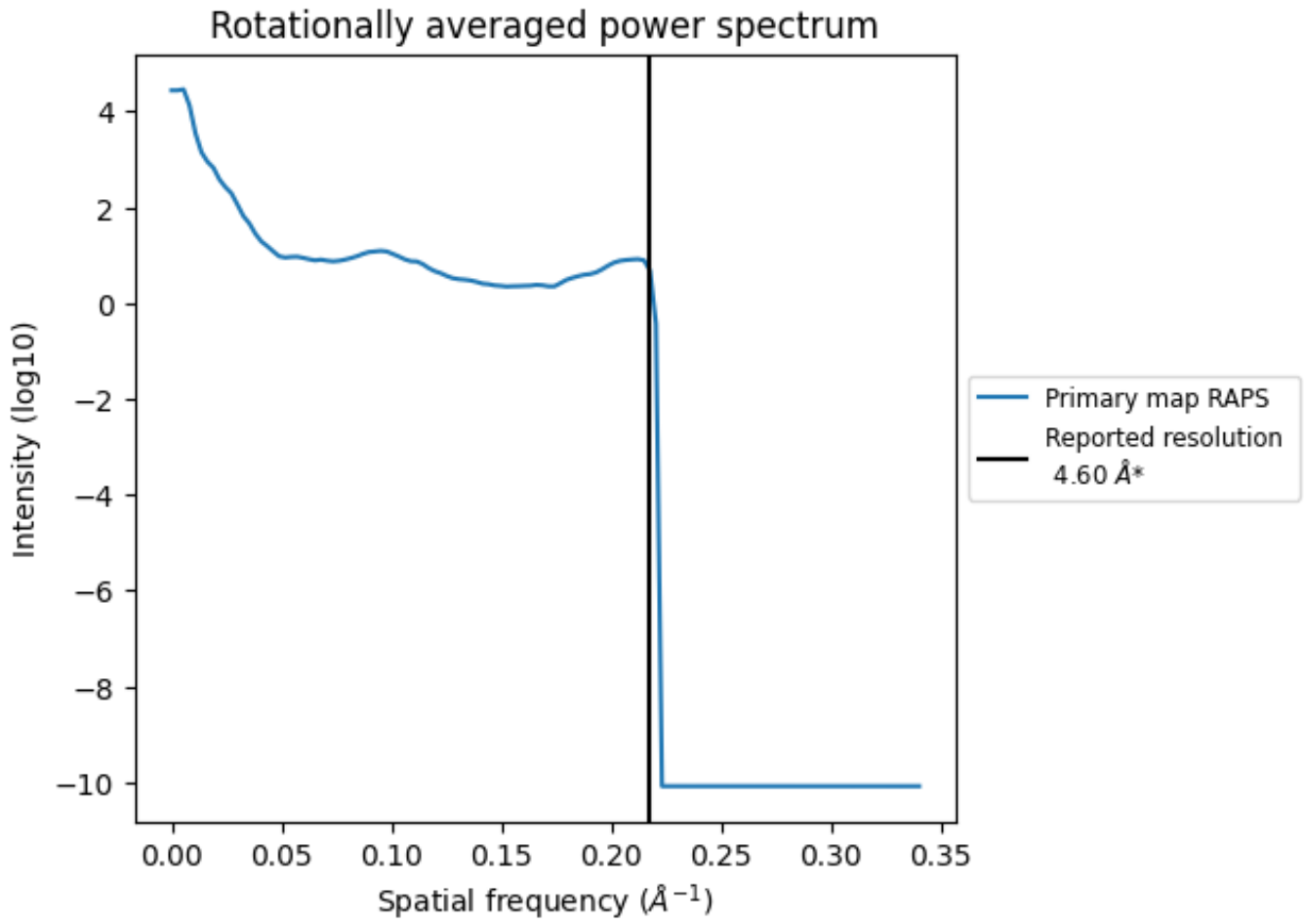
7.2 Volume estimate



The volume at the recommended contour level is 508 nm^3; this corresponds to an approximate mass of 459 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

