



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:15 PM UTC

PDB ID : 7ZWD / pdb_00007zwd
EMDB ID : EMD-14997
Title : Structure of SNAPc containing Pol II pre-initiation complex bound to U5 snRNA promoter (CC)
Authors : Rengachari, S.; Schilbach, S.; Kaliyappan, T.; Gouge, J.; Zumer, K.; Schwarz, J.; Urlaub, H.; Dienemann, C.; Vannini, A.; Cramer, P.
Deposited on : 2022-05-19
Resolution : 3.00 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

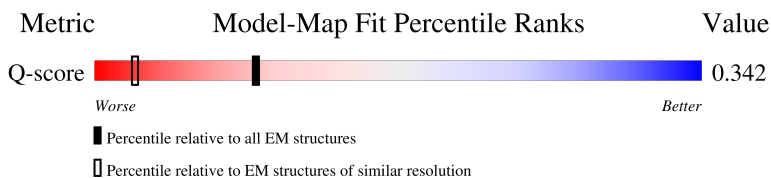
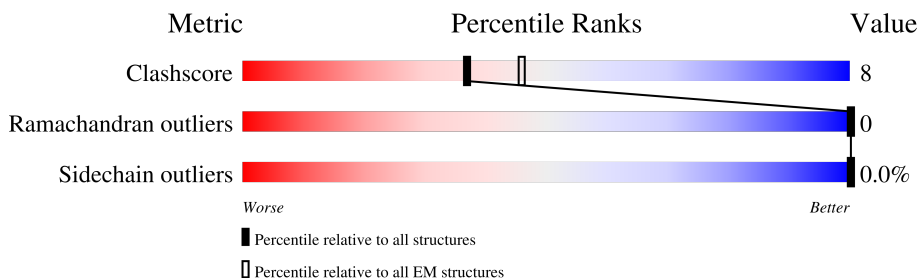
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



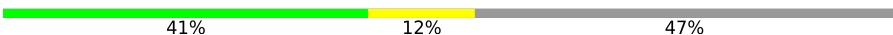
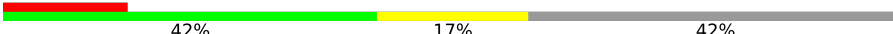
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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 $\leq 5\%$. 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	1970	 5% 63% 10% 28%
2	B	1174	 85% 12% .
3	C	275	 85% 9% 7%
4	D	142	 35% 78% 12% 10%

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Mol	Chain	Length	Quality of chain
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	316	
14	N	96	
15	O	339	
16	Q	517	
17	R	249	
18	T	96	
19	U	376	
20	V	109	
21	a	368	
22	b	411	
23	c	1469	
24	d	98	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 49279 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1423	Total	C	N	O	S	0	0
			11274	7092	2016	2094	72		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1136	Total	C	N	O	S	0	0
			9076	5739	1597	1676	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	128	Total	C	N	O	S	0	0
			1050	656	178	212	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	79	Total	C	N	O	S	0	0
			636	406	108	117	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	114	Total	C	N	O	S	0	0
			928	571	166	180	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 11 is a protein called RNA polymerase II subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			373	231	72	64	6		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	242	Total	C	N	O	S	0	0
			1879	1182	332	349	16		

- Molecule 14 is a DNA chain called Non-template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	66	Total	C	N	O	P	0	0
			1351	646	242	397	66		

- Molecule 15 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	179	Total	C	N	O	S	0	0
			1422	923	251	241	7		

- Molecule 16 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 17 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 18 is a DNA chain called Template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	66	Total	C	N	O	P	0	0
			1355	647	247	395	66		

- Molecule 19 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	88	Total	C	N	O	S	0	0
			735	470	124	137	4		

- Molecule 20 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	97	Total	C	N	O	S	0	0
			793	502	140	149	2		

- Molecule 21 is a protein called snRNA-activating protein complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	a	215	Total	C	N	O	S	0	0
			1807	1165	313	319	10		

- Molecule 22 is a protein called snRNA-activating protein complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	b	365	Total	C	N	O	S	0	0
			2978	1890	510	558	20		

- Molecule 23 is a protein called snRNA-activating protein complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	c	303	Total	C	N	O	S	0	0
			2516	1574	453	479	10		

- Molecule 24 is a protein called snRNA-activating protein complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	d	52	Total	C	N	O	S	0	0
			424	259	81	81	3		

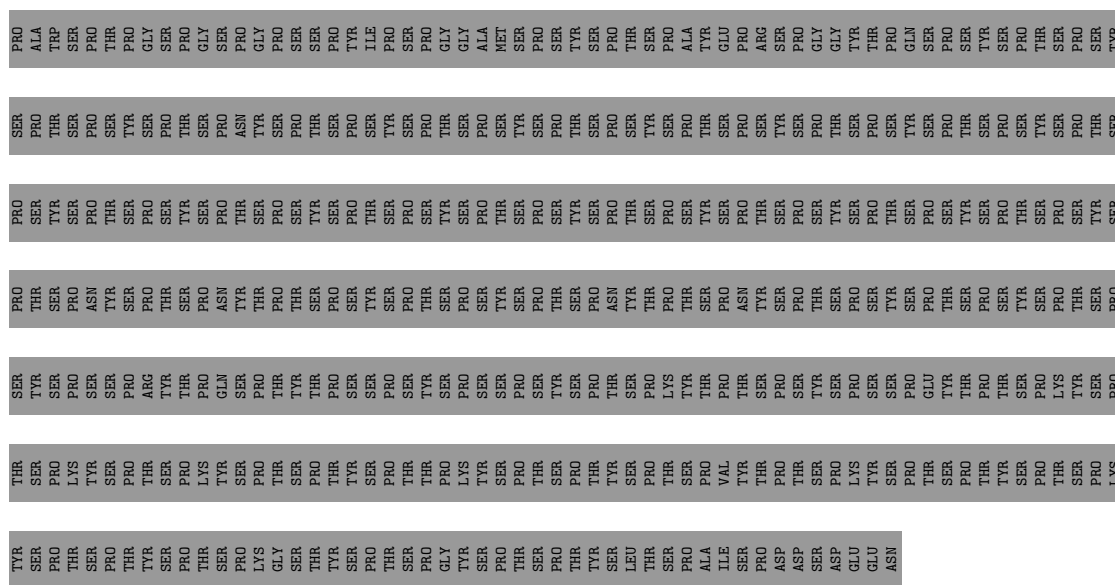
- Molecule 25 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
25	A	2	Total	Zn	0
			2	2	
25	B	1	Total	Zn	0
			1	1	
25	C	1	Total	Zn	0
			1	1	
25	I	2	Total	Zn	0
			2	2	
25	J	1	Total	Zn	0
			1	1	
25	L	1	Total	Zn	0
			1	1	
25	M	1	Total	Zn	0
			1	1	
25	b	2	Total	Zn	0
			2	2	

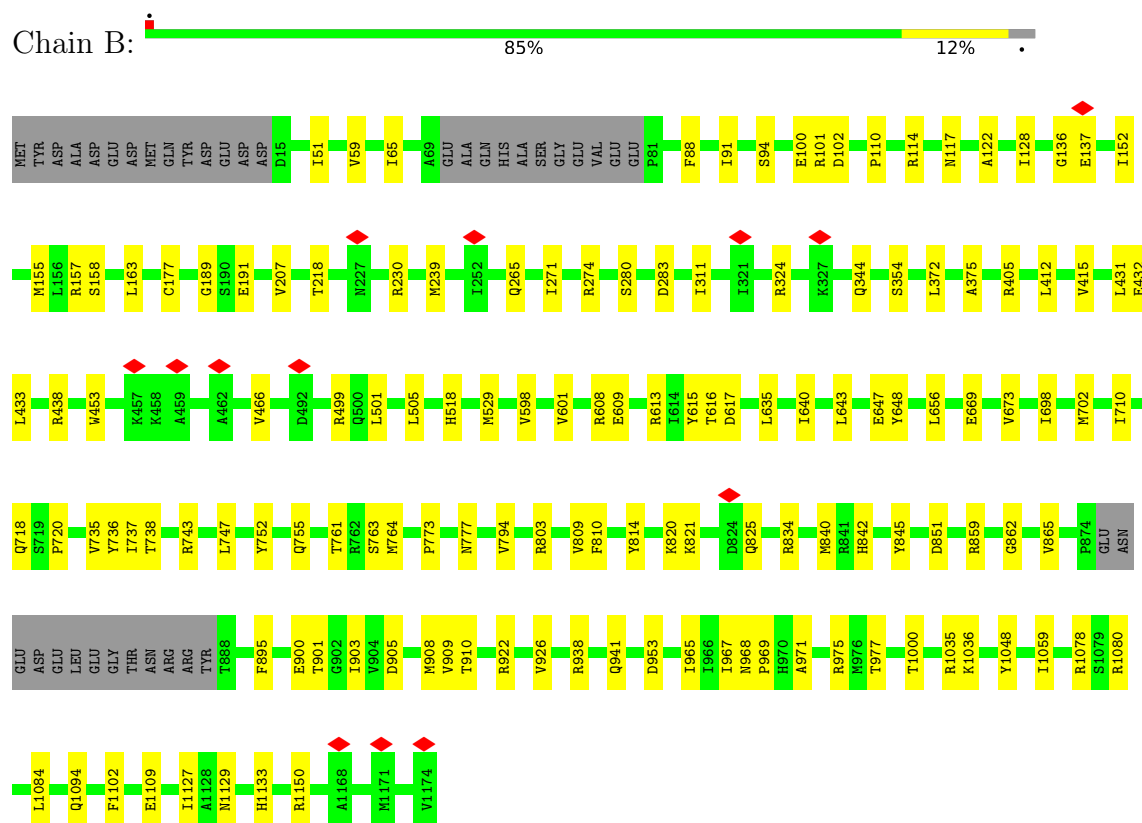
- Molecule 26 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of

Interest" by depositor).

