W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB EM Validation Report (i)

Nov 22, 2022 – 12:39 AM JST

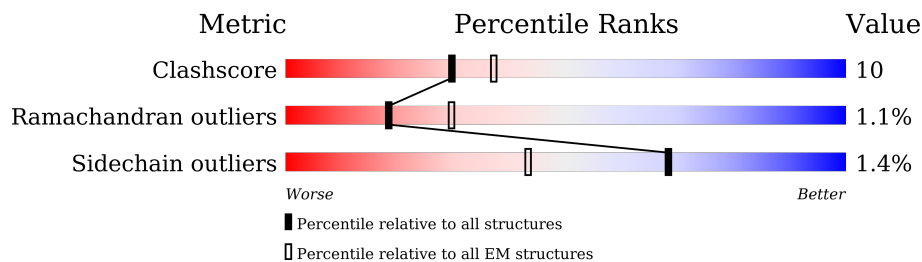|		
PDB ID	:	7E2C
EMDB ID	:	EMD-30954
Title	:	Monomer of TRAPPII (open)
Authors	:	Sui, S.F.; Sun, S.; Mi, C.C.
Deposited on	:	2021-02-05
Resolution	:	4.18 Å(reported)

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 4.18 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	Percentile Ranks	Value
Clashscore		10
Ramachandran outliers		1.1%
Sidechain outliers		1.4%

Worse   *Better*

∎ Percentile relative to all structures
⧠ Percentile relative to all EM structures

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	152	10% 68% 28% • •
2	B	268	• 53% 18% • 27%
3	C	193	• 76% 19% • 5%
3	F	193	• 75% 18% • 6%
4	D	159	74% 19% • 5%
5	E	219	58% 16% 26%
6	G	283	57% 14% • 28%
7	H	175	• 61% 19% • 17%

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Mol	Chain	Length	Quality of chain
8	I	1102	66%　　　6% •　　27%
9	J	1289	56%　　　11% •　　32%
10	K	559	39%　　6% •　　55%

2 Entry composition ⓘ

There are 10 unique types of molecules in this entry. The entry contains 23020 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 TRAPP-associated protein TCA17.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	150	Total 1206	C 781	N 188	O 233	S 4	0	0

- Molecule 2 is a protein called Trafficking protein particle complex subunit 33.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	195	Total 1458	C 939	N 247	O 264	S 8	0	0

- Molecule 3 is a protein called Trafficking protein particle complex subunit BET3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	184	Total 1482	C 947	N 244	O 280	S 11	0	0
3	F	182	Total 1470	C 939	N 242	O 278	S 11	0	0

- Molecule 4 is a protein called Trafficking protein particle complex subunit BET5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	151	Total 1234	C 792	N 209	O 227	S 6	0	0

- Molecule 5 is a protein called Trafficking protein particle complex subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	161	Total 1295	C 838	N 206	O 242	S 9	0	0

- Molecule 6 is a protein called Trafficking protein particle complex subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	203	Total 1612	C 1029	N 282	O 292	S 9	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	41	TYR	ILE	conflict	UNP Q03337
G	42	ILE	PRO	conflict	UNP Q03337

- Molecule 7 is a protein called Trafficking protein particle complex subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	146	Total 1172	C 758	N 194	O 215	S 5	0	0

- Molecule 8 is a protein called Trafficking protein particle complex II-specific subunit 130.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	799	Total 4258	C 2590	N 822	O 844	S 2	0	0

- Molecule 9 is a protein called Trafficking protein particle complex II-specific subunit 120.

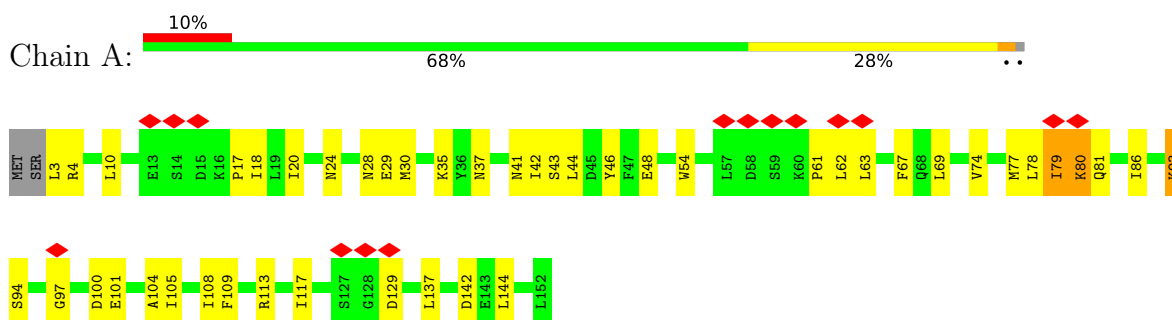| Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	873	Total 6265	C 3988	N 1085	O 1173	S 19	0	0

- Molecule 10 is a protein called Trafficking protein particle complex II-specific subunit 65.

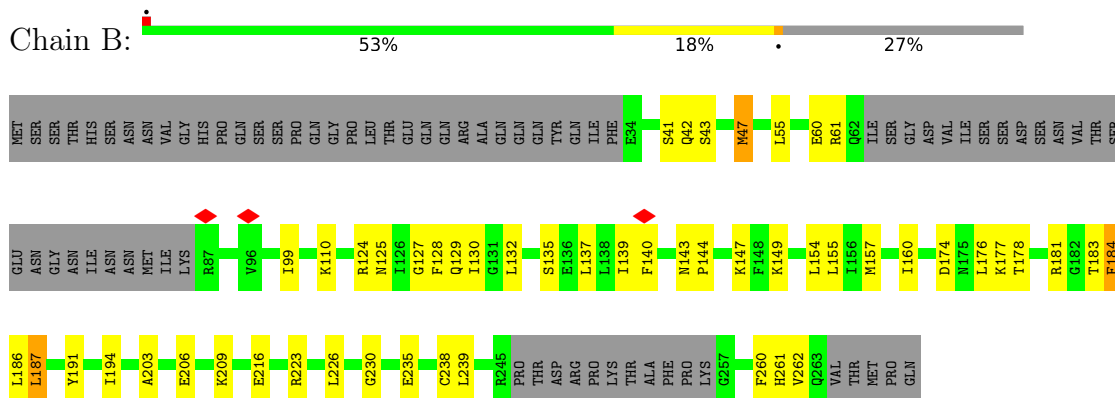| Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	251	Total 1568	C 988	N 278	O 300	S 2	0	0

3 Residue-property plots ⓘ

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.
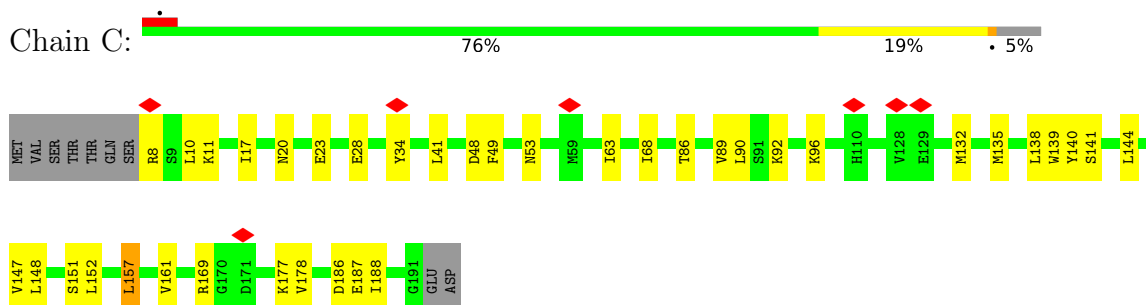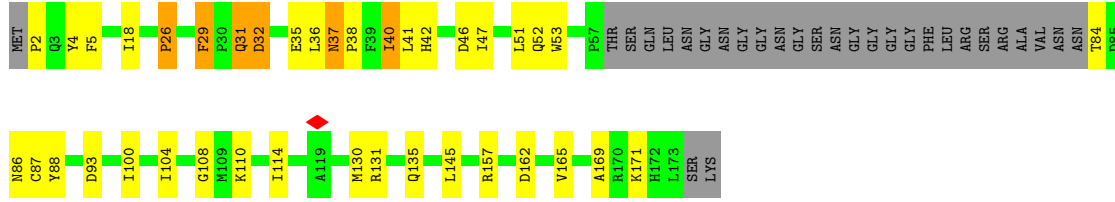
• Molecule 1: TRAPP-associated protein TCA17

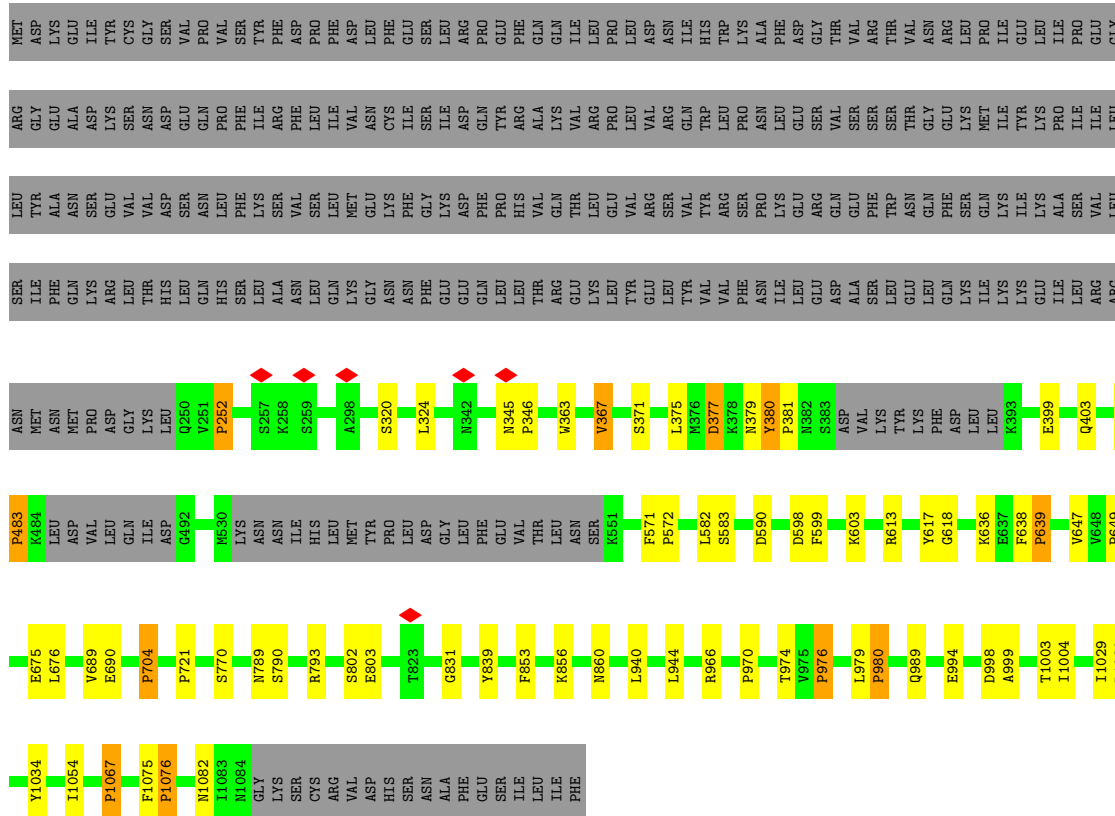• Molecule 2: Trafficking protein particle complex subunit 33