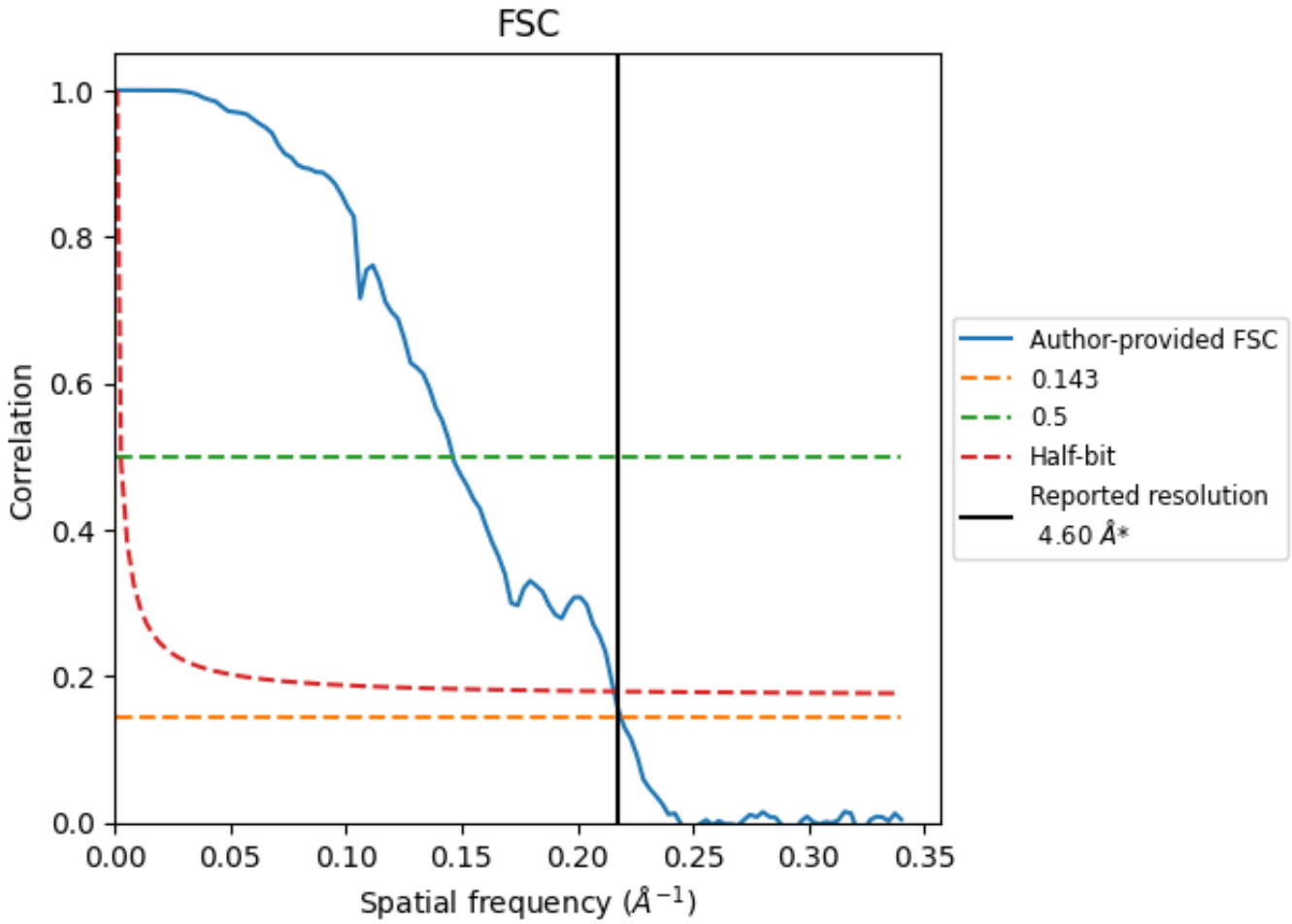


*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

8 Fourier-Shell correlation

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 0.217 Å^{-1}

8.2 Resolution estimates (i)

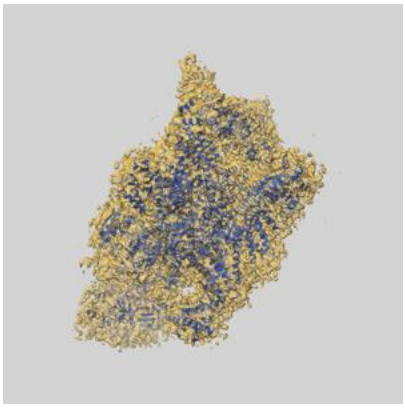
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.57	6.84	4.63
Unmasked-calculated*	-	-	-

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

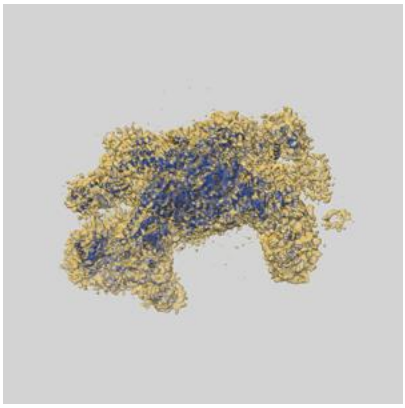
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9841 and PDB model 6K72. Per-residue inclusion information can be found in section 3 on page 6.