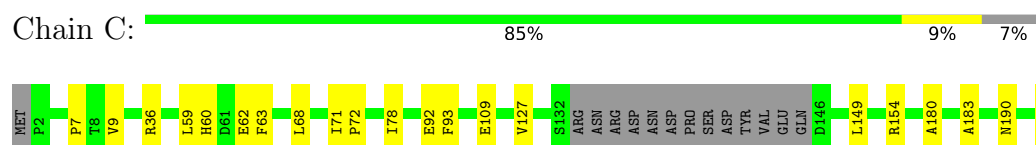
Mol	Chain	Residues	Atoms		AltConf
26	A	1	Total	Mg	0
			1	1	

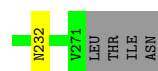


- Molecule 2: DNA-directed RNA polymerase subunit beta

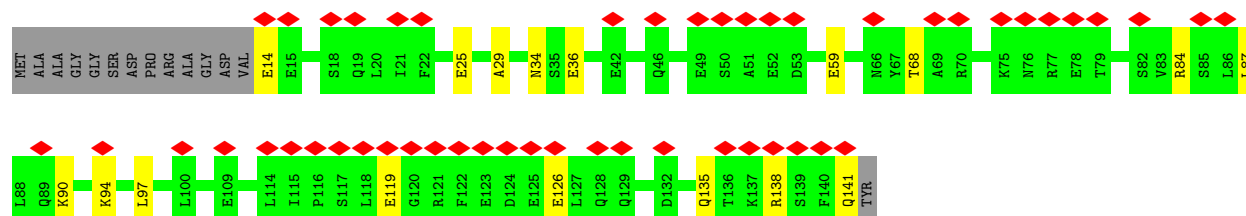
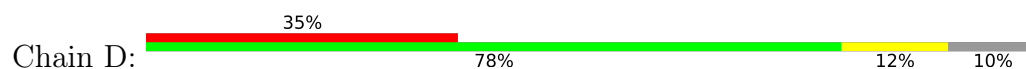


- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

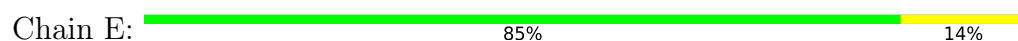




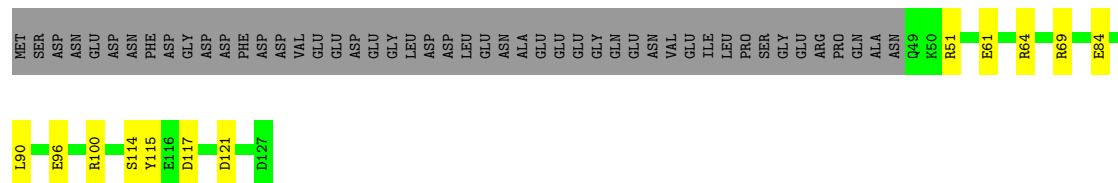
- Molecule 4: RNA polymerase II subunit D



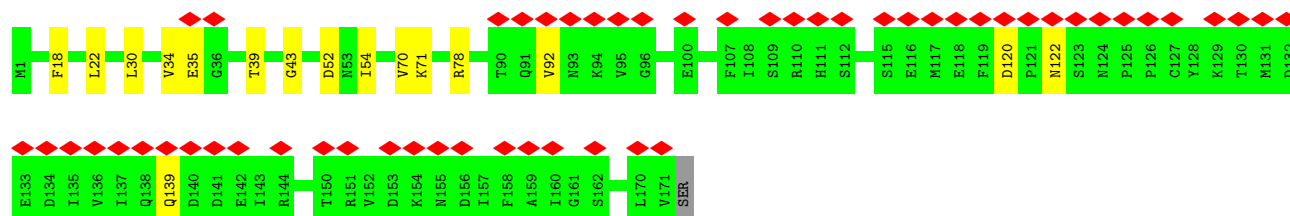
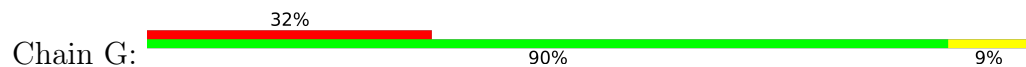
- Molecule 5: DNA-directed RNA polymerase II subunit E



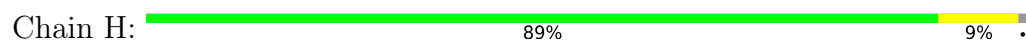
- Molecule 6: DNA-directed RNA polymerase II subunit F



- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:  82% 9% 9%



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  73% 22% .



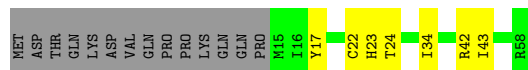
- Molecule 11: RNA polymerase II subunit J

Chain K:  86% 12% .



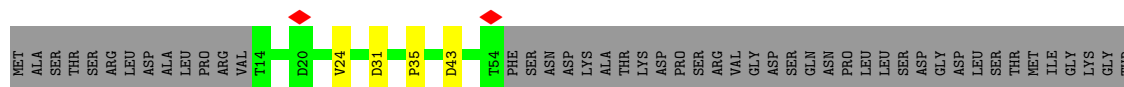
- Molecule 12: RNA polymerase II subunit K

Chain L:  64% 12% 24%



- Molecule 13: Transcription initiation factor IIB

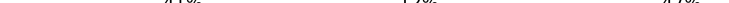
Chain M:  56% 21% 23%

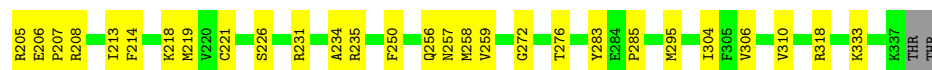
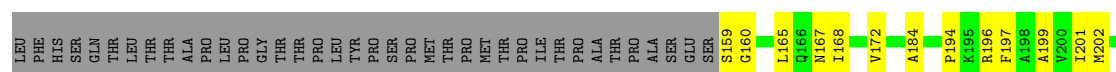
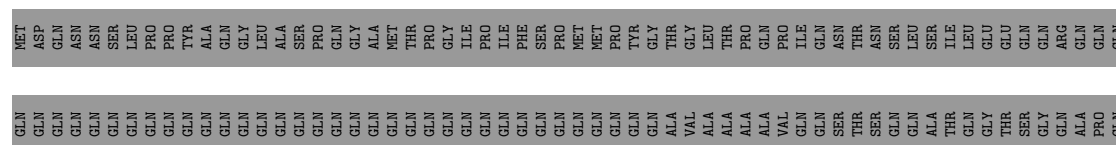