• Molecule 3: Trafficking protein particle complex subunit BET3
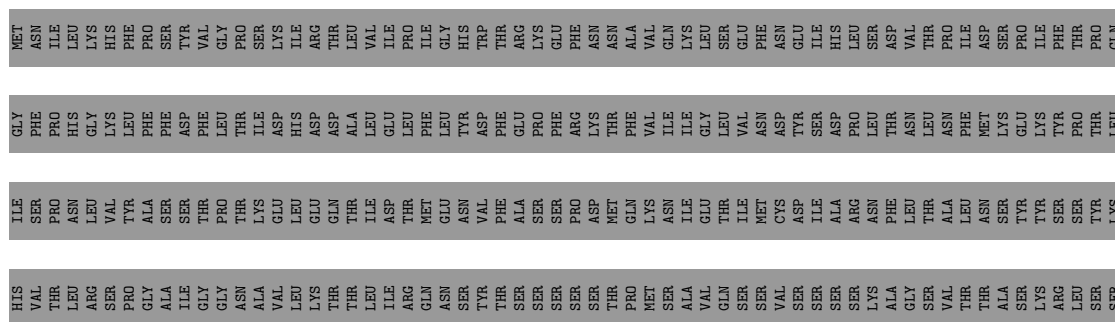

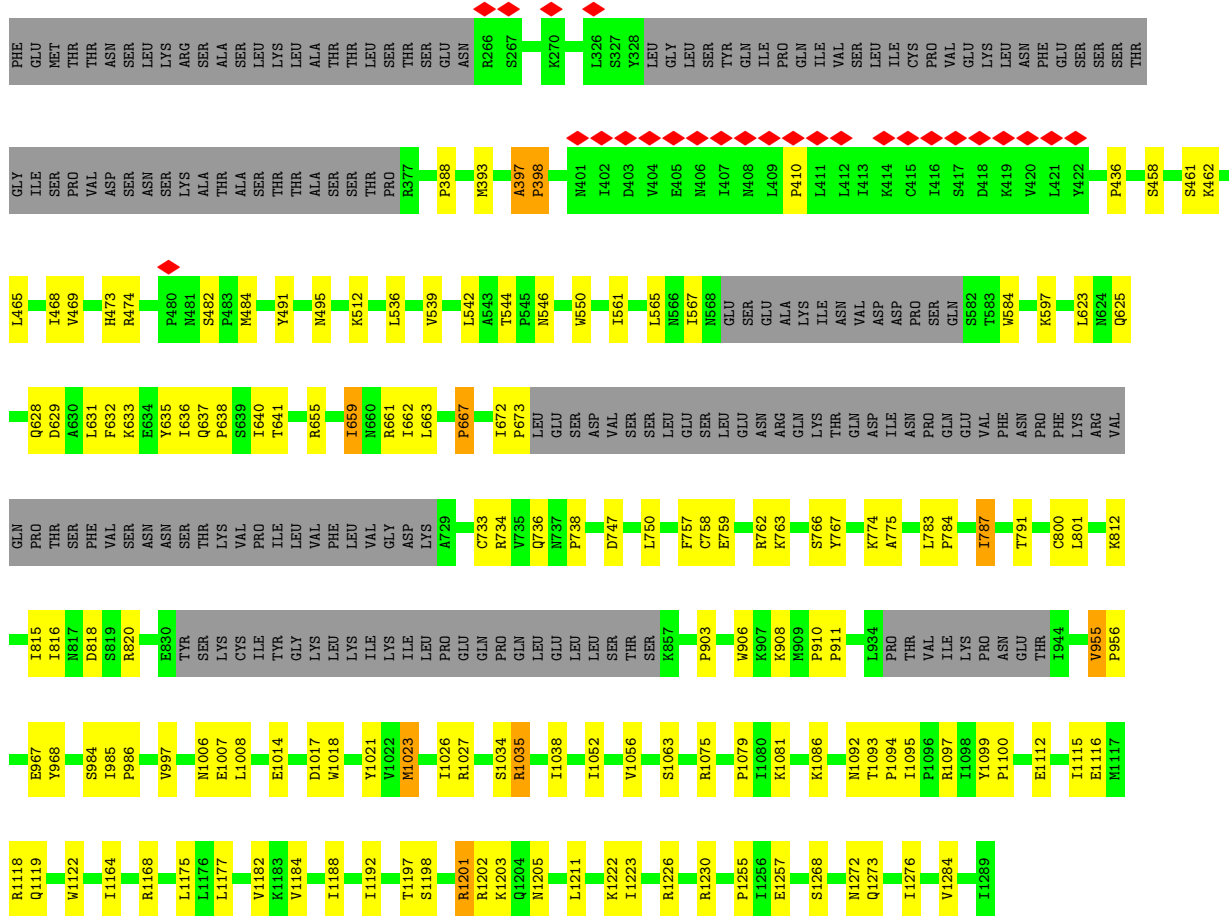• Molecule 3: Trafficking protein particle complex subunit BET3

Chain F: 75% 18% 6%

MET VAL SER THR THR GLN SER R8 M13 I17 N26 T27 E28 L29 F49 N53 M59 F71 T75 R79 N82 K85 T86 S87 E88 V89 L90 A94 F95 K96 L99 N100 I101 W108 S109 K112 D113 T114 L119 D120 E121 D126

S137 L138 L144 V147 D166 R169 T174 R182 I183 L184 K185 P189 ILE GLY GLU ASP

• Molecule 4: Trafficking protein particle complex subunit BET5

Chain D: 74% 19% 5%

MET G2 W7 D10 R11 I16 F17 D18 R19 E20 A24 S29 GLY THR ILE ASN SER K35 I48 R52 K64 I67 R68 S69 I70 S71 G85 L86 S92 D93 F94 K95 Y99 V102 L103 I106 I110 K113 Y114 N117 N118 L119 L120

R133 N142 F145 V148 V157 ASN GLN

• Molecule 5: Trafficking protein particle complex subunit 23

Chain E: 58% 16% 26%

MET A2 V8 I9 N10 I16 Y17 N20 N23 E32 I35 L36 K53 A54 L55 GLN LEU THR GLN GLN THR ASN ILE GLU N65 M75 SER SER ASN ARG SER ASP THR ARG ASN GLY GLY ASN ASN ASN LYS HIS THR ASN ASN GLU LYS LEU GLY SER PHE

LYS GLY D104 T112 N113 W114 M115 R120 Q121 L122 C123 T124 D125 Q126 F130 Q133 T134 L135 T136 G137 L138 K139 F140 V141 A142 M148 PRO GLN ARG GLN PRO THR ILE ALA THR THR ASP LYS PRO ASP ARG PRO LYS SER THR SER N169 F178 L179 V190 I202

Q219

• Molecule 6: Trafficking protein particle complex subunit 31

Chain G: 57% 14% 28%

MET SER GLN ARG ILE ILE GLN PRO SER ALA SER ASP GLN GLN PHE PRO GLY LYS SER ASP GLY TYR GLU TYR THR V26 G27 P28 I42 M62 D89 I94 R97 L98 L101 S107 V108 SER PRO SER LEU PRO ARG ALA SER ALA PHE LEU SER GLN ASN GLU

SER SER SER LYS LEU SER ASN ASN ALA SER ASN SER PRO GLY MET LEU ALA ASN SER SER THR ALA THR SER SER ALA ASN GLU LEU ARG LEU GLU GLU LYS GLN THR GLU LEU SER LEU S163 I166 T167 K168 M169 R170 R171 R172 D173 L180 H184 L191 S196 D197 D198 L199 V200

K201 R205 D206 N207 N214 E225 I236 F246 V250 R254 S261 Q262 L267 I268 V274 L275 D276 R277 E278 G279 L280 R281 F282 GLY

• Molecule 7: Trafficking protein particle complex subunit 20

Chain H: 61% 19% 17%

MET P2 Q3 Y4 F5 I18 P26 F29 P30 Q31 D32 E35 L36 N37 P38 F39 I40 L41 H42 D46 I47 L51 Q52 W53 P57 THR SER GLN LEU ASN GLY ASN GLY GLY ASN SER ASN GLY GLY GLY PHE LEU ARG SER ARG ALA VAL ASN ASN T84 D85

N86 C87 Y88 D93 I100 I104 G108 M109 K110 I114 A119 M130 R131 Q135 L145 R157 D162 V165 A169 R170 K171 H172 L173 SER LYS

• Molecule 8: Trafficking protein particle complex II-specific subunit 130

Chain I:

66%　　　　6% •　　　27%

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

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

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

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

ASN MET ASN MET PRO ASP GLY LYS LEU Q250 V251 P252 S257 K258 S259 A298 S320 L324 N342 N345 P346 W363 V367 S371 L375 M376 D377 K378 N379 Y380 P381 N382 S383 ASP VAL LYS TYR LYS PHE ASP LEU LEU K393 E399 Q403 W464

P483 K484 LEU ASP VAL LEU GLN ILE ASP G492 M530 LYS ASN ASN ILE HIS LEU MET TYR PRO LEU ASP GLY LEU PHE GLU VAL THR LEU ASN SER K551 F571 P572 L582 S583 D590 D598 F599 K603 R613 Y617 G618 K636 E637 F638 P639 V647 V648 P649

E675 L676 V669 E690 P704 P721 S770 N789 S790 R793 S802 E803 T823 G831 Y839 F853 K856 N860 L940 L944 R966 P970 T974 V975 P976 L979 P980 Q989 E994 D998 A999 T1003 I1004 I1029 D1030

Y1034 I1054 P1067 F1075 P1076 N1082 I1083 N1084 GLY LYS SER CYS ARG VAL ASP HIS SER ASN ALA PHE GLU SER ILE LEU ILE PHE

• Molecule 9: Trafficking protein particle complex II-specific subunit 120

Chain J:

56%　　　11% •　　　32%

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

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

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

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

• Molecule 10: Trafficking protein particle complex II-specific subunit 65

Chain K:

39% 6% • 55%

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91346	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.068	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	523.68, 523.68, 523.68	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	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	0.40	0/1226	0.80	3/1655 (0.2%)
2	B	0.43	0/1480	0.81	2/1998 (0.1%)
3	C	0.39	0/1509	0.73	1/2040 (0.0%)
3	F	0.43	0/1497	0.83	6/2024 (0.3%)
4	D	0.46	0/1262	0.79	3/1702 (0.2%)
5	E	0.46	0/1319	0.79	1/1779 (0.1%)
6	G	0.46	0/1645	0.87	11/2217 (0.5%)
7	H	0.49	0/1202	0.83	3/1629 (0.2%)
8	I	0.36	0/4279	0.67	13/5936 (0.2%)
9	J	0.44	0/6368	0.86	25/8672 (0.3%)
10	K	0.45	0/1582	0.88	9/2169 (0.4%)
All	All	0.43	0/23369	0.80	77/31821 (0.2%)