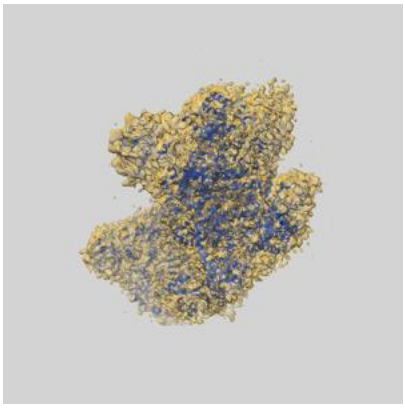
9.1 Map-model overlay



X



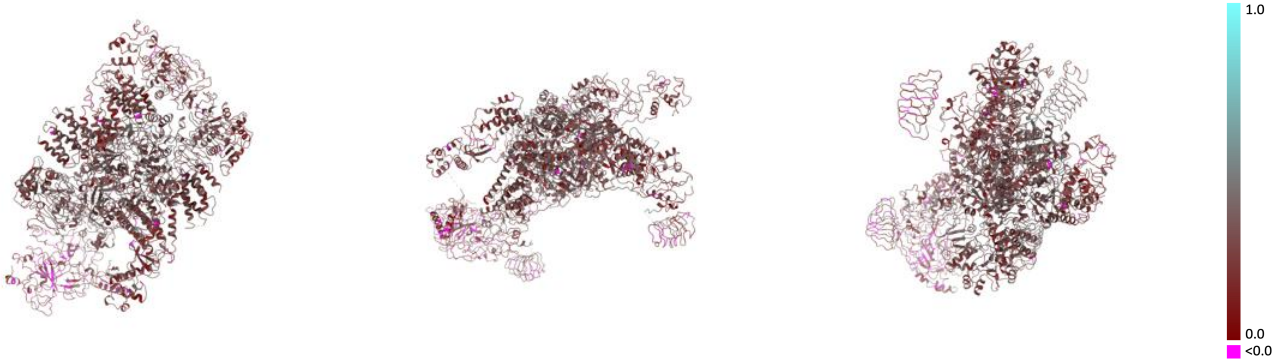
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0104 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.

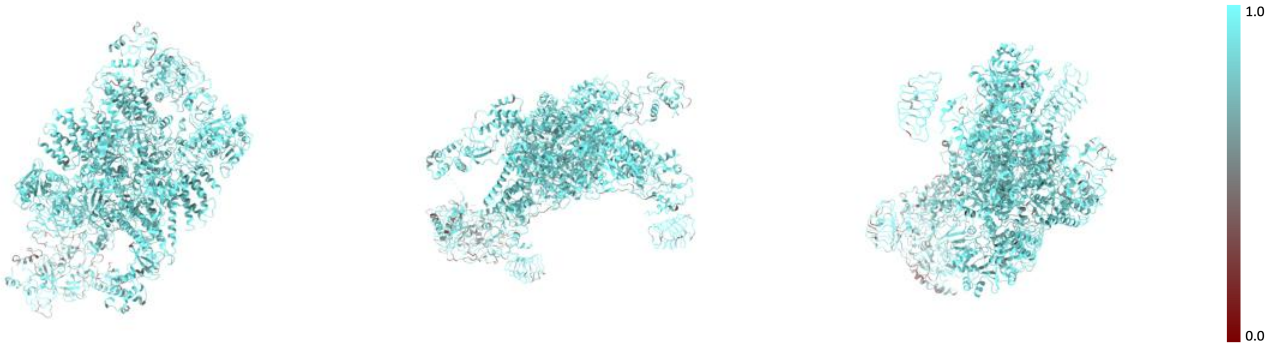
9.2 Q-score mapped to coordinate model (i)



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.