- Molecule 14: Non-template strand

Chain N:  14% 54% 15% 31%

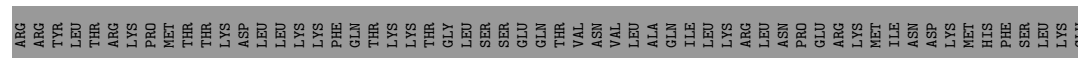
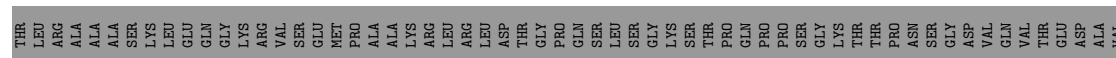
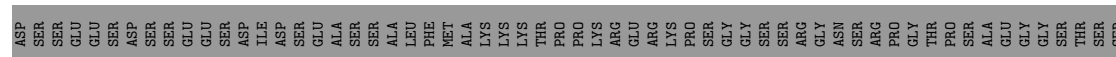
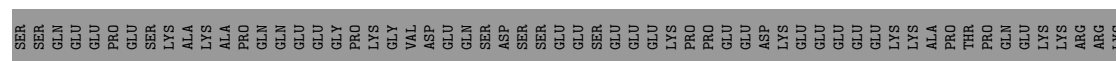
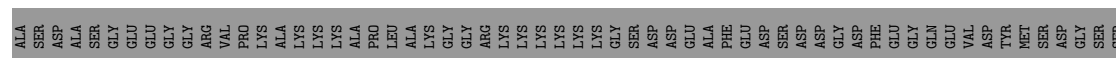
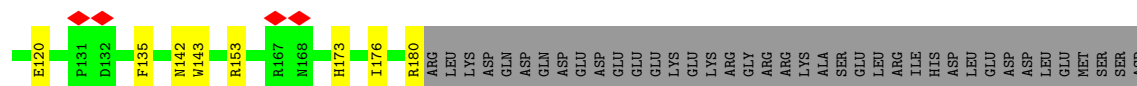
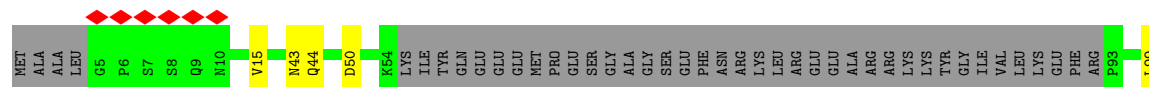
- Molecule 15: TATA-box-binding protein

Chain O:  41% 12% 47%

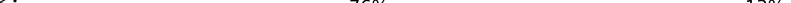


- Molecule 16: General transcription factor IIF subunit 1

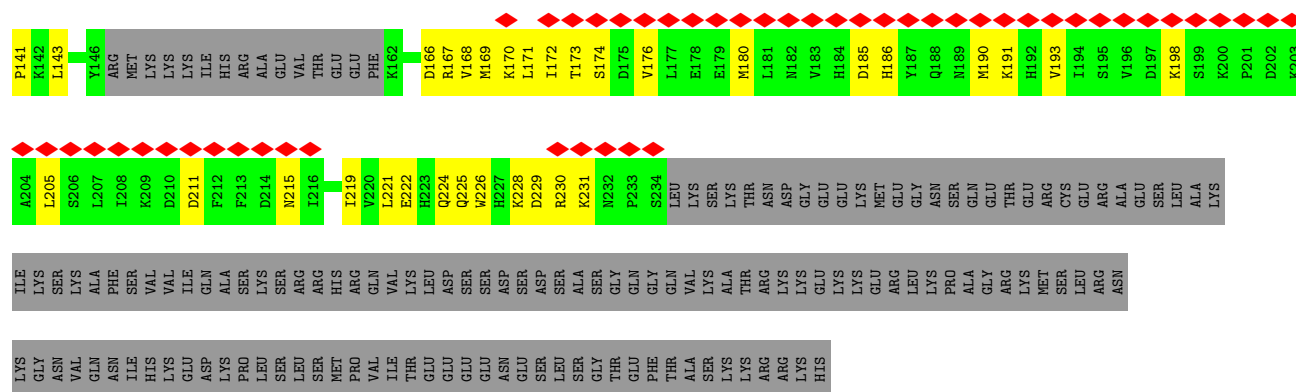
Chain Q: 24% 73%



- Molecule 17: General transcription factor IIF subunit 2

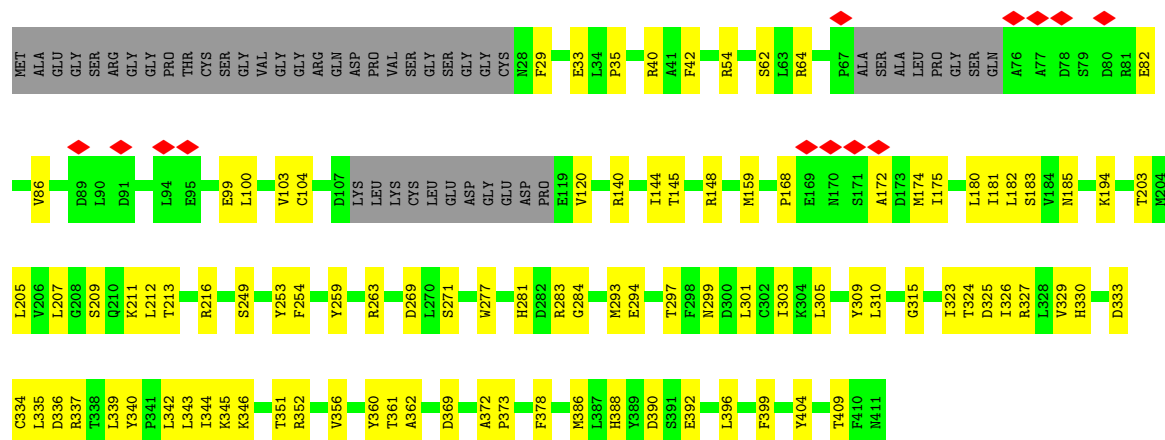
Chain B: 





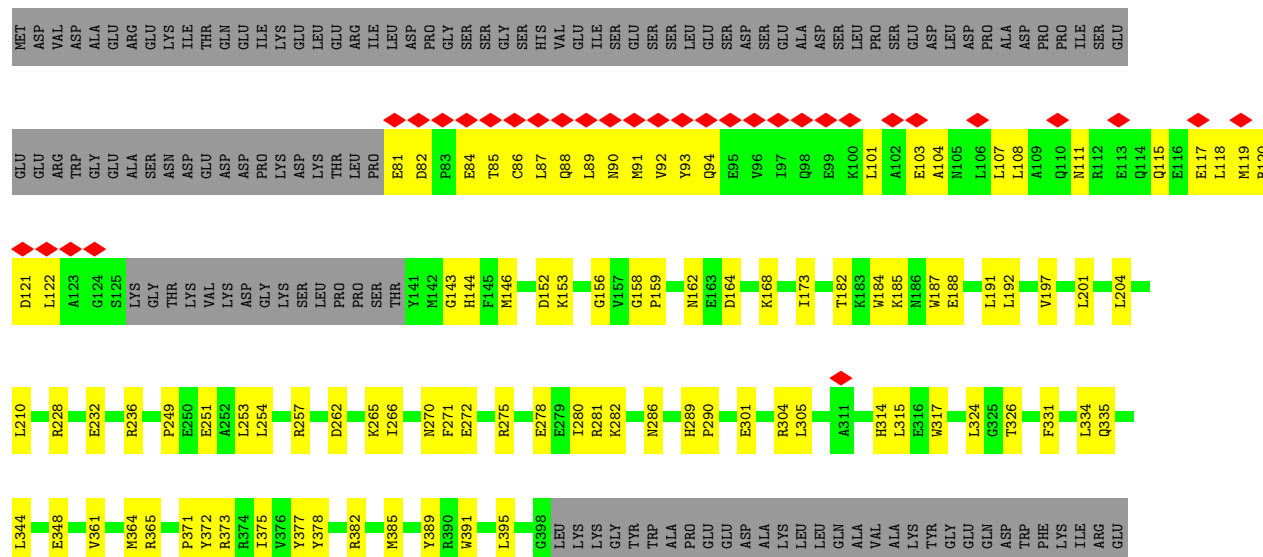
• Molecule 22: snRNA-activating protein complex subunit 3