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	783	LEU	CA-CB-CG	10.40	139.22	115.30
7	H	46	ASP	CB-CG-OD1	10.29	127.56	118.30
6	G	42	ILE	CG1-CB-CG2	-9.81	89.83	111.40
4	D	16	ILE	CG1-CB-CG2	-9.11	91.35	111.40
6	G	101	LEU	CA-CB-CG	8.25	134.27	115.30
9	J	787	ILE	CG1-CB-CG2	-8.06	93.68	111.40
8	I	976	PRO	N-CA-CB	7.91	112.80	103.30
9	J	750	LEU	CA-CB-CG	7.79	133.21	115.30
9	J	550	TRP	C-N-CA	7.65	140.83	121.70
8	I	1076	PRO	N-CA-CB	7.29	112.05	103.30
7	H	26	PRO	N-CA-CB	7.17	111.90	103.30
9	J	1052	ILE	CG1-CB-CG2	-7.15	95.66	111.40
10	K	325	PRO	N-CA-CB	7.08	111.80	103.30
9	J	673	PRO	N-CA-CB	6.90	111.58	103.30
4	D	120	LEU	CA-CB-CG	6.86	131.08	115.30
8	I	704	PRO	N-CA-CB	6.85	111.52	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	267	LEU	CA-CB-CG	6.75	130.81	115.30
9	J	667	PRO	N-CA-CB	6.71	111.35	103.30
6	G	199	LEU	CA-CB-CG	6.67	130.63	115.30
4	D	110	ILE	CG1-CB-CG2	-6.62	96.84	111.40
8	I	252	PRO	N-CA-CB	6.58	111.20	103.30
10	K	330	PRO	N-CA-CB	6.56	111.18	103.30
9	J	997	VAL	CG1-CB-CG2	-6.54	100.44	110.90
3	F	99	LEU	CA-CB-CG	6.52	130.29	115.30
3	F	17	ILE	CG1-CB-CG2	-6.40	97.32	111.40
10	K	282	PRO	N-CA-CB	6.39	110.97	103.30
10	K	310	PRO	N-CA-CB	6.37	110.95	103.30
8	I	483	PRO	N-CA-CB	6.34	110.92	103.30
7	H	46	ASP	CB-CG-OD2	-6.30	112.63	118.30
3	F	185	LYS	CA-CB-CG	6.13	126.90	113.40
2	B	155	LEU	CA-CB-CG	6.12	129.38	115.30
8	I	1067	PRO	N-CA-CB	6.09	110.61	103.30
8	I	970	PRO	N-CA-CB	6.05	110.56	103.30
10	K	243	LEU	CA-CB-CG	6.03	129.17	115.30
10	K	305	PRO	N-CA-CB	6.00	110.50	103.30
8	I	649	PRO	N-CA-CB	6.00	110.50	103.30
6	G	101	LEU	CB-CG-CD2	-5.93	100.92	111.00
1	A	144	LEU	CA-CB-CG	5.92	128.93	115.30
9	J	635	TYR	CB-CG-CD2	-5.92	117.45	121.00
10	K	279	PRO	N-CA-CB	5.89	110.36	103.30
6	G	28	PRO	N-CA-CB	5.88	110.35	103.30
9	J	659	ILE	CG1-CB-CG2	-5.86	98.52	111.40
3	F	59	MET	CA-CB-CG	5.77	123.11	113.30
6	G	236	ILE	CG1-CB-CG2	-5.76	98.72	111.40
9	J	1255	PRO	N-CA-CB	5.74	110.18	103.30
8	I	346	PRO	N-CA-CB	5.73	110.18	103.30
9	J	410	PRO	N-CA-CB	5.70	110.14	103.30
9	J	623	LEU	CA-CB-CG	5.69	128.40	115.30
9	J	436	PRO	N-CA-CB	5.67	110.11	103.30
9	J	388	PRO	N-CA-CB	5.67	110.10	103.30
8	I	980	PRO	N-CA-CB	5.67	110.10	103.30
3	F	90	LEU	CA-CB-CG	5.66	128.31	115.30
10	K	250	PRO	N-CA-CB	5.64	110.06	103.30
8	I	721	PRO	N-CA-CB	5.62	110.04	103.30
9	J	398	PRO	N-CA-CB	5.56	109.97	103.30
8	I	639	PRO	N-CA-CB	5.55	109.96	103.30
8	I	572	PRO	N-CA-CB	5.54	109.94	103.30
9	J	908	LYS	C-N-CA	5.52	135.51	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	956	PRO	N-CA-CB	5.49	109.89	103.30
6	G	62	MET	CA-CB-CG	5.45	122.56	113.30
6	G	173	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	137	LEU	CA-CB-CG	5.41	127.75	115.30
3	C	157	LEU	CA-CB-CG	5.40	127.72	115.30
9	J	986	PRO	N-CA-CB	5.38	109.75	103.30
9	J	1100	PRO	N-CA-CB	5.34	109.71	103.30
9	J	763	LYS	CA-CB-CG	5.32	125.10	113.40
5	E	36	LEU	CB-CG-CD1	5.28	119.97	111.00
9	J	1023	MET	CB-CG-SD	5.23	128.10	112.40
10	K	286	PRO	N-CA-CB	5.16	109.50	103.30
9	J	1211	LEU	CA-CB-CG	5.14	127.12	115.30
9	J	631	LEU	CA-CB-CG	5.13	127.11	115.30
6	G	98	LEU	CA-CB-CG	5.09	127.00	115.30
6	G	170	ARG	CG-CD-NE	5.08	122.47	111.80
2	B	47	MET	CG-SD-CE	5.05	108.28	100.20
1	A	69	LEU	CA-CB-CG	5.04	126.90	115.30
9	J	815	ILE	CG1-CB-CG2	-5.03	100.34	111.40
3	F	13	MET	CA-CB-CG	5.02	121.83	113.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1206	0	1228	87	0
2	B	1458	0	1380	59	0
3	C	1482	0	1490	28	0
3	F	1470	0	1476	23	0
4	D	1234	0	1201	24	0
5	E	1295	0	1293	23	0
6	G	1612	0	1554	39	0
7	H	1172	0	1121	54	0
8	I	4258	0	2190	39	0
9	J	6265	0	5496	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	K	1568	0	1147	13	0
All	All	23020	0	19576	426	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 (426) 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:35:LYS:HE2	8:I:377:ASP:CB	1.15	1.60
1:A:35:LYS:CE	8:I:377:ASP:CB	1.83	1.53
1:A:79:ILE:CG2	1:A:81:GLN:OE1	1.67	1.39
1:A:63:LEU:HD12	1:A:77:MET:CE	1.58	1.33
1:A:35:LYS:NZ	8:I:377:ASP:HA	1.45	1.30
7:H:37:ASN:HB3	7:H:38:PRO:CD	1.73	1.19
6:G:108:VAL:HG21	6:G:169:MET:HG3	1.20	1.18
2:B:177:LYS:CB	2:B:185:TYR:HE1	1.60	1.15
7:H:32:ASP:OD1	7:H:36:LEU:HD23	1.46	1.15
6:G:108:VAL:CG2	6:G:169:MET:HG3	1.77	1.13
2:B:177:LYS:HB2	2:B:185:TYR:HE1	0.96	1.10
2:B:177:LYS:HB2	2:B:185:TYR:CE1	1.85	1.09
1:A:63:LEU:HA	1:A:77:MET:CE	1.84	1.08
1:A:63:LEU:HD12	1:A:77:MET:HE1	1.30	1.07
7:H:37:ASN:CB	7:H:38:PRO:HD2	1.83	1.07
1:A:63:LEU:CD1	1:A:77:MET:HE1	1.84	1.06
7:H:37:ASN:CB	7:H:38:PRO:CD	2.35	1.05
1:A:35:LYS:NZ	8:I:377:ASP:CA	2.21	1.02
1:A:61:PRO:HB2	1:A:79:ILE:HD13	1.41	1.02
1:A:79:ILE:HG23	1:A:81:GLN:OE1	0.86	1.01
1:A:79:ILE:HG23	1:A:81:GLN:CD	1.79	1.01
1:A:79:ILE:HG22	1:A:81:GLN:H	1.22	0.99
1:A:63:LEU:CD1	1:A:77:MET:CE	2.39	0.99
1:A:35:LYS:HE3	8:I:377:ASP:CB	1.94	0.98
1:A:63:LEU:HA	1:A:77:MET:HE1	1.43	0.97
6:G:108:VAL:HG22	6:G:169:MET:HA	1.44	0.96
7:H:37:ASN:HB3	7:H:38:PRO:HD2	0.96	0.96
7:H:37:ASN:O	7:H:41:LEU:HG	1.66	0.95
1:A:35:LYS:CE	8:I:377:ASP:CA	2.47	0.93
1:A:63:LEU:HD12	1:A:77:MET:HE2	1.49	0.93
1:A:35:LYS:HZ1	8:I:377:ASP:HA	1.03	0.91
1:A:54:TRP:NE1	1:A:78:LEU:HD12	1.86	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:LEU:HB2	2:B:186:LEU:CD1	2.01	0.89
2:B:174:ASP:O	2:B:187:LEU:HD23	1.73	0.89
1:A:62:LEU:O	1:A:77:MET:SD	2.31	0.87
2:B:177:LYS:CB	2:B:185:TYR:CE1	2.49	0.87
1:A:61:PRO:HG2	1:A:79:ILE:HA	1.55	0.86
2:B:187:LEU:HD23	2:B:187:LEU:O	1.77	0.84
1:A:35:LYS:HE2	8:I:377:ASP:CA	2.06	0.84
7:H:37:ASN:CG	7:H:38:PRO:HD3	1.98	0.83
1:A:61:PRO:HG2	1:A:79:ILE:HD12	1.60	0.83
2:B:176:LEU:HB2	2:B:186:LEU:HD11	1.59	0.82
1:A:79:ILE:CG2	1:A:81:GLN:HB2	2.10	0.81
1:A:61:PRO:CG	1:A:79:ILE:HD12	2.11	0.81
6:G:108:VAL:HG12	6:G:108:VAL:O	1.79	0.81
2:B:181:ARG:HA	2:B:184:PHE:CE1	2.16	0.81
7:H:32:ASP:O	7:H:36:LEU:HG	1.83	0.79
7:H:38:PRO:HB3	9:J:584:TRP:CZ2	2.18	0.79
1:A:61:PRO:HD2	1:A:79:ILE:HD12	1.64	0.78
7:H:38:PRO:O	7:H:42:HIS:N	2.16	0.78
1:A:35:LYS:HZ3	8:I:377:ASP:HA	1.48	0.78
2:B:174:ASP:O	2:B:187:LEU:CD2	2.32	0.78
2:B:177:LYS:O	2:B:185:TYR:CE1	2.37	0.77
8:I:379:ASN:O	8:I:380:TYR:O	2.02	0.76
1:A:61:PRO:CD	1:A:79:ILE:HD12	2.15	0.76
1:A:61:PRO:CB	1:A:79:ILE:HD13	2.16	0.76
1:A:54:TRP:CE2	1:A:78:LEU:HD12	2.19	0.75
1:A:63:LEU:CA	1:A:77:MET:HE1	2.18	0.74
6:G:108:VAL:HG22	6:G:169:MET:HG3	1.71	0.72
9:J:491:TYR:O	9:J:495:ASN:HB2	1.88	0.72
1:A:61:PRO:HG2	1:A:79:ILE:CD1	2.19	0.72
1:A:61:PRO:CG	1:A:79:ILE:CD1	2.67	0.72
7:H:37:ASN:CG	7:H:38:PRO:CD	2.57	0.72
2:B:176:LEU:HD13	2:B:186:LEU:HD13	1.73	0.70
1:A:61:PRO:CG	1:A:79:ILE:HA	2.21	0.70
1:A:54:TRP:HE1	1:A:78:LEU:HD12	1.58	0.69
7:H:38:PRO:O	7:H:42:HIS:HB2	1.94	0.69
1:A:77:MET:HB3	1:A:109:PHE:CE1	2.28	0.68
9:J:800:CYS:SG	9:J:801:LEU:N	2.67	0.67
1:A:79:ILE:HG21	1:A:81:GLN:HB2	1.76	0.66
1:A:93:LYS:HE3	1:A:93:LYS:C	2.16	0.66
7:H:2:PRO:HB2	7:H:29:PHE:CE1	2.31	0.66
1:A:54:TRP:CZ2	1:A:78:LEU:CD1	2.80	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:PRO:HD2	1:A:79:ILE:CD1	2.25	0.65
1:A:79:ILE:HG22	1:A:81:GLN:N	2.03	0.65
7:H:52:GLN:HG3	7:H:104:ILE:HG21	1.78	0.65
2:B:47:MET:HB2	3:C:63:ILE:HD11	1.78	0.64
1:A:61:PRO:HG2	1:A:79:ILE:CA	2.27	0.64
4:D:20:GLU:HB2	4:D:24:ALA:CB	2.28	0.64
9:J:628:GLN:O	9:J:632:PHE:HB2	1.98	0.64
6:G:108:VAL:CG1	6:G:166:ILE:HD12	2.29	0.63
7:H:36:LEU:HD12	7:H:36:LEU:C	2.19	0.63
3:C:49:PHE:HB3	3:C:138:LEU:HB2	1.81	0.63
2:B:177:LYS:O	2:B:185:TYR:CD1	2.52	0.62
9:J:662:ILE:O	9:J:736:GLN:CD	2.37	0.62
6:G:108:VAL:HG13	6:G:168:LYS:O	2.00	0.62
5:E:140:PHE:HB3	5:E:179:LEU:HD12	1.81	0.62
7:H:36:LEU:HA	7:H:40:ILE:HG21	1.80	0.62
9:J:393:MET:O	9:J:397:ALA:HB3	2.00	0.62