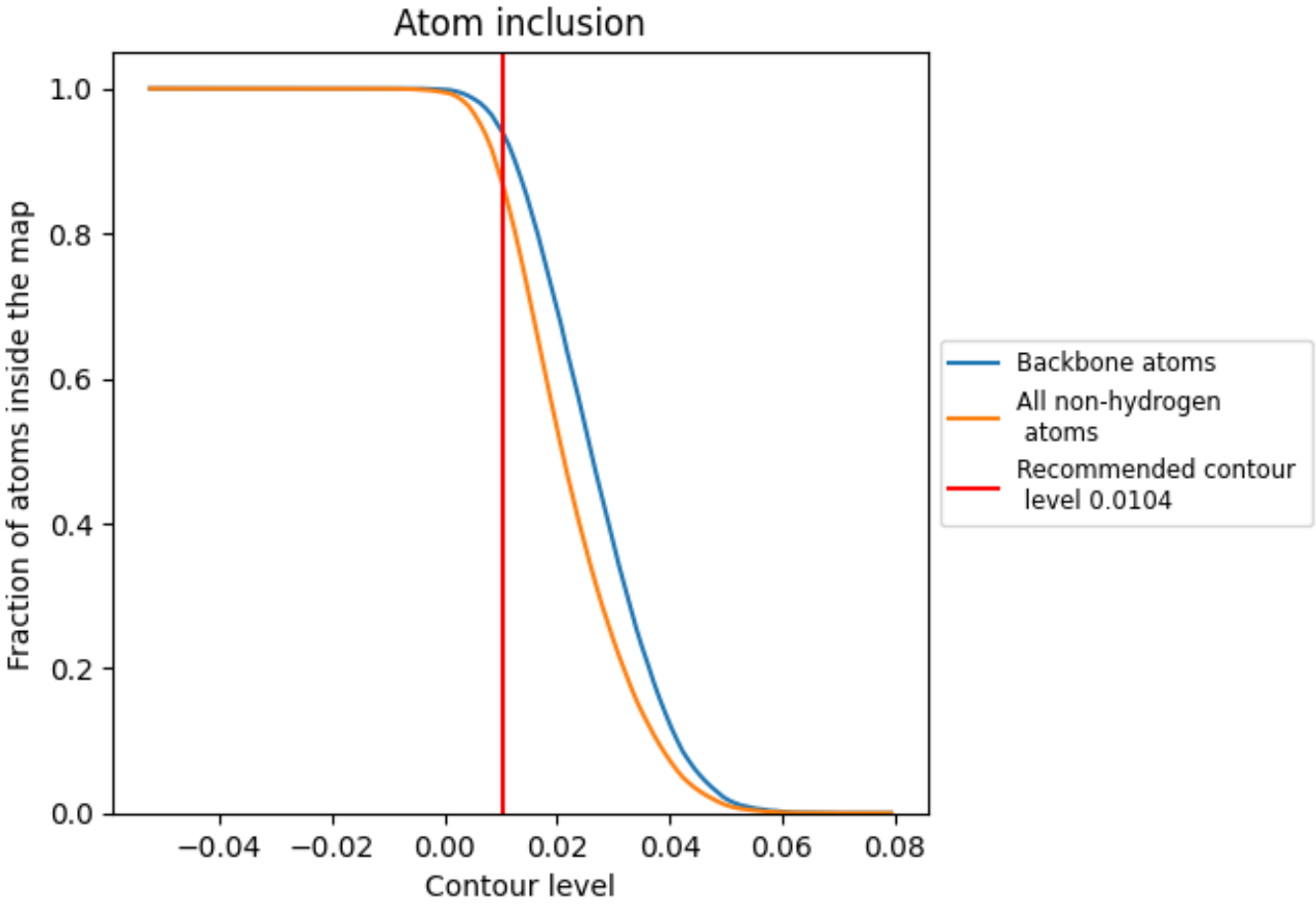
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0104).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 87% 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 (0.0104) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8675	0.2980
A	0.8916	0.3130
B	0.8976	0.3210
C	0.8823	0.3330
D	0.8991	0.3270
E	0.8754	0.2640
F	0.8679	0.2880
G	0.8785	0.3280
H	0.8818	0.3370
I	0.9165	0.3400
J	0.9075	0.3160
K	0.8110	0.2530
L	0.7905	0.2730
M	0.7194	0.1790
P	0.7471	0.1760