Chain b: 65% 23% 11%



• Molecule 23: snRNA-activating protein complex subunit 4

Chain c: 14% 7% 79%







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85787	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.93	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.222	Depositor
Minimum map value	-0.102	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0153	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.15	0/11479	0.26	0/15496
2	B	0.17	0/9257	0.28	0/12493
3	C	0.17	0/2102	0.28	0/2857
4	D	0.09	0/1064	0.18	0/1428
5	E	0.13	0/1752	0.25	0/2366
6	F	0.16	0/646	0.26	0/871
7	G	0.11	0/1382	0.20	0/1874
8	H	0.16	0/1207	0.29	0/1628
9	I	0.12	0/949	0.27	0/1284
10	J	0.19	0/516	0.28	0/696
11	K	0.16	0/939	0.26	0/1271
12	L	0.17	0/378	0.29	0/500
13	M	0.33	0/1909	0.45	0/2580
14	N	0.43	0/1514	0.69	1/2334 (0.0%)
15	O	0.40	0/1448	0.46	0/1948
16	Q	0.10	0/1167	0.22	0/1576
17	R	0.30	0/1817	0.47	0/2445
18	T	0.45	0/1520	0.67	1/2344 (0.0%)
19	U	0.37	0/748	0.45	0/1005
20	V	0.41	0/803	0.48	0/1088
21	a	0.27	0/1851	0.42	0/2493
22	b	0.39	0/3054	0.55	3/4131 (0.1%)
23	c	0.32	0/2562	0.45	0/3440
24	d	0.17	0/425	0.43	0/564
All	All	0.25	0/50489	0.37	5/68712 (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
17	R	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	T	5	DT	C2'-C3'-O3'	-6.34	101.99	111.50
22	b	172	ALA	N-CA-C	-5.45	107.28	114.31
22	b	120	VAL	CA-C-N	5.34	123.61	120.24
22	b	120	VAL	C-N-CA	5.34	123.61	120.24
14	N	-12	DG	C2'-C3'-O3'	5.18	119.27	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	R	172	ASP	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11274	0	11406	122	0
2	B	9076	0	9116	120	0
3	C	2059	0	2007	22	0
4	D	1050	0	1033	11	0
5	E	1721	0	1737	21	0
6	F	636	0	665	9	0
7	G	1351	0	1358	12	0
8	H	1186	0	1147	9	0
9	I	928	0	859	8	0
10	J	507	0	523	20	0
11	K	920	0	942	13	0
12	L	373	0	378	10	0
13	M	1879	0	1915	71	0
14	N	1351	0	747	22	0
15	O	1422	0	1514	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	Q	1138	0	1103	7	0
17	R	1788	0	1818	42	0
18	T	1355	0	746	25	0
19	U	735	0	729	26	0
20	V	793	0	801	26	0
21	a	1807	0	1800	51	0
22	b	2978	0	2839	87	0
23	c	2516	0	2483	108	0
24	d	424	0	447	36	0
25	A	2	0	0	0	0
25	B	1	0	0	0	0
25	C	1	0	0	0	0
25	I	2	0	0	0	0
25	J	1	0	0	0	0
25	L	1	0	0	0	0
25	M	1	0	0	0	0
25	b	2	0	0	0	0
26	A	1	0	0	0	0
All	All	49279	0	48113	735	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 8.