9:J:1182:VAL:HG11	9:J:1188:ILE:HD11	1.82	0.62
3:C:187:GLU:H	4:D:133:ARG:HH11	1.48	0.61
1:A:93:LYS:HE3	1:A:93:LYS:O	2.00	0.61
7:H:35:GLU:O	7:H:40:ILE:CG2	2.49	0.61
10:K:445:VAL:HG12	10:K:540:VAL:HG12	1.83	0.60
1:A:54:TRP:CE2	1:A:78:LEU:CD1	2.85	0.60
7:H:87:CYS:SG	7:H:88:TYR:N	2.74	0.60
2:B:183:THR:C	2:B:184:PHE:HD1	2.06	0.59
7:H:4:TYR:HB3	7:H:114:ILE:HB	1.84	0.59
9:J:1075:ARG:HD2	10:K:505:ASN:HB2	1.83	0.58
9:J:1175:LEU:HG	9:J:1192:ILE:HG22	1.85	0.58
9:J:1112:GLU:O	9:J:1116:GLU:HB2	2.02	0.58
3:F:108:TRP:HB3	3:F:112:LYS:HA	1.85	0.58
1:A:105:ILE:HA	1:A:108:ILE:HG12	1.85	0.58
3:F:101:ILE:HD11	3:F:121:GLU:HG3	1.85	0.58
3:C:68:ILE:HD13	3:C:151:SER:HB2	1.84	0.58
3:C:92:LYS:O	3:C:96:LYS:HB2	2.04	0.58
7:H:47:ILE:O	7:H:51:LEU:HB2	2.04	0.58
2:B:181:ARG:HA	2:B:184:PHE:HE1	1.67	0.58
1:A:35:LYS:HZ3	8:I:377:ASP:CA	2.09	0.57
1:A:61:PRO:CB	1:A:79:ILE:HA	2.34	0.57
8:I:1003:THR:O	9:J:1230:ARG:NH2	2.37	0.57
9:J:659:ILE:HG23	9:J:738:PRO:HB3	1.86	0.57
9:J:661:ARG:NH2	9:J:733:CYS:HA	2.20	0.57
1:A:61:PRO:HB2	1:A:79:ILE:CD1	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:19:ARG:HH22	4:D:20:GLU:HG2	1.69	0.57
4:D:20:GLU:HB2	4:D:24:ALA:HB1	1.86	0.57
2:B:157:MET:HA	2:B:160:ILE:HG22	1.87	0.56
2:B:238:CYS:SG	2:B:239:LEU:N	2.78	0.56
6:G:107:SER:HB2	6:G:170:ARG:HB2	1.86	0.56
7:H:29:PHE:N	7:H:29:PHE:CD1	2.73	0.56
2:B:42:GLN:H	3:C:23:GLU:HB3	1.69	0.56
3:F:29:LEU:HD12	6:G:191:LEU:HD22	1.88	0.56
1:A:79:ILE:HG21	1:A:81:GLN:OE1	1.90	0.56
9:J:458:SER:O	9:J:462:LYS:NZ	2.39	0.56
5:E:10:ASN:HA	5:E:138:LEU:HD23	1.88	0.56
7:H:88:TYR:OH	7:H:130:MET:SD	2.62	0.55
6:G:250:VAL:HG13	6:G:268:ILE:HG22	1.89	0.55
6:G:277:ARG:HH11	7:H:53:TRP:HB3	1.71	0.55
9:J:1017:ASP:N	9:J:1017:ASP:OD1	2.40	0.55
9:J:1115:ILE:HD11	9:J:1201:ARG:HH21	1.72	0.55
10:K:416:ASN:O	10:K:420:LYS:NZ	2.37	0.55
2:B:184:PHE:HD1	2:B:184:PHE:N	2.05	0.54
9:J:1008:LEU:O	9:J:1023:MET:SD	2.65	0.54
1:A:80:LYS:O	1:A:80:LYS:HG2	2.08	0.54
3:F:26:ASN:ND2	3:F:28:GLU:OE2	2.41	0.54
2:B:181:ARG:C	2:B:184:PHE:HE1	2.11	0.54
8:I:599:PHE:HA	8:I:636:LYS:HA	1.88	0.54
4:D:103:LEU:HD23	4:D:106:ILE:HD11	1.90	0.54
9:J:638:PRO:HA	9:J:641:THR:HG22	1.90	0.53
3:F:71:PHE:O	3:F:75:THR:OG1	2.25	0.53
9:J:542:LEU:HD11	9:J:597:LYS:HB3	1.89	0.53
4:D:92:SER:OG	4:D:93:ASP:N	2.40	0.53
4:D:114:TYR:O	4:D:118:ASN:ND2	2.41	0.53
1:A:61:PRO:CB	1:A:79:ILE:CD1	2.86	0.53
2:B:187:LEU:CD2	2:B:187:LEU:H	2.22	0.53
3:C:48:ASP:OD1	3:C:48:ASP:N	2.38	0.53
5:E:190:VAL:HG21	5:E:202:ILE:HG23	1.90	0.53
6:G:94:ILE:HA	6:G:97:ARG:HD3	1.90	0.53
2:B:184:PHE:N	2:B:184:PHE:CD1	2.76	0.53
3:C:8:ARG:HE	3:C:10:LEU:H	1.57	0.53
3:C:186:ASP:OD1	4:D:133:ARG:NH1	2.42	0.53
3:F:49:PHE:O	3:F:53:ASN:ND2	2.42	0.53
6:G:89:ASP:N	6:G:89:ASP:OD1	2.42	0.53
3:C:161:VAL:HG12	3:C:178:VAL:HG13	1.91	0.53
8:I:379:ASN:C	8:I:380:TYR:O	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:37:ASN:OD1	7:H:38:PRO:HD3	2.08	0.52
5:E:20:ASN:HB2	5:E:23:ASN:HD21	1.74	0.52
9:J:1203:LYS:HG2	9:J:1205:ASN:H	1.73	0.52
1:A:62:LEU:C	1:A:77:MET:SD	2.88	0.52
1:A:63:LEU:HA	1:A:77:MET:HE2	1.85	0.52
5:E:113:ASN:ND2	5:E:115:ASN:OD1	2.43	0.52
7:H:31:GLN:CA	7:H:31:GLN:NE2	2.73	0.52
1:A:10:LEU:HA	1:A:86:ILE:HG22	1.92	0.52
1:A:54:TRP:CZ2	1:A:78:LEU:HD12	2.43	0.52
9:J:1006:ASN:ND2	10:K:498:GLU:OE2	2.43	0.52
7:H:37:ASN:O	7:H:41:LEU:CG	2.49	0.52
2:B:139:ILE:HG22	2:B:147:LYS:HB2	1.92	0.52
3:F:49:PHE:HB3	3:F:138:LEU:HB2	1.92	0.52
7:H:2:PRO:CB	7:H:29:PHE:CE1	2.92	0.51
1:A:61:PRO:CD	1:A:79:ILE:CD1	2.85	0.51
3:C:147:VAL:O	3:C:151:SER:HB3	2.10	0.51
4:D:69:SER:OG	5:E:123:CYS:SG	2.66	0.51
3:C:132:MET:HA	3:C:135:MET:HB2	1.92	0.51
1:A:42:ILE:O	1:A:46:TYR:CB	2.59	0.51
2:B:187:LEU:CD2	2:B:187:LEU:N	2.73	0.51
6:G:167:THR:O	7:H:131:ARG:NH2	2.42	0.51
9:J:474:ARG:HH12	9:J:491:TYR:HA	1.75	0.51
9:J:633:LYS:HA	9:J:636:ILE:HG12	1.93	0.51
3:C:86:THR:HA	3:C:89:VAL:HG12	1.92	0.51
5:E:115:ASN:HA	5:E:133:GLN:HE21	1.75	0.51
6:G:108:VAL:HG22	6:G:169:MET:CA	2.28	0.51
3:F:82:ASN:OD1	3:F:85:LYS:N	2.41	0.51
6:G:108:VAL:CG2	6:G:169:MET:CG	2.70	0.51
2:B:186:LEU:O	2:B:260:PHE:HB2	2.11	0.51
6:G:108:VAL:HG21	6:G:169:MET:CG	2.14	0.51
8:I:994:GLU:CB	8:I:1030:ASP:HA	2.41	0.51
10:K:401:SER:O	10:K:553:ASN:ND2	2.44	0.51
1:A:100:ASP:O	1:A:104:ALA:HB2	2.11	0.50
2:B:187:LEU:HD23	2:B:187:LEU:C	2.31	0.50
9:J:1034:SER:OG	9:J:1035:ARG:N	2.44	0.50
3:C:53:ASN:ND2	3:C:139:TRP:O	2.42	0.50
2:B:55:LEU:HD11	3:C:41:LEU:HD21	1.94	0.50
2:B:137:LEU:HD13	2:B:140:PHE:HD2	1.76	0.50
3:C:138:LEU:O	3:C:169:ARG:NH1	2.40	0.50
4:D:71:SER:HB2	5:E:121:GLN:HG2	1.93	0.50
2:B:177:LYS:HB3	2:B:185:TYR:CE1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:53:ASN:HD21	3:F:138:LEU:HA	1.76	0.50
9:J:1272:ASN:ND2	9:J:1273:GLN:O	2.44	0.50
2:B:135:SER:HB2	2:B:149:LYS:HE2	1.92	0.50
2:B:181:ARG:CA	2:B:184:PHE:HE1	2.23	0.50
4:D:11:ARG:HG2	4:D:85:GLY:HA3	1.93	0.50
9:J:1268:SER:HA	9:J:1276:ILE:HA	1.94	0.50
2:B:185:TYR:HB3	2:B:261:HIS:HA	1.92	0.50
4:D:113:LYS:HA	4:D:117:ASN:HD22	1.77	0.50
5:E:137:GLY:O	5:E:139:LYS:NZ	2.44	0.50
2:B:124:ARG:NH1	2:B:216:GLU:OE2	2.45	0.50
7:H:32:ASP:HA	7:H:35:GLU:CD	2.33	0.50
2:B:184:PHE:O	2:B:262:VAL:HG12	2.11	0.49
5:E:8:VAL:HG23	5:E:16:ILE:HB	1.94	0.49
9:J:1014:GLU:OE2	9:J:1027:ARG:NH1	2.45	0.49
2:B:154:LEU:O	2:B:184:PHE:CE2	2.65	0.49
3:C:17:ILE:HA	3:C:20:ASN:HB2	1.95	0.49
5:E:2:ALA:N	5:E:219:GLN:OE1	2.45	0.49
6:G:97:ARG:NH2	7:H:145:LEU:O	2.45	0.49
7:H:2:PRO:CB	7:H:29:PHE:HE1	2.26	0.49
9:J:818:ASP:HB3	9:J:820:ARG:HG3	1.94	0.49
1:A:37:ASN:O	1:A:41:ASN:ND2	2.45	0.49
3:F:144:LEU:HA	3:F:147:VAL:HG12	1.95	0.49
2:B:178:THR:OG1	2:B:184:PHE:CD1	2.52	0.49
2:B:144:PRO:HD2	2:B:147:LYS:HB3	1.93	0.49
9:J:565:LEU:HB2	9:J:567:ILE:HG12	1.94	0.49
8:I:363:TRP:O	8:I:367:VAL:CB	2.61	0.49
4:D:99:TYR:HB3	4:D:102:VAL:HB	1.95	0.48
6:G:108:VAL:O	6:G:108:VAL:CG1	2.52	0.48
9:J:967:GLU:N	9:J:985:ILE:O	2.45	0.48
7:H:31:GLN:NE2	7:H:31:GLN:N	2.61	0.48
9:J:968:TYR:HA	9:J:984:SER:HA	1.95	0.48
3:F:109:SER:HG	3:F:114:THR:HG1	1.61	0.48
2:B:177:LYS:C	2:B:185:TYR:CE1	2.86	0.48
6:G:172:ARG:NH2	7:H:86:ASN:O	2.46	0.48
6:G:168:LYS:HD3	7:H:131:ARG:NH2	2.28	0.48
9:J:1094:PRO:HD3	9:J:1122:TRP:HE1	1.78	0.48
6:G:261:SER:HG	6:G:262:GLN:HE21	1.59	0.48
9:J:762:ARG:HE	9:J:791:THR:HG21	1.79	0.48
10:K:500:ILE:HG22	10:K:526:GLY:HA2	1.96	0.48
2:B:181:ARG:CA	2:B:184:PHE:CE1	2.92	0.47
7:H:157:ARG:NH1	7:H:162:ASP:OD2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:1056:VAL:O	9:J:1063:SER:OG	2.32	0.47
4:D:17:PHE:CZ	4:D:20:GLU:HA	2.49	0.47
3:F:182:ARG:NH1	3:F:183:ILE:O	2.47	0.47
10:K:542:ASP:HB3	10:K:547:GLU:HB3	1.96	0.47
3:F:96:LYS:HG2	3:F:100:ASN:HD22	1.78	0.47
6:G:275:LEU:O	6:G:279:GLY:N	2.46	0.47
1:A:63:LEU:CB	1:A:77:MET:HE1	2.43	0.47
3:F:53:ASN:ND2	3:F:137:SER:O	2.47	0.47
1:A:63:LEU:HD13	1:A:77:MET:HE1	1.83	0.47
2:B:223:ARG:HE	2:B:235:GLU:HB3	1.79	0.47
2:B:226:LEU:O	2:B:230:GLY:N	2.48	0.47
3:F:82:ASN:O	3:F:86:THR:OG1	2.33	0.47
8:I:940:LEU:O	8:I:944:LEU:N	2.47	0.47
9:J:393:MET:O	9:J:397:ALA:CB	2.62	0.47
6:G:108:VAL:HG12	6:G:166:ILE:HD12	1.96	0.47
7:H:32:ASP:OD1	7:H:36:LEU:CD2	2.39	0.47
2:B:110:LYS:O	2:B:209:LYS:NZ	2.44	0.47
8:I:989:GLN:N	8:I:1082:ASN:O	2.47	0.47
9:J:1021:TYR:HD2	9:J:1079:PRO:HG2	1.79	0.47
10:K:218:ARG:HA	10:K:232:LEU:HA	1.97	0.47
1:A:63:LEU:HA	1:A:77:MET:SD	2.53	0.47
2:B:127:GLY:HA2	2:B:130:ILE:HD12	1.96	0.47
9:J:662:ILE:O	9:J:736:GLN:NE2	2.49	0.47
1:A:35:LYS:HZ1	8:I:377:ASP:CA	1.94	0.46
1:A:79:ILE:CG2	1:A:81:GLN:CB	2.88	0.46
4:D:20:GLU:HB2	4:D:24:ALA:HB3	1.97	0.46
7:H:32:ASP:HA	7:H:35:GLU:OE2	2.15	0.46
9:J:628:GLN:O	9:J:632:PHE:CB	2.63	0.46
4:D:67:ILE:HA	5:E:124:THR:HG22	1.96	0.46
3:F:90:LEU:O	3:F:94:ALA:CB	2.64	0.46
6:G:171:ARG:HD3	7:H:86:ASN:HB2	1.96	0.46
9:J:1092:ASN:O	9:J:1122:TRP:NE1	2.49	0.46
2:B:60:GLU:OE1	2:B:61:ARG:NH2	2.48	0.46
6:G:180:LEU:HD12	6:G:199:LEU:HD12	1.98	0.46
9:J:1197:THR:OG1	9:J:1198:SER:N	2.49	0.46
1:A:61:PRO:CG	1:A:79:ILE:HD13	2.42	0.46
9:J:1119:GLN:OE1	9:J:1168:ARG:NH1	2.49	0.46
2:B:185:TYR:HB2	2:B:260:PHE:O	2.16	0.46
5:E:32:GLU:HA	5:E:35:ILE:HD12	1.98	0.45
6:G:184:HIS:NE2	6:G:196:SER:O	2.50	0.45
8:I:860:ASN:ND2	8:I:966:ARG:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:757:PHE:HA	9:J:766:SER:HB3	1.98	0.45
9:J:1115:ILE:HA	9:J:1118:ARG:HB3	1.98	0.45
6:G:172:ARG:HH12	7:H:104:ILE:HG22	1.81	0.45
7:H:38:PRO:HB3	9:J:584:TRP:CE2	2.49	0.45
3:C:144:LEU:HA	3:C:147:VAL:HG22	1.99	0.45
1:A:24:ASN:ND2	1:A:28:ASN:OD1	2.50	0.45
3:F:85:LYS:HA	3:F:88:GLU:HG2	1.98	0.45
9:J:536:LEU:HA	9:J:539:VAL:HG12	1.99	0.45
9:J:910:PRO:HA	9:J:911:PRO:HD3	1.79	0.45
2:B:174:ASP:O	2:B:187:LEU:O	2.34	0.45
7:H:29:PHE:CD2	7:H:36:LEU:CD2	3.00	0.45
8:I:598:ASP:HA	8:I:603:LYS:HA	1.97	0.45
9:J:903:PRO:HA	9:J:906:TRP:HB3	1.98	0.45
3:C:8:ARG:HG3	3:C:11:LYS:H	1.81	0.45
7:H:165:VAL:O	7:H:169:ALA:N	2.48	0.45
8:I:676:LEU:HA	8:I:689:VAL:HA	1.97	0.45
8:I:793:ARG:NH2	8:I:831:GLY:O	2.49	0.45
5:E:53:LYS:HG2	5:E:55:LEU:HB3	1.99	0.45
1:A:30:MET:SD	1:A:30:MET:N	2.85	0.45
4:D:7:TRP:HA	4:D:17:PHE:HB2	1.99	0.45
4:D:64:LYS:O	5:E:126:GLN:NE2	2.50	0.45
5:E:8:VAL:HG22	5:E:17:TYR:HB3	1.99	0.45
7:H:31:GLN:N	7:H:31:GLN:HE21	2.14	0.45
1:A:79:ILE:HG22	1:A:81:GLN:HB2	1.97	0.44
5:E:112:THR:OG1	5:E:113:ASN:N	2.51	0.44
9:J:663:LEU:HA	9:J:734:ARG:HH21	1.82	0.44
1:A:129:ASP:OD1	1:A:129:ASP:N	2.50	0.44
7:H:31:GLN:NE2	7:H:31:GLN:HA	2.29	0.44
7:H:38:PRO:HB3	9:J:584:TRP:CH2	2.49	0.44
9:J:758:CYS:HA	9:J:801:LEU:HB2	1.99	0.44
1:A:67:PHE:HD2	1:A:74:VAL:HG23	1.82	0.44
5:E:130:PHE:N	5:E:142:ALA:O	2.50	0.44
3:F:119:LEU:O	3:F:174:THR:OG1	2.35	0.44
6:G:167:THR:OG1	6:G:168:LYS:N	2.50	0.44
8:I:399:GLU:O	8:I:403:GLN:N	2.51	0.44
8:I:590:ASP:H	8:I:613:ARG:HA	1.81	0.44
3:F:166:ASP:OD1	3:F:169:ARG:N	2.45	0.44
6:G:197:ASP:OD2	6:G:214:ASN:ND2	2.49	0.44
9:J:774:LYS:HD3	9:J:775:ALA:H	1.81	0.44
1:A:61:PRO:HG2	1:A:79:ILE:O	2.18	0.44
1:A:77:MET:HE3	1:A:77:MET:HB2	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:LEU:HD12	2:B:186:LEU:HA	1.78	0.44
4:D:110:ILE:HD11	4:D:148:VAL:HG13	2.00	0.44
6:G:254:ARG:HD3	6:G:262:GLN:HA	2.00	0.44
7:H:171:LYS:HE3	7:H:171:LYS:HB3	1.90	0.44
9:J:662:ILE:O	9:J:736:GLN:OE1	2.36	0.44
1:A:42:ILE:O	1:A:46:TYR:HB3	2.17	0.44
7:H:5:PHE:HB3	7:H:18:ILE:HG22	1.99	0.44
9:J:561:ILE:HD13	9:J:561:ILE:HA	1.88	0.44
3:F:28:GLU:H	3:F:28:GLU:HG2	1.58	0.44
7:H:36:LEU:C	7:H:36:LEU:CD1	2.86	0.44
1:A:17:PRO:HB3	1:A:20:ILE:HD11	2.00	0.43
9:J:1177:LEU:HD13	9:J:1284:VAL:HG11	2.00	0.43
8:I:803:GLU:O	8:I:856:LYS:N	2.52	0.43
2:B:128:PHE:O	2:B:132:LEU:N	2.47	0.43
4:D:142:ASN:HB2	4:D:145:PHE:HB3	1.99	0.43
6:G:246:PHE:HA	6:G:274:VAL:HG11	2.00	0.43
10:K:267:LYS:H	10:K:273:SER:HA	1.83	0.43
10:K:499:GLY:O	10:K:527:ILE:N	2.51	0.43
1:A:93:LYS:HD2	1:A:93:LYS:HA	1.71	0.43
8:I:583:SER:HA	8:I:617:TYR:HA	2.01	0.43
9:J:738:PRO:HG2	9:J:784:PRO:HG2	1.99	0.43
7:H:93:ASP:HB2	7:H:100:ILE:HD11	2.00	0.43
9:J:1093:THR:OG1	9:J:1118:ARG:NH2	2.47	0.43
9:J:1184:VAL:HG13	9:J:1257:GLU:H	1.84	0.43
9:J:1202:ARG:H	9:J:1202:ARG:HG2	1.58	0.43
4:D:17:PHE:CE2	4:D:20:GLU:HA	2.54	0.43
8:I:853:PHE:O	8:I:974:THR:N	2.51	0.43
3:C:11:LYS:HD2	3:C:92:LYS:HE3	2.00	0.43
6:G:171:ARG:NH2	7:H:84:THR:O	2.46	0.43
9:J:1081:LYS:HB3	9:J:1081:LYS:HE2	1.87	0.43
2:B:178:THR:OG1	2:B:184:PHE:CE1	2.66	0.43
2:B:191:TYR:HD2	2:B:194:ILE:HG12	1.83	0.43
4:D:10:ASP:HA	4:D:86:LEU:HD13	2.01	0.43
9:J:758:CYS:SG	9:J:759:GLU:N	2.91	0.43
2:B:143:ASN:HA	2:B:147:LYS:HD3	2.00	0.43
5:E:115:ASN:HB2	5:E:120:ARG:CZ	2.48	0.43
8:I:379:ASN:O	8:I:380:TYR:C	2.57	0.43
9:J:1222:LYS:NZ	9:J:1223:ILE:O	2.42	0.43
1:A:42:ILE:O	1:A:46:TYR:HB2	2.19	0.42
1:A:43:SER:HA	1:A:46:TYR:HB3	2.01	0.42
2:B:187:LEU:H	2:B:187:LEU:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:177:LYS:HB3	3:C:177:LYS:HE2	1.89	0.42
3:C:188:ILE:HG23	4:D:133:ARG:HG2	2.01	0.42
3:F:90:LEU:O	3:F:94:ALA:HB2	2.19	0.42
10:K:306:LYS:HA	10:K:332:ARG:HA	2.01	0.42
3:F:26:ASN:OD1	3:F:26:ASN:N	2.50	0.42
9:J:1018:TRP:HB2	9:J:1079:PRO:HG3	2.01	0.42
8:I:675:GLU:O	8:I:690:GLU:N	2.52	0.42
9:J:625:GLN:NE2	9:J:747:ASP:O	2.48	0.42
9:J:465:LEU:HA	9:J:468:ILE:HG22	2.01	0.42
9:J:767:TYR:HB2	9:J:787:ILE:HD11	2.02	0.42
6:G:201:LYS:NZ	6:G:206:ASP:OD1	2.46	0.42
7:H:157:ARG:HD2	7:H:157:ARG:HA	1.74	0.42
9:J:544:THR:HG22	9:J:546:ASN:H	1.83	0.42
9:J:629:ASP:HA	9:J:632:PHE:HB3	2.01	0.42
9:J:637:GLN:HA	9:J:640:ILE:HG12	2.01	0.42
9:J:800:CYS:HB3	9:J:812:LYS:HB3	2.02	0.42
6:G:207:ASN:OD1	6:G:207:ASN:N	2.52	0.42
8:I:770:SER:N	8:I:789:ASN:O	2.52	0.42
3:C:141:SER:HB3	3:C:144:LEU:HG	2.02	0.42
9:J:458:SER:O	9:J:461:SER:OG	2.35	0.42
3:C:34:TYR:OH	3:C:140:TYR:O	2.34	0.42
5:E:178:PHE:HD2	5:E:179:LEU:HD22	1.85	0.42
6:G:108:VAL:HG22	6:G:169:MET:CG	2.46	0.42
6:G:169:MET:HE3	7:H:135:GLN:HB3	2.02	0.42
9:J:1026:ILE:HD12	9:J:1026:ILE:HA	1.94	0.42
1:A:10:LEU:HB2	1:A:18:ILE:HB	2.02	0.41
1:A:117:ILE:HD12	1:A:117:ILE:HA	1.94	0.41
2:B:137:LEU:HD12	3:C:28:GLU:HG3	2.02	0.41
5:E:9:ILE:HB	5:E:139:LYS:HB2	2.01	0.41
9:J:655:ARG:HH11	9:J:816:ILE:HG21	1.84	0.41
9:J:1038:ILE:HD11	9:J:1164:ILE:HD12	2.02	0.41
10:K:220:ILE:HA	10:K:230:SER:HA	2.02	0.41
1:A:17:PRO:HD2	8:I:464:TRP:HB2	2.01	0.41
4:D:48:ILE:O	4:D:52:ARG:N	2.53	0.41
8:I:979:LEU:O	8:I:1075:PHE:N	2.52	0.41
1:A:41:ASN:HA	1:A:44:LEU:HB2	2.01	0.41
1:A:142:ASP:OD1	1:A:142:ASP:N	2.53	0.41
8:I:802:SER:O	8:I:839:TYR:OH	2.38	0.41
1:A:97:GLY:N	1:A:101:GLU:OE1	2.53	0.41
3:C:63:ILE:HD12	3:C:63:ILE:HA	1.94	0.41
9:J:1095:ILE:O	9:J:1097:ARG:NH1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:172:ARG:HH22	7:H:104:ILE:HB	1.85	0.41
8:I:998:ASP:O	8:I:999:ALA:HB3	2.21	0.41
9:J:1086:LYS:HA	9:J:1086:LYS:HD3	1.74	0.41
2:B:203:ALA:HB3	2:B:206:GLU:HG2	2.02	0.41
3:C:152:LEU:HD22	3:C:157:LEU:HD11	2.03	0.41
6:G:225:GLU:HA	6:G:254:ARG:HH22	1.86	0.41
9:J:512:LYS:HA	9:J:512:LYS:HD2	1.82	0.41
2:B:125:ASN:O	2:B:129:GLN:NE2	2.54	0.41
2:B:160:ILE:HD12	2:B:160:ILE:HA	1.99	0.41
8:I:989:GLN:HA	8:I:1034:TYR:HA	2.02	0.41
1:A:3:LEU:HD23	1:A:4:ARG:HH12	1.86	0.40
7:H:108:GLY:O	7:H:110:LYS:NZ	2.55	0.40
8:I:582:LEU:O	8:I:618:GLY:N	2.54	0.40
9:J:662:ILE:CB	9:J:736:GLN:OE1	2.69	0.40
10:K:248:ILE:O	10:K:253:HIS:N	2.53	0.40
2:B:41:SER:OG	2:B:43:SER:OG	2.36	0.40
3:C:90:LEU:HD21	3:C:148:LEU:HD22	2.04	0.40
8:I:320:SER:HA	8:I:324:LEU:H	1.86	0.40
1:A:48:GLU:HB2	1:A:54:TRP:HZ3	1.86	0.40
2:B:176:LEU:CB	2:B:186:LEU:CD1	2.87	0.40
1:A:28:ASN:HB3	1:A:29:GLU:H	1.79	0.40
5:E:23:ASN:OD1	5:E:23:ASN:N	2.54	0.40
5:E:135:LEU:HD11	3:F:79:ARG:HE	1.86	0.40
8:I:790:SER:O	8:I:793:ARG:NH1	2.45	0.40
9:J:469:VAL:O	9:J:473:HIS:ND1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	148/152 (97%)	128 (86%)	20 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	189/268 (70%)	165 (87%)	23 (12%)	1 (0%)	29	68
3	C	182/193 (94%)	169 (93%)	13 (7%)	0	100	100
3	F	180/193 (93%)	164 (91%)	16 (9%)	0	100	100
4	D	147/159 (92%)	125 (85%)	22 (15%)	0	100	100
5	E	153/219 (70%)	139 (91%)	14 (9%)	0	100	100
6	G	199/283 (70%)	176 (88%)	23 (12%)	0	100	100
7	H	142/175 (81%)	124 (87%)	16 (11%)	2 (1%)	11	47
8	I	791/1102 (72%)	641 (81%)	129 (16%)	21 (3%)	5	34
9	J	861/1289 (67%)	691 (80%)	164 (19%)	6 (1%)	22	62
10	K	243/559 (44%)	183 (75%)	55 (23%)	5 (2%)	7	39
All	All	3235/4592 (70%)	2705 (84%)	495 (15%)	35 (1%)	18	51