All (735) 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)
23:c:184:TRP:CZ3	23:c:192:LEU:HD11	1.45	1.51
14:N:10:DA:H4'	17:R:174:LYS:CD	1.49	1.41
2:B:820:LYS:NZ	13:M:137:ARG:NH2	1.70	1.38
14:N:10:DA:C4'	17:R:174:LYS:HD2	1.52	1.38
2:B:820:LYS:NZ	13:M:137:ARG:HH21	1.26	1.30
2:B:820:LYS:HZ3	13:M:137:ARG:NH2	1.33	1.22
2:B:438:ARG:NH2	13:M:126:ASP:OD1	1.76	1.18
2:B:432:GLU:O	17:R:153:TYR:OH	1.66	1.14
2:B:438:ARG:CZ	13:M:126:ASP:OD1	1.99	1.10
23:c:187:TRP:O	23:c:191:LEU:HD13	1.56	1.05
23:c:184:TRP:CZ3	23:c:192:LEU:CD1	2.41	1.03
14:N:-18:DG:OP1	22:b:145:THR:HG22	1.61	0.98
23:c:184:TRP:HZ3	23:c:192:LEU:HD11	1.24	0.97
2:B:438:ARG:NE	13:M:126:ASP:OD2	1.97	0.96
2:B:820:LYS:HZ2	13:M:137:ARG:HH22	1.05	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:820:LYS:HZ2	13:M:137:ARG:NH2	1.45	0.90
2:B:438:ARG:HG2	13:M:126:ASP:OD2	1.71	0.89
2:B:438:ARG:CZ	13:M:126:ASP:CG	2.45	0.89
14:N:-25:DC:H2'	23:c:389:TYR:OH	1.74	0.87
22:b:168:PRO:CA	22:b:336:ASP:OD1	2.24	0.85
1:A:911:PRO:O	1:A:963:ARG:NH2	2.10	0.85
18:T:8:DG:H5'	23:c:144:HIS:CD2	2.11	0.85
1:A:39:GLY:O	1:A:42:LYS:NZ	2.09	0.84
2:B:438:ARG:CG	13:M:126:ASP:OD2	2.25	0.84
2:B:274:ARG:NH1	2:B:311:ILE:O	2.09	0.84
18:T:8:DG:C5'	23:c:144:HIS:CD2	2.60	0.84
2:B:814:TYR:OH	2:B:900:GLU:OE1	1.96	0.83
2:B:438:ARG:CD	13:M:126:ASP:OD2	2.28	0.82
21:a:166:ASP:H	21:a:169:MET:HE3	1.45	0.82
1:A:710:LYS:NZ	1:A:824:GLU:OE1	2.13	0.81
3:C:193:ARG:NH2	3:C:218:ALA:O	2.13	0.81
1:A:893:GLU:OE1	5:E:197:SER:OG	1.99	0.81
3:C:36:ARG:NH1	11:K:41:THR:OG1	2.14	0.80
18:T:20:DC:OP2	23:c:372:TYR:HE1	1.63	0.80
1:A:535:MET:O	1:A:669:TYR:OH	1.98	0.80
23:c:192:LEU:CD2	23:c:271:PHE:CZ	2.65	0.80
23:c:187:TRP:O	23:c:191:LEU:CD1	2.29	0.80
13:M:127:ARG:HG2	17:R:153:TYR:CZ	2.18	0.79
21:a:190:MET:HE1	23:c:86:CYS:HA	1.65	0.79
23:c:192:LEU:HD23	23:c:271:PHE:CE1	2.18	0.79
22:b:168:PRO:HB3	22:b:336:ASP:OD1	1.84	0.77
23:c:192:LEU:HD23	23:c:271:PHE:CZ	2.20	0.77
22:b:168:PRO:HA	22:b:336:ASP:OD1	1.82	0.77
5:E:46:ASP:O	5:E:52:ARG:NH1	2.17	0.77
2:B:344:GLN:NE2	2:B:354:SER:O	2.18	0.77
21:a:100:ALA:HB2	21:a:141:PRO:HD3	1.65	0.76
2:B:433:LEU:HA	13:M:127:ARG:HH22	1.51	0.76
23:c:184:TRP:CH2	23:c:192:LEU:HD11	2.19	0.76
23:c:104:ALA:HB1	24:d:19:LYS:HZ2	1.51	0.76
1:A:113:PHE:O	1:A:227:ARG:NH1	2.18	0.75
1:A:1147:SER:OG	1:A:1351:ASP:OD2	2.04	0.75
2:B:438:ARG:CZ	13:M:126:ASP:OD2	2.33	0.75
18:T:8:DG:H5''	23:c:144:HIS:CD2	2.22	0.75
7:G:30:LEU:HD22	7:G:70:VAL:HG11	1.69	0.74
1:A:513:ALA:HB2	6:F:90:LEU:HD21	1.67	0.74
2:B:909:VAL:HG12	12:L:34:ILE:HD13	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:64:PRO:O	12:L:23:HIS:NE2	2.20	0.74
2:B:821:LYS:O	2:B:825:GLN:NE2	2.20	0.73
1:A:322:LEU:O	1:A:327:ARG:NH2	2.21	0.73
15:O:259:VAL:HG21	18:T:-4:DA:C2	2.22	0.73
21:a:190:MET:HE3	23:c:89:LEU:HD23	1.71	0.73
22:b:168:PRO:CB	22:b:336:ASP:OD1	2.37	0.73
1:A:1234:LYS:NZ	1:A:1298:LEU:O	2.21	0.73
2:B:777:ASN:O	10:J:47:ARG:NH1	2.22	0.73
18:T:8:DG:H5'	23:c:144:HIS:NE2	2.03	0.72
20:V:80:GLU:OE2	22:b:283:ARG:NH2	2.23	0.72
15:O:259:VAL:HG21	18:T:-4:DA:H2	1.55	0.72
22:b:175:ILE:HG22	22:b:337:ARG:HG3	1.71	0.72
1:A:1411:LEU:O	1:A:1421:ARG:NH2	2.23	0.71
17:R:163:ILE:CG2	17:R:167:ARG:NH2	2.52	0.71
19:U:338:GLN:HG3	19:U:355:ASP:OD1	1.91	0.71
1:A:1178:ASP:OD2	1:A:1260:ARG:NH2	2.23	0.70
5:E:52:ARG:HD3	5:E:53:PRO:HD3	1.73	0.70
13:M:127:ARG:HG2	17:R:153:TYR:CE1	2.26	0.70
23:c:115:GLN:HA	23:c:118:LEU:HD12	1.71	0.70
1:A:373:LEU:O	1:A:485:ASN:ND2	2.24	0.70
22:b:315:GLY:O	23:c:162:ASN:ND2	2.24	0.70
1:A:86:GLY:O	1:A:255:VAL:N	2.25	0.70
2:B:613:ARG:NH1	2:B:615:TYR:OH	2.24	0.70
14:N:34:DT:H3	18:T:-34:DA:H61	1.40	0.69
10:J:14:VAL:HG13	10:J:49:LEU:HD11	1.73	0.69
24:d:2:LEU:HD22	24:d:6:GLN:HE21	1.57	0.69
14:N:-25:DC:C2'	23:c:389:TYR:OH	2.41	0.69
23:c:254:LEU:HD13	23:c:290:PRO:HG2	1.73	0.69
23:c:94:GLN:HG2	24:d:29:LEU:HD13	1.74	0.68
17:R:190:ALA:O	17:R:197:TYR:OH	2.09	0.68
22:b:203:THR:HG22	22:b:345:LYS:HB3	1.75	0.67
23:c:192:LEU:CD2	23:c:271:PHE:HZ	2.07	0.67
20:V:4:GLN:OE1	20:V:7:ARG:NH1	2.27	0.67
2:B:851:ASP:OD2	12:L:17:TYR:OH	2.11	0.67
22:b:352:ARG:NH1	22:b:404:TYR:OH	2.26	0.67
23:c:373:ARG:NH2	23:c:377:TYR:OH	2.27	0.67
1:A:22:GLN:NE2	1:A:1446:GLY:O	2.28	0.67
22:b:340:TYR:O	22:b:342:LEU:N	2.27	0.67
14:N:14:DA:C2	18:T:-13:DA:C2	2.83	0.67
1:A:481:THR:O	1:A:483:ARG:NH1	2.27	0.66
1:A:1226:LEU:HD23	1:A:1230:GLN:HE21	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:102:ASP:OD2	8:H:110:THR:OG1	2.12	0.66
21:a:222:GLU:OE1	24:d:17:ARG:NH1	2.27	0.66
1:A:233:CYS:SG	1:A:244:ARG:NH1	2.69	0.66
3:C:180:ALA:O	10:J:42:ARG:NH2	2.28	0.66
22:b:303:ILE:HD12	22:b:323:ILE:HG13	1.76	0.66
19:U:20:ASP:OD2	20:V:51:ARG:NH2	2.27	0.66
20:V:71:VAL:HG23	20:V:98:CYS:HB2	1.77	0.66
22:b:174:MET:HE1	22:b:335:LEU:HD13	1.77	0.66
1:A:432:HIS:NE2	13:M:35:PRO:O	2.29	0.66
17:R:177:ARG:HG2	17:R:209:PRO:HG2	1.77	0.66
21:a:219:ILE:HD13	24:d:17:ARG:HB3	1.78	0.66
2:B:529:MET:HE1	2:B:698:ILE:HD12	1.77	0.66
6:F:100:ARG:NH2	6:F:121:ASP:O	2.28	0.65
23:c:152:ASP:HB2	23:c:156:GLY:H	1.61	0.65
14:N:-6:DG:N2	18:T:7:DG:C2	2.64	0.65
21:a:167:ARG:HA	21:a:170:LYS:HD2	1.77	0.65
1:A:621:ILE:HG23	1:A:621:ILE:O	1.97	0.65
2:B:953:ASP:OD1	3:C:36:ARG:NH2	2.30	0.65
14:N:-25:DC:C6	23:c:389:TYR:OH	2.50	0.65
19:U:355:ASP:HB2	20:V:48:LEU:HB3	1.77	0.65
13:M:248:ARG:NH1	18:T:1:DA:OP2	2.31	0.64
2:B:794:VAL:HG13	2:B:965:ILE:HG23	1.77	0.64
21:a:167:ARG:N	24:d:11:GLU:OE2	2.30	0.64