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	26	PRO
7	H	37	ASN
8	I	252	PRO
8	I	380	TYR
8	I	381	PRO
8	I	638	PHE
8	I	647	VAL
8	I	976	PRO
8	I	980	PRO
8	I	1067	PRO
8	I	1076	PRO
9	J	667	PRO
9	J	1099	TYR
10	K	325	PRO
8	I	639	PRO
8	I	704	PRO
8	I	1054	ILE
10	K	269	ILE
8	I	371	SER
8	I	571	PHE
9	J	398	PRO
9	J	672	ILE
10	K	282	PRO

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Mol	Chain	Res	Type
10	K	286	PRO
8	I	377	ASP
8	I	1004	ILE
9	J	397	ALA
8	I	375	LEU
2	B	99	ILE
8	I	367	VAL
9	J	955	VAL
10	K	281	CYS
8	I	1029	ILE
8	I	345	ASN
8	I	483	PRO

5.3.2　Protein sidechains　ⓘ

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	140/142 (99%)	135 (96%)	5 (4%)	35	60
2	B	142/248 (57%)	139 (98%)	3 (2%)	53	71
3	C	169/178 (95%)	169 (100%)	0	100	100
3	F	168/178 (94%)	167 (99%)	1 (1%)	86	92
4	D	135/145 (93%)	132 (98%)	3 (2%)	52	70
5	E	144/199 (72%)	144 (100%)	0	100	100
6	G	169/249 (68%)	165 (98%)	4 (2%)	49	68
7	H	126/152 (83%)	122 (97%)	4 (3%)	39	62
8	I	78/1023 (8%)	78 (100%)	0	100	100
9	J	551/1213 (45%)	544 (99%)	7 (1%)	69	82
10	K	93/517 (18%)	93 (100%)	0	100	100
All	All	1915/4244 (45%)	1888 (99%)	27 (1%)	68	80