14:N:-6:DG:N2	18:T:7:DG:N1	2.45	0.64
17:R:163:ILE:CG2	17:R:167:ARG:HH22	2.11	0.64
12:L:22:CYS:SG	12:L:24:THR:OG1	2.54	0.64
22:b:183:SER:O	22:b:324:THR:OG1	2.16	0.64
14:N:-25:DC:H6	23:c:389:TYR:OH	1.79	0.64
13:M:226:LYS:HG3	13:M:230:MET:HE3	1.80	0.63
14:N:-14:DT:H3'	22:b:194:LYS:HB2	1.80	0.63
4:D:34:ASN:O	4:D:68:THR:OG1	2.15	0.63
21:a:51:LYS:HD2	21:a:90:LEU:HB2	1.81	0.63
20:V:29:THR:HG23	20:V:32:LEU:H	1.64	0.62
19:U:368:SER:HB3	20:V:52:VAL:HG12	1.81	0.62
19:U:46:TRP:CD1	20:V:14:SER:HG	2.18	0.62
13:M:127:ARG:CG	17:R:153:TYR:CE2	2.82	0.62
16:Q:153:ARG:NH1	16:Q:180:ARG:O	2.33	0.62
23:c:278:GLU:OE2	23:c:281:ARG:NH1	2.31	0.62
2:B:529:MET:HE2	2:B:702:MET:HG3	1.82	0.62
3:C:9:VAL:HG11	11:K:105:PHE:HD1	1.64	0.62
3:C:59:LEU:HD13	3:C:63:PHE:CD2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:78:ILE:HG21	3:C:127:VAL:HG22	1.82	0.61
1:A:1375:ARG:NE	1:A:1403:ASP:OD1	2.27	0.61
13:M:169:ARG:HG3	13:M:174:PRO:HB3	1.81	0.61
22:b:249:SER:OG	23:c:164:ASP:OD2	2.18	0.61
23:c:304:ARG:NH2	23:c:324:LEU:O	2.33	0.61
17:R:158:ASN:ND2	17:R:163:ILE:HG13	2.15	0.61
2:B:862:GLY:O	2:B:1078:ARG:NH2	2.33	0.61
13:M:158:ALA:HB2	13:M:190:GLU:OE2	2.00	0.61
22:b:253:TYR:HB3	22:b:310:LEU:HB3	1.83	0.61
8:H:74:GLU:OE1	8:H:76:ASN:ND2	2.34	0.61
13:M:134:ILE:HG12	13:M:171:GLU:HG3	1.83	0.61
18:T:20:DC:OP2	23:c:372:TYR:CE1	2.52	0.61
22:b:390:ASP:HB3	22:b:396:LEU:HD21	1.82	0.61
2:B:735:VAL:HG21	10:J:55:LEU:CD1	2.30	0.61
20:V:82:ARG:NH1	23:c:158:GLY:O	2.22	0.61
15:O:213:ILE:HG12	15:O:219:MET:HG3	1.83	0.60
22:b:361:THR:HB	23:c:377:TYR:CZ	2.36	0.60
1:A:902:GLU:OE2	1:A:985:ARG:NH2	2.34	0.60
1:A:400:ASP:OD1	1:A:401:ARG:N	2.35	0.60
22:b:175:ILE:HD11	22:b:329:VAL:HG21	1.84	0.60
1:A:1192:TRP:HZ3	1:A:1246:ILE:HG22	1.67	0.60
3:C:9:VAL:HG11	11:K:105:PHE:CD1	2.36	0.60
4:D:29:ALA:O	4:D:94:LYS:NZ	2.28	0.60
13:M:127:ARG:NH2	17:R:153:TYR:OH	2.35	0.59
22:b:284:GLY:HA3	23:c:153:LYS:HG2	1.85	0.59
1:A:875:TYR:OH	6:F:61:GLU:OE2	2.08	0.59
3:C:59:LEU:HD13	3:C:63:PHE:CE2	2.37	0.59
5:E:31:ASP:OD1	5:E:32:GLU:N	2.36	0.59
13:M:267:GLU:OE1	13:M:269:ARG:NH2	2.34	0.59
13:M:169:ARG:HB3	13:M:206:VAL:HG11	1.84	0.59
2:B:432:GLU:C	17:R:153:TYR:OH	2.44	0.59
13:M:247:GLY:HA3	15:O:306:VAL:HG21	1.85	0.59
16:Q:142:ASN:OD1	16:Q:143:TRP:N	2.36	0.59
23:c:81:GLU:HG2	23:c:82:ASP:H	1.66	0.59
2:B:100:GLU:OE1	12:L:42:ARG:NH1	2.36	0.58
14:N:10:DA:C5'	17:R:174:LYS:HD2	2.28	0.58
17:R:163:ILE:HG21	17:R:167:ARG:HH22	1.66	0.58
20:V:50:GLN:HB3	23:c:265:LYS:HG3	1.85	0.58
22:b:33:GLU:O	23:c:120:ARG:NH1	2.36	0.58
1:A:869:GLU:OE1	1:A:1455:SER:OG	2.21	0.58
13:M:127:ARG:HG3	17:R:153:TYR:CE2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:901:THR:HG23	2:B:901:THR:O	2.01	0.58
9:I:60:HIS:O	9:I:60:HIS:ND1	2.36	0.58
2:B:738:THR:HG21	10:J:58:LYS:HG3	1.84	0.58
7:G:54:ILE:HD13	7:G:70:VAL:HG13	1.86	0.58
23:c:184:TRP:HZ3	23:c:192:LEU:CD1	2.01	0.58
2:B:157:ARG:NH2	2:B:177:CYS:O	2.37	0.58
4:D:14:GLU:N	4:D:14:GLU:OE1	2.36	0.58
21:a:98:ARG:NH2	21:a:140:MET:O	2.32	0.58
22:b:203:THR:HG23	22:b:344:ILE:HB	1.85	0.58
22:b:209:SER:H	22:b:299:ASN:HB2	1.65	0.58
2:B:643:LEU:HD11	2:B:656:LEU:HD11	1.85	0.57
23:c:192:LEU:HD21	23:c:271:PHE:CZ	2.37	0.57
1:A:1242:ASP:HA	1:A:1262:MET:HE2	1.86	0.57
2:B:432:GLU:HB3	17:R:153:TYR:CZ	2.39	0.57
13:M:127:ARG:HG2	17:R:153:TYR:CE2	2.38	0.57
18:T:8:DG:C5'	23:c:144:HIS:NE2	2.67	0.57
4:D:59:GLU:N	4:D:59:GLU:OE1	2.38	0.57
13:M:137:ARG:NH1	13:M:171:GLU:OE1	2.37	0.57
2:B:102:ASP:HA	13:M:173:VAL:HB	1.84	0.57
2:B:764:MET:HE1	2:B:938:ARG:NH1	2.18	0.57
1:A:1242:ASP:O	1:A:1262:MET:N	2.37	0.57
15:O:196:ARG:HG2	18:T:-7:DG:H5''	1.87	0.57
17:R:156:VAL:CG1	17:R:158:ASN:O	2.52	0.57
23:c:361:VAL:O	23:c:365:ARG:HG3	2.05	0.57
1:A:1235:ILE:HG13	1:A:1296:MET:HE1	1.85	0.57
22:b:185:ASN:HA	22:b:203:THR:HA	1.86	0.57
22:b:327:ARG:NH2	22:b:333:ASP:OD2	2.37	0.57
22:b:361:THR:HB	23:c:377:TYR:CE1	2.39	0.57
1:A:1160:ARG:NH2	1:A:1350:LYS:O	2.38	0.57
16:Q:43:ASN:OD1	16:Q:44:GLN:N	2.38	0.56
2:B:747:LEU:HD22	2:B:810:PHE:HZ	1.71	0.56
13:M:140:ASN:ND2	13:M:144:GLN:OE1	2.36	0.56
5:E:94:MET:O	5:E:98:ASN:N	2.39	0.56
19:U:344:ARG:HG2	19:U:345:SER:O	2.06	0.56
2:B:265:GLN:OE1	2:B:324:ARG:NH1	2.38	0.56
2:B:1035:ARG:NH1	2:B:1036:LYS:O	2.39	0.56
13:M:286:ARG:NH2	14:N:-6:DG:OP2	2.39	0.56
17:R:177:ARG:CG	17:R:209:PRO:HG2	2.36	0.56
11:K:63:VAL:HG23	11:K:63:VAL:O	2.05	0.56
23:c:117:GLU:HA	23:c:120:ARG:HG2	1.88	0.56
22:b:269:ASP:OD1	22:b:271:SER:OG	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:926:VAL:HG21	3:C:62:GLU:HG3	1.88	0.55
23:c:118:LEU:O	23:c:122:LEU:HG	2.06	0.55
23:c:371:PRO:O	23:c:375:ILE:HG12	2.04	0.55
24:d:28:ARG:O	24:d:32:GLU:HG3	2.05	0.55
15:O:201:ILE:HD13	18:T:-6:DT:H5''	1.88	0.55
20:V:5:LEU:HD22	20:V:98:CYS:HB3	1.86	0.55
13:M:115:MET:HE3	13:M:116:ASN:H	1.72	0.55
22:b:254:PHE:HB2	22:b:259:TYR:HE2	1.71	0.55
1:A:1248:ASN:ND2	1:A:1254:LYS:O	2.36	0.55
22:b:182:LEU:HG	22:b:326:ILE:HG12	1.89	0.55
1:A:549:THR:O	1:A:589:LYS:NZ	2.38	0.55
1:A:1137:PRO:HB2	1:A:1341:VAL:HG13	1.88	0.55
23:c:281:ARG:NH1	23:c:282:LYS:HE3	2.22	0.55
23:c:364:MET:HE1	23:c:378:TYR:CE1	2.42	0.55
22:b:82:GLU:O	22:b:86:VAL:HG23	2.07	0.55
13:M:127:ARG:CG	17:R:153:TYR:CZ	2.89	0.55
21:a:225:GLN:HG2	21:a:228:LYS:HE3	1.87	0.55
21:a:228:LYS:HA	21:a:231:LYS:HE2	1.89	0.55
10:J:8:PHE:CD2	10:J:48:MET:HE1	2.42	0.55
21:a:25:ARG:HB3	21:a:27:GLU:HG2	1.89	0.55
2:B:909:VAL:HG12	12:L:34:ILE:CD1	2.37	0.55
24:d:15:LEU:O	24:d:19:LYS:HG3	2.07	0.54
2:B:432:GLU:C	17:R:153:TYR:HH	2.09	0.54
13:M:178:LYS:HB3	17:R:155:PRO:HB3	1.89	0.54
15:O:205:ARG:NH2	20:V:63:ASN:O	2.41	0.54
1:A:348:GLY:O	1:A:352:GLY:N	2.39	0.54
2:B:101:ARG:HG2	13:M:131:PRO:HG3	1.89	0.54
2:B:755:GLN:HE22	10:J:48:MET:HE2	1.73	0.54
7:G:39:THR:O	7:G:43:GLY:N	2.40	0.54
14:N:7:DC:H1'	15:O:214:PHE:CE1	2.42	0.54
2:B:65:ILE:HD11	2:B:412:LEU:HG	1.89	0.54
22:b:29:PHE:HZ	22:b:54:ARG:HH22	1.54	0.54
2:B:433:LEU:HD12	17:R:153:TYR:HE1	1.72	0.54
2:B:735:VAL:HG21	10:J:55:LEU:HD13	1.88	0.54
15:O:167:ASN:OD1	15:O:168:ILE:N	2.40	0.54
15:O:206:GLU:HB2	15:O:207:PRO:HD3	1.90	0.54
19:U:10:VAL:HG22	19:U:366:ILE:HG12	1.89	0.54
22:b:334:CYS:SG	22:b:339:LEU:HD11	2.48	0.54
23:c:188:GLU:O	23:c:192:LEU:HG	2.08	0.54
8:H:91:VAL:HG22	8:H:144:LEU:HD23	1.89	0.54
17:R:37:ARG:NE	17:R:39:GLU:O	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:156:VAL:HG12	17:R:158:ASN:O	2.08	0.54
13:M:231:ALA:O	13:M:235:ILE:HG13	2.07	0.54
22:b:33:GLU:HB2	22:b:40:ARG:HG3	1.90	0.54
23:c:257:ARG:HB3	23:c:289:HIS:CD2	2.43	0.54
1:A:790:GLN:NE2	1:A:791:GLN:O	2.40	0.53
23:c:168:LYS:HE3	23:c:173:ILE:HG21	1.90	0.53
1:A:1357:THR:O	5:E:142:HIS:NE2	2.41	0.53
19:U:338:GLN:NE2	19:U:355:ASP:OD2	2.41	0.53
23:c:115:GLN:O	23:c:119:MET:HG2	2.08	0.53
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.91	0.53
8:H:2:ALA:O	8:H:84:ARG:NH2	2.39	0.53
22:b:159:MET:HE2	22:b:346:LYS:HG2	1.90	0.53
5:E:54:ARG:O	5:E:57:ASP:N	2.42	0.53
22:b:253:TYR:O	22:b:309:TYR:HB3	2.09	0.53
23:c:85:THR:HA	23:c:88:GLN:HG3	1.88	0.53
23:c:201:LEU:HG	23:c:253:LEU:HD21	1.90	0.53
23:c:314:HIS:O	23:c:317:TRP:NE1	2.41	0.53
23:c:348:GLU:O	23:c:382:ARG:NH2	2.41	0.53
23:c:364:MET:HB2	23:c:375:ILE:HD11	1.90	0.53
24:d:2:LEU:O	24:d:6:GLN:HG2	2.08	0.53
11:K:8:GLU:O	11:K:37:LYS:NZ	2.36	0.53
13:M:211:THR:HG21	13:M:236:ALA:HB1	1.91	0.53
1:A:1236:ASN:O	1:A:1240:GLY:N	2.42	0.53
1:A:467:MET:HG2	1:A:534:VAL:HG11	1.91	0.52
17:R:97:THR:OG1	17:R:107:GLU:OE2	2.21	0.52
19:U:355:ASP:OD1	19:U:355:ASP:O	2.25	0.52
24:d:40:ILE:O	24:d:44:ARG:HG2	2.09	0.52
1:A:547:LYS:O	1:A:553:VAL:HG21	2.10	0.52
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.90	0.52
5:E:71:GLN:HB2	5:E:99:ILE:HD12	1.91	0.52
17:R:163:ILE:HG22	17:R:167:ARG:NH2	2.25	0.52
23:c:187:TRP:CZ3	23:c:191:LEU:HD22	2.45	0.52
1:A:1189:ASP:O	1:A:1193:VAL:HG23	2.09	0.52
2:B:598:VAL:CG2	2:B:601:VAL:HG23	2.39	0.52
2:B:910:THR:HG22	12:L:43:ILE:HA	1.91	0.52
5:E:106:VAL:O	5:E:132:GLN:N	2.42	0.52
13:M:251:ILE:HD12	13:M:251:ILE:H	1.73	0.52
22:b:360:TYR:OH	23:c:344:LEU:O	2.25	0.52
22:b:369:ASP:HA	22:b:399:PHE:HB3	1.91	0.52
21:a:105:ASP:OD1	22:b:54:ARG:NH1	2.42	0.52
21:a:211:ASP:O	21:a:215:ASN:N	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ASN:N	1:A:338:SER:OG	2.42	0.52
1:A:362:SER:HB2	2:B:1084:LEU:HD12	1.92	0.52
2:B:59:VAL:HG21	2:B:91:ILE:HD11	1.91	0.52
5:E:52:ARG:CD	5:E:53:PRO:HD3	2.39	0.52
5:E:103:LEU:HD11	5:E:130:PHE:CE2	2.44	0.52
13:M:115:MET:C	13:M:117:ALA:H	2.18	0.52
22:b:369:ASP:OD1	22:b:388:HIS:NE2	2.37	0.52
23:c:188:GLU:HG2	23:c:271:PHE:HE2	1.73	0.52
2:B:738:THR:HG21	10:J:58:LYS:CG	2.40	0.52
8:H:71:ASP:O	8:H:72:ASP:OD1	2.28	0.52
13:M:247:GLY:O	18:T:0:DA:H5"	2.10	0.52
17:R:217:LEU:O	17:R:221:GLY:N	2.43	0.52
21:a:96:LYS:HE3	22:b:330:HIS:CD2	2.45	0.52
22:b:356:VAL:HG11	23:c:334:LEU:HG	1.92	0.52
23:c:232:GLU:O	23:c:236:ARG:HG2	2.09	0.52
22:b:62:SER:HB2	22:b:64:ARG:HE	1.75	0.52
2:B:155:MET:O	2:B:158:SER:OG	2.17	0.51
1:A:350:VAL:HG21	1:A:1435:THR:HG21	1.91	0.51
21:a:66:PHE:CE1	21:a:79:LEU:HB2	2.45	0.51
23:c:197:VAL:HG13	23:c:253:LEU:HD23	1.92	0.51
24:d:32:GLU:O	24:d:36:LEU:HG	2.09	0.51
5:E:9:ARG:O	5:E:13:ILE:HD12	2.10	0.51
11:K:105:PHE:CD2	11:K:109:ILE:HD11	2.45	0.51
1:A:825:ASN:ND2	1:A:835:GLU:OE1	2.42	0.51
1:A:1182:GLN:O	1:A:1190:GLN:NE2	2.37	0.51
1:A:1453:GLY:O	1:A:1457:ASN:ND2	2.41	0.51
4:D:119:GLU:N	4:D:119:GLU:OE1	2.43	0.51
23:c:90:ASN:HD22	24:d:33:GLU:CD	2.18	0.51
1:A:122:ASN:O	1:A:127:LYS:NZ	2.44	0.51
15:O:219:MET:HE3	15:O:221:CYS:HB2	1.93	0.51
5:E:103:LEU:HD12	5:E:128:GLU:HB2	1.93	0.51
18:T:-37:DA:H2"	18:T:-36:DA:C8	2.46	0.50
5:E:41:LYS:O	5:E:45:GLY:N	2.43	0.50
23:c:84:GLU:OE1	24:d:44:ARG:NH1	2.44	0.50
1:A:479:TRP:HB2	1:A:483:ARG:NH2	2.26	0.50
9:I:27:LYS:N	9:I:36:LEU:O	2.44	0.50
13:M:270:THR:HG23	13:M:272:LYS:H	1.76	0.50
23:c:103:GLU:O	23:c:107:LEU:HG	2.11	0.50
2:B:743:ARG:O	2:B:922:ARG:NH1	2.44	0.50
7:G:30:LEU:O	7:G:34:VAL:HG22	2.11	0.50
8:H:49:PRO:O	8:H:147:LYS:NZ	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:159:SER:OG	15:O:160:GLY:N	2.25	0.50
22:b:183:SER:HB3	22:b:325:ASP:OD2	2.10	0.50
2:B:845:TYR:CE1	2:B:865:VAL:HG21	2.47	0.50
22:b:281:HIS:O	22:b:283:ARG:HG3	2.11	0.50
23:c:266:ILE:HA	23:c:270:ASN:HD22	1.75	0.50
11:K:105:PHE:CE2	11:K:109:ILE:HD11	2.47	0.50
19:U:40:MET:O	19:U:44:THR:HG23	2.12	0.50
21:a:224:GLN:O	21:a:228:LYS:HG2	2.12	0.50
1:A:1172:ASN:ND2	1:A:1215:GLU:OE1	2.43	0.50
2:B:1129:ASN:O	2:B:1133:HIS:N	2.45	0.50
22:b:390:ASP:N	22:b:390:ASP:OD1	2.44	0.50
2:B:271:ILE:HD11	2:B:311:ILE:HD13	1.95	0.49
23:c:87:LEU:O	23:c:91:MET:HG2	2.12	0.49
2:B:128:ILE:HG21	2:B:431:LEU:HD21	1.94	0.49
2:B:94:SER:O	2:B:122:ALA:HB1	2.13	0.49
13:M:114:MET:HE1	13:M:143:LYS:HG2	1.94	0.49
13:M:244:LEU:HD23	13:M:292:ILE:HG22	1.93	0.49
15:O:194:PRO:HA	15:O:197:PHE:O	2.12	0.49
23:c:90:ASN:O	23:c:94:GLN:HG3	2.13	0.49