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ILE
1	A	80	LYS
1	A	93	LYS
1	A	94	SER
1	A	113	ARG
2	B	184	PHE
2	B	185	TYR
2	B	187	LEU
4	D	19	ARG
4	D	20	GLU
4	D	95	LYS
3	F	185	LYS
6	G	172	ARG
6	G	205	ARG
6	G	277	ARG
6	G	281	ARG
7	H	29	PHE
7	H	31	GLN
7	H	32	ASP
7	H	40	ILE
9	J	482	SER
9	J	484	MET
9	J	955	VAL
9	J	1007	GLU
9	J	1035	ARG
9	J	1201	ARG
9	J	1226	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	117	ASN
3	F	100	ASN
7	H	31	GLN
9	J	772	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30954. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

6.1.1 Primary map

| X | Y | Z |
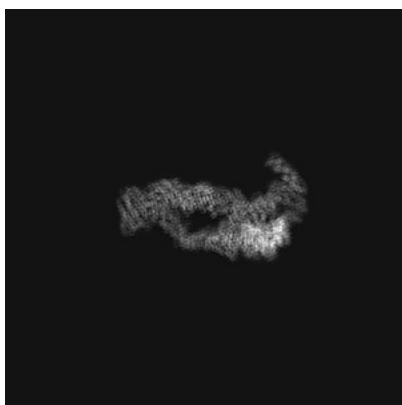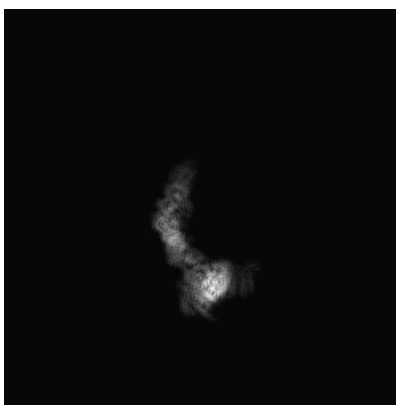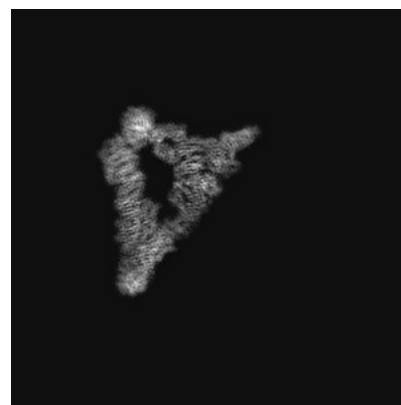
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

| X Index: 240 | Y Index: 240 | Z Index: 240 |
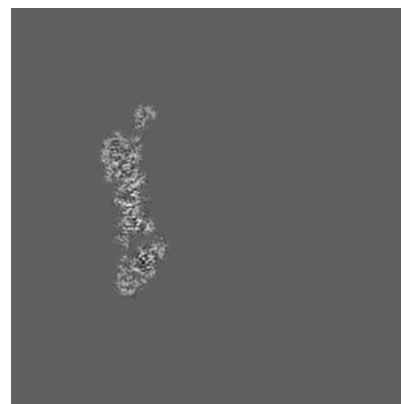
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

6.3.1 Primary map

| X Index: 147 | Y Index: 322 | Z Index: 201 |

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

6.4 Orthogonal surface views ⓘ
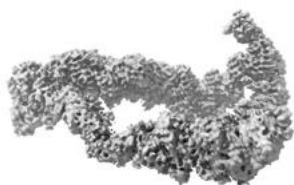
6.4.1 Primary map

| X | Y | Z |
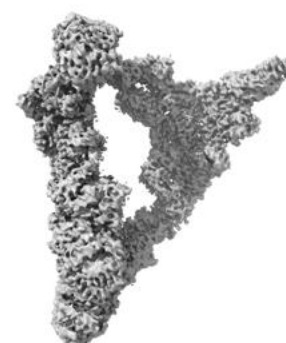
The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5 Mask visualisation ⓘ

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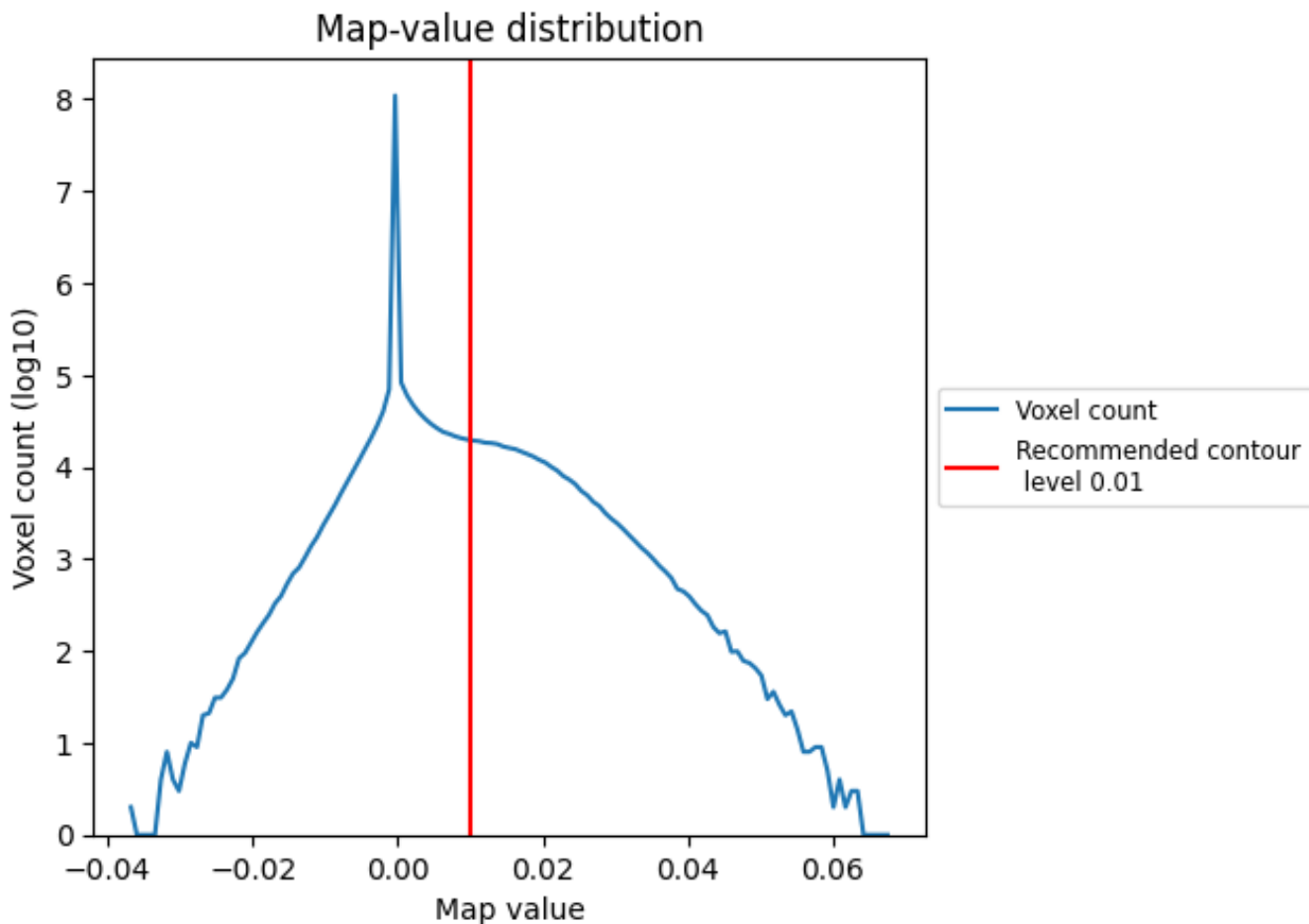
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
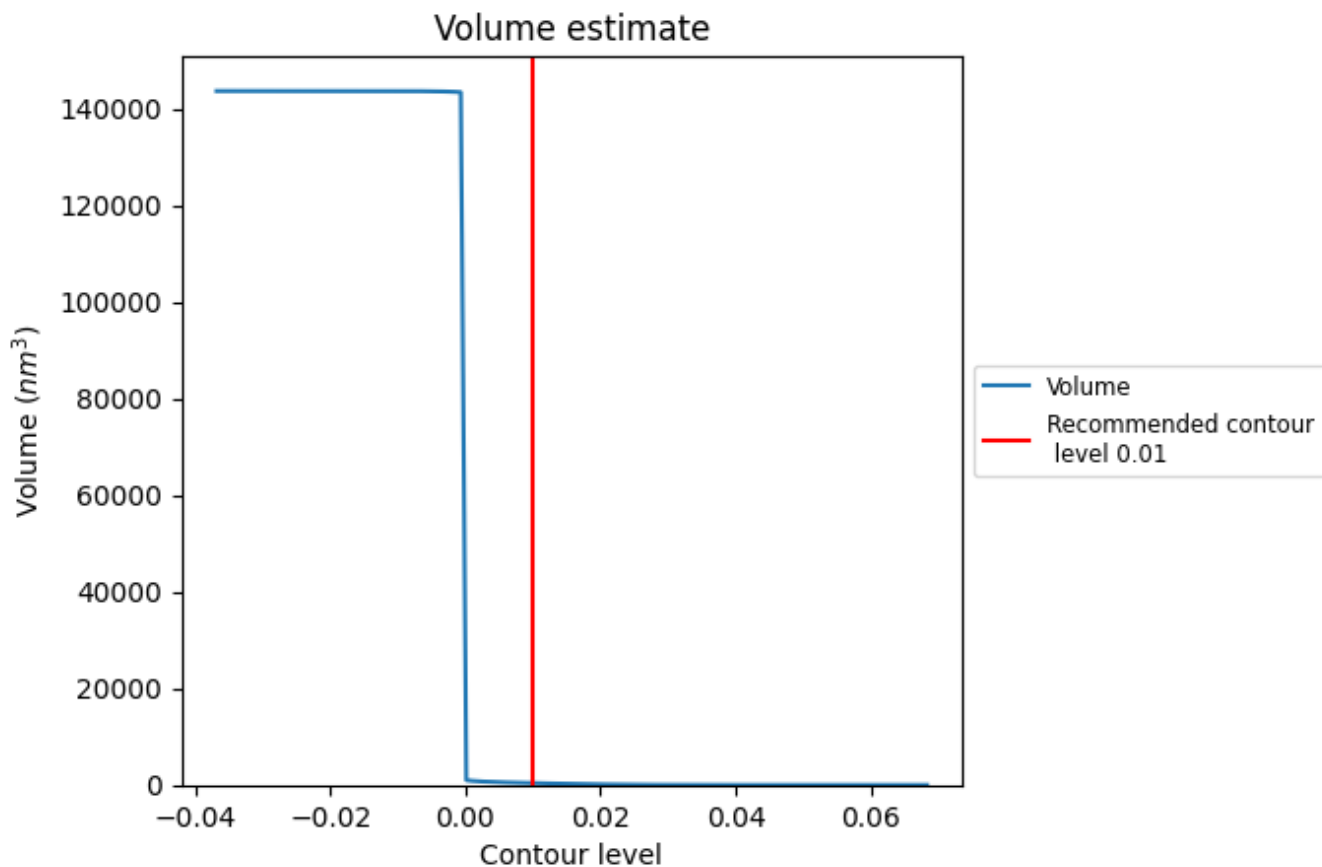
The volume at the recommended contour level is 386 nm^3; this corresponds to an approximate mass of 349 kDa.