20:V:41:ASP:O	20:V:45:ASN:ND2	2.45	0.49
1:A:1251:ASN:OD1	1:A:1252:ALA:N	2.45	0.49
2:B:433:LEU:HD23	13:M:185:ARG:HB3	1.93	0.49
2:B:601:VAL:HG22	2:B:616:THR:HG23	1.95	0.49
1:A:42:LYS:O	1:A:288:ASN:ND2	2.43	0.49
1:A:668:PHE:CE1	1:A:672:ILE:HD11	2.47	0.49
3:C:78:ILE:HG21	3:C:127:VAL:CG2	2.43	0.49
2:B:669:GLU:O	2:B:673:VAL:HG23	2.12	0.49
21:a:59:LEU:HD11	21:a:89:GLN:NE2	2.28	0.49
21:a:215:ASN:O	21:a:219:ILE:HG13	2.13	0.48
22:b:140:ARG:HG3	22:b:144:ILE:HG13	1.95	0.48
22:b:209:SER:N	22:b:299:ASN:HB2	2.26	0.48
23:c:182:THR:HG23	23:c:275:ARG:HH22	1.78	0.48
16:Q:173:HIS:O	16:Q:176:ILE:HG22	2.13	0.48
1:A:786:ALA:O	1:A:787:VAL:HG23	2.13	0.48
17:R:158:ASN:HD22	17:R:163:ILE:CG1	2.26	0.48
1:A:1454:VAL:HG12	1:A:1458:ILE:HD12	1.94	0.48
20:V:3:TYR:OH	20:V:98:CYS:O	2.31	0.48
10:J:6:ARG:HD3	10:J:13:ILE:HD13	1.96	0.48
13:M:174:PRO:O	13:M:217:ARG:NH2	2.44	0.48
1:A:1208:SER:O	1:A:1260:ARG:NH1	2.47	0.48
2:B:834:ARG:HH11	2:B:840:MET:HE2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:d:6:GLN:O	24:d:9:ARG:HG3	2.13	0.48
19:U:28:ILE:HD11	23:c:210:LEU:HG	1.94	0.48
20:V:51:ARG:NE	23:c:262:ASP:OD1	2.47	0.48
21:a:125:ILE:HD11	22:b:104:CYS:HB3	1.96	0.48
24:d:29:LEU:O	24:d:33:GLU:HG2	2.12	0.48
1:A:44:PRO:O	1:A:57:LEU:HD12	2.14	0.48
22:b:212:LEU:O	22:b:213:THR:OG1	2.20	0.48
1:A:514:GLU:OE1	2:B:1102:PHE:N	2.43	0.48
1:A:1218:ARG:NH2	1:A:1252:ALA:O	2.47	0.48
5:E:103:LEU:HD11	5:E:130:PHE:CD2	2.49	0.48
18:T:20:DC:H4'	22:b:148:ARG:CZ	2.44	0.48
23:c:192:LEU:HD23	23:c:271:PHE:HE1	1.73	0.48
2:B:608:ARG:NH2	2:B:609:GLU:OE2	2.46	0.47
23:c:187:TRP:HZ3	23:c:191:LEU:HD22	1.79	0.47
1:A:529:GLN:NE2	1:A:1097:GLU:OE1	2.45	0.47
1:A:1382:LEU:HD21	1:A:1401:LEU:HD23	1.96	0.47
1:A:1382:LEU:HD23	1:A:1398:LEU:HD13	1.96	0.47
2:B:499:ARG:NH1	2:B:518:HIS:O	2.44	0.47
2:B:865:VAL:HG22	2:B:895:PHE:CE2	2.49	0.47
6:F:51:ARG:NH2	6:F:117:ASP:O	2.38	0.47
1:A:84:HIS:HD1	2:B:1127:ILE:HG22	1.79	0.47
13:M:311:ASP:HB3	24:d:3:SER:HA	1.96	0.47
21:a:98:ARG:CZ	21:a:138:THR:HG21	2.43	0.47
22:b:174:MET:O	22:b:337:ARG:NH2	2.48	0.47
22:b:386:MET:HA	23:c:315:LEU:HD13	1.96	0.47
21:a:226:TRP:CH2	21:a:230:ARG:HD2	2.49	0.47
1:A:274:ASP:OD2	1:A:342:ARG:NH2	2.48	0.47
1:A:274:ASP:OD1	1:A:275:ASP:N	2.46	0.47
2:B:820:LYS:HZ3	13:M:137:ARG:HH21	0.54	0.47
21:a:171:LEU:HD13	24:d:18:LEU:HD12	1.96	0.47
2:B:968:ASN:OD1	2:B:969:PRO:HD2	2.15	0.47
11:K:81:TYR:OH	11:K:89:ASN:OD1	2.27	0.47
21:a:16:SER:HA	21:a:19:GLN:HG2	1.96	0.47
22:b:362:ALA:HB1	22:b:378:PHE:HB3	1.97	0.47
23:c:282:LYS:HD3	23:c:286:ASN:ND2	2.30	0.47
23:c:305:LEU:HD11	23:c:317:TRP:HZ3	1.80	0.47
1:A:261:ARG:HD2	1:A:261:ARG:O	2.15	0.47
10:J:40:LEU:CD1	10:J:49:LEU:HD13	2.44	0.47
15:O:304:ILE:HG23	15:O:310:VAL:HG22	1.96	0.47
17:R:198:ASN:OD1	17:R:199:LEU:N	2.48	0.47
1:A:1468:THR:HG23	6:F:64:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:141:GLN:OE1	4:D:141:GLN:N	2.48	0.47
24:d:30:LYS:O	24:d:34:LEU:HG	2.14	0.47
1:A:408:ARG:NH1	1:A:414:PRO:O	2.48	0.46
13:M:121:ILE:HD13	13:M:138:THR:HG22	1.96	0.46
14:N:7:DC:H1'	15:O:214:PHE:CZ	2.50	0.46
14:N:20:DT:H2''	14:N:21:DA:C8	2.50	0.46
4:D:36:GLU:OE1	4:D:84:ARG:NH2	2.47	0.46
14:N:-18:DG:OP1	22:b:145:THR:CG2	2.50	0.46
24:d:36:LEU:O	24:d:40:ILE:HG12	2.16	0.46
3:C:109:GLU:OE1	3:C:109:GLU:N	2.48	0.46
17:R:39:GLU:OE1	17:R:40:VAL:N	2.48	0.46
21:a:68:PRO:HA	21:a:70:TYR:H	1.80	0.46
21:a:167:ARG:HD3	23:c:107:LEU:HB3	1.96	0.46
1:A:495:ASP:OD1	1:A:497:ASP:OD1	2.33	0.46
23:c:192:LEU:CD2	23:c:271:PHE:CE1	2.90	0.46
1:A:1382:LEU:HD23	1:A:1398:LEU:CD1	2.46	0.46
2:B:752:TYR:HE1	2:B:809:VAL:HG22	1.79	0.46
22:b:209:SER:HB2	22:b:299:ASN:HD22	1.81	0.46
23:c:192:LEU:HD22	23:c:280:ILE:HG23	1.98	0.46
2:B:110:PRO:HG2	2:B:163:LEU:HD11	1.97	0.46
4:D:90:LYS:NZ	4:D:126:GLU:OE2	2.49	0.46
15:O:219:MET:HE1	15:O:234:ALA:HA	1.98	0.46
19:U:371:ILE:HD12	20:V:55:ARG:HH11	1.81	0.46
17:R:80:GLU:OE2	17:R:81:HIS:N	2.49	0.46
2:B:842:HIS:CD2	13:M:24:VAL:HG13	2.50	0.46
22:b:334:CYS:HB3	22:b:340:TYR:CE1	2.51	0.46
24:d:9:ARG:O	24:d:13:GLU:HG2	2.16	0.46
2:B:239:MET:HB2	2:B:372:LEU:HD21	1.98	0.46
2:B:280:SER:OG	2:B:283:ASP:OD2	2.33	0.46
21:a:59:LEU:HD11	21:a:89:GLN:HE22	1.81	0.46
22:b:277:TRP:CZ2	22:b:283:ARG:HD3	2.50	0.46
22:b:283:ARG:HG2	23:c:152:ASP:OD1	2.16	0.46
24:d:6:GLN:HA	24:d:9:ARG:HG3	1.97	0.46
2:B:1059:ILE:O	2:B:1080:ARG:NH2	2.49	0.45
5:E:17:ILE:HD11	5:E:135:LEU:HD21	1.98	0.45
17:R:163:ILE:HG21	17:R:167:ARG:NH2	2.26	0.45
22:b:180:LEU:HD22	22:b:326:ILE:HG22	1.96	0.45
1:A:1289:GLU:OE2	1:A:1293:LEU:HD11	2.16	0.45
18:T:18:DC:OP1	22:b:351:THR:HG23	2.16	0.45
22:b:343:LEU:HD12	22:b:343:LEU:HA	1.80	0.45
1:A:467:MET:SD	1:A:467:MET:N	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1129:ASN:O	1:A:1130:ILE:C	2.59	0.45
2:B:803:ARG:NH1	10:J:8:PHE:O	2.44	0.45
15:O:184:ALA:O	20:V:66:ARG:HD2	2.17	0.45
1:A:508:SER:OG	1:A:511:THR:HG22	2.15	0.45
1:A:541:THR:HG21	1:A:672:ILE:HG22	1.98	0.45
1:A:1468:THR:HG22	6:F:64:ARG:HD2	1.96	0.45
2:B:114:ARG:NE	2:B:191:GLU:OE2	2.49	0.45
2:B:809:VAL:HG21	3:C:60:HIS:CE1	2.52	0.45
2:B:840:MET:HE3	2:B:845:TYR:CE2	2.51	0.45
5:E:50:GLU:OE1	5:E:50:GLU:N	2.50	0.45
9:I:58:ILE:HD12	9:I:58:ILE:H	1.81	0.45
11:K:37:LYS:N	11:K:69:HIS:O	2.50	0.45
1:A:1379:GLU:OE2	1:A:1395:TYR:HE1	1.99	0.45
3:C:72:PRO:HG3	10:J:13:ILE:HD11	1.98	0.45
4:D:25:GLU:OE2	7:G:78:ARG:NH2	2.49	0.45
9:I:69:ILE:HG22	9:I:71:ASP:H	1.81	0.45
22:b:62:SER:HB2	22:b:64:ARG:NE	2.31	0.45
3:C:