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 ⓘ
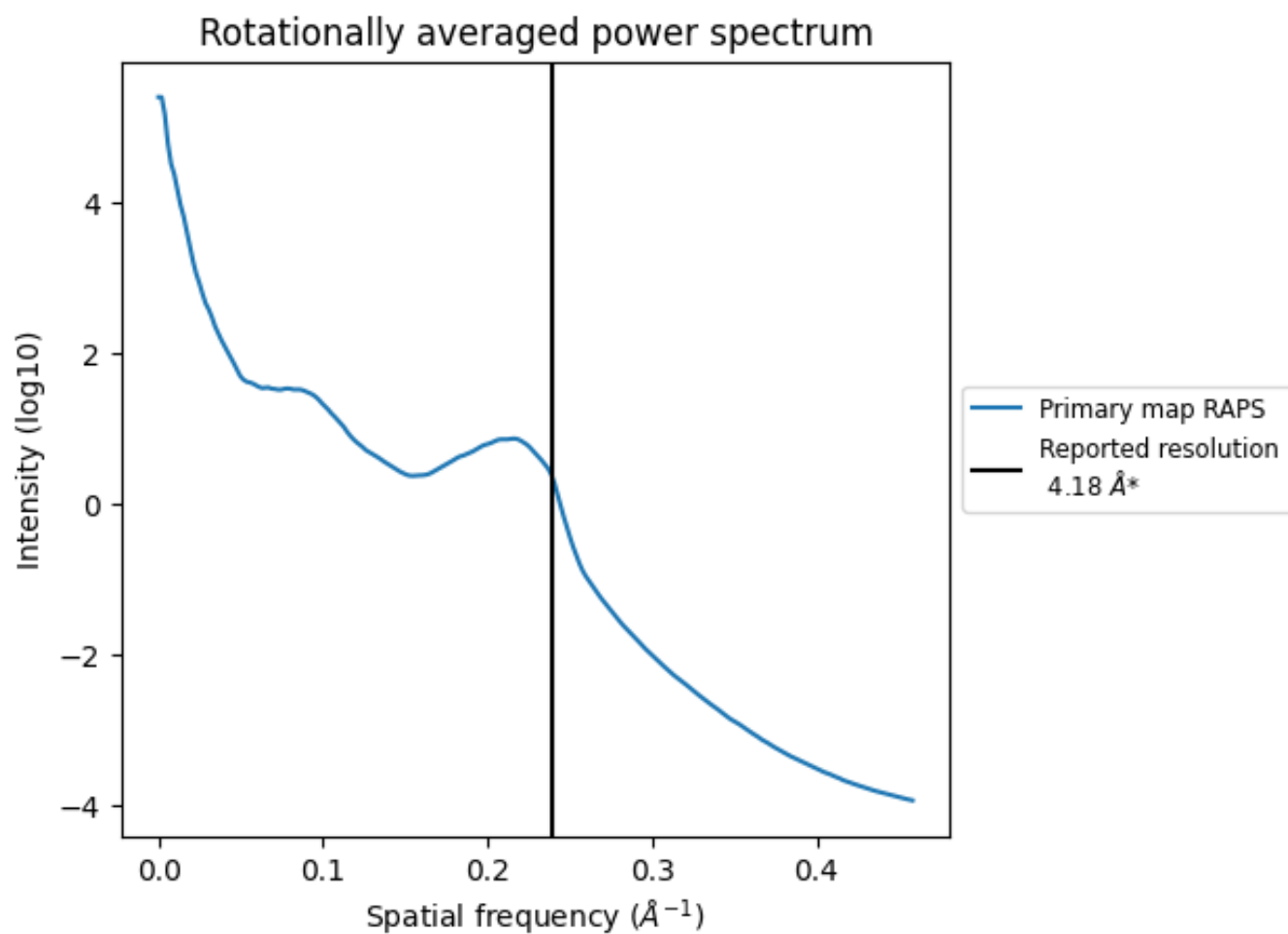
*Reported resolution corresponds to spatial frequency of 0.239 Å^{-1}

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9　Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-30954 and PDB model 7E2C. Per-residue inclusion information can be found in section 3 on page 6.

9.1　Map-model overlay ⓘ

| X | Y | Z |
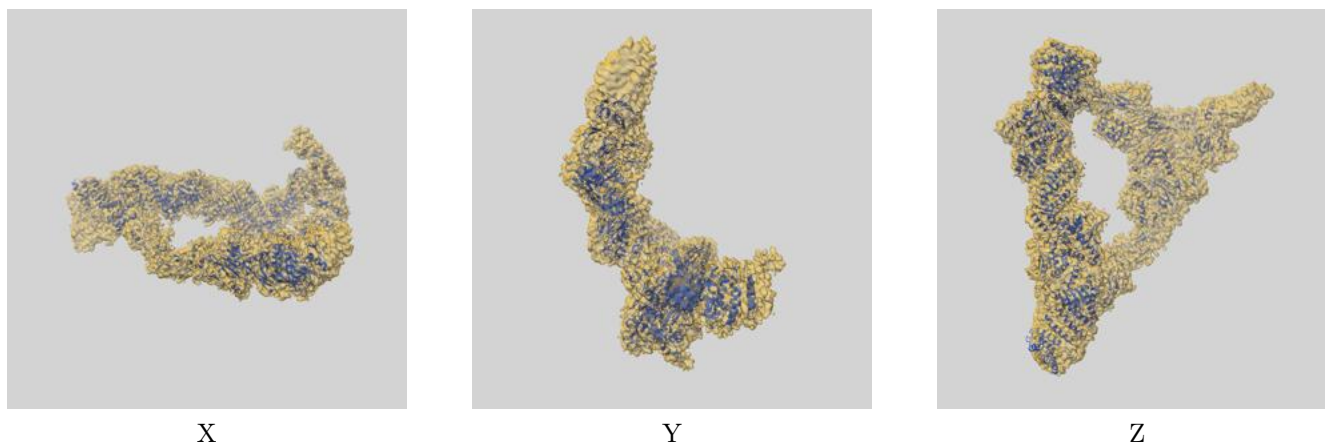
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

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 ⓘ

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 (0.01).

9.4 Atom inclusion ⓘ
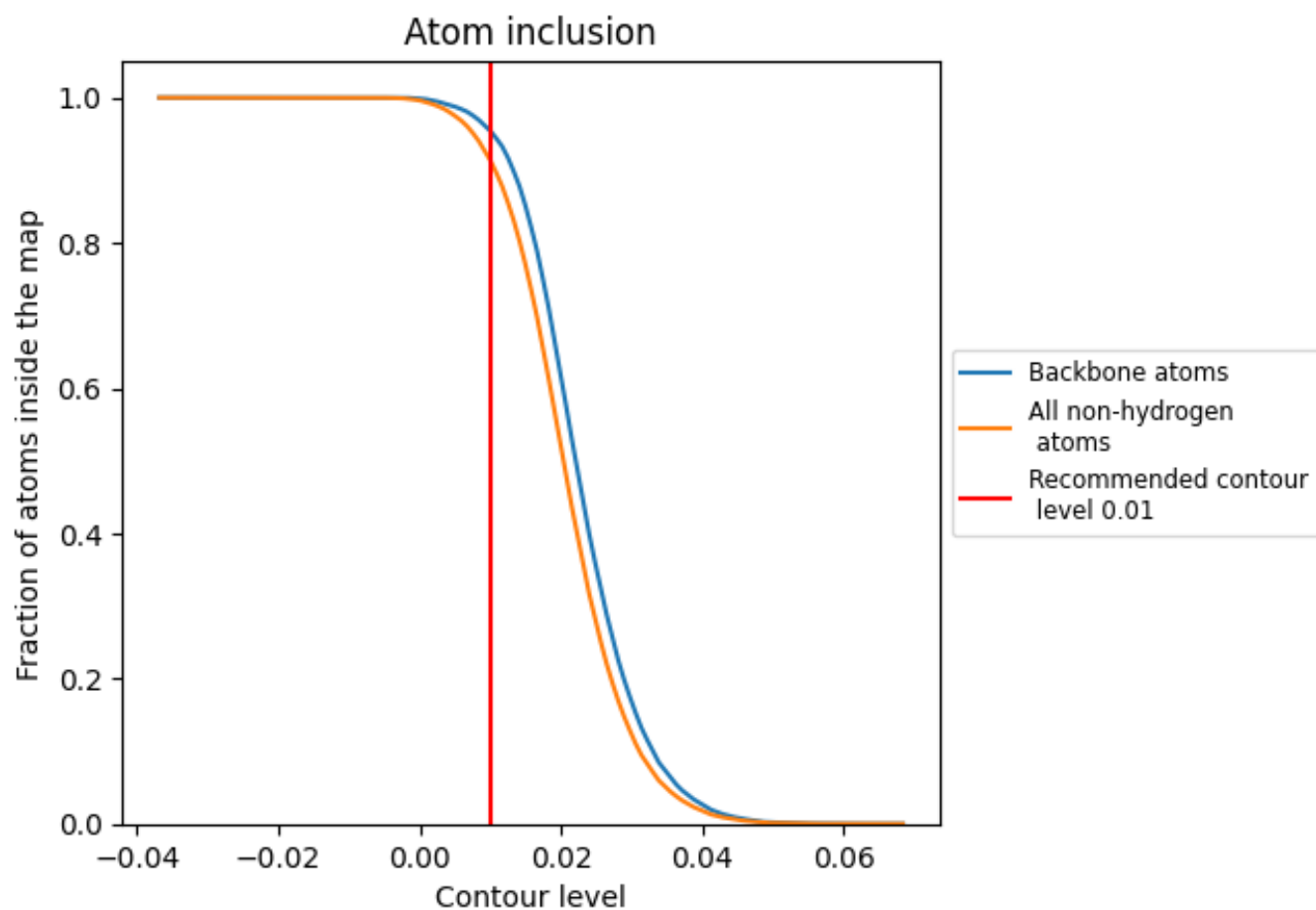
At the recommended contour level, 95% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9136	0.3570
A	0.7569	0.2690
B	0.8825	0.2850
C	0.8211	0.2630
D	0.9303	0.3600
E	0.9154	0.3770
F	0.9143	0.3540
G	0.9187	0.3750
H	0.9054	0.3620
I	0.9609	0.3870
J	0.9249	0.3850
K	0.9614	0.3490

1.0

0.0
<0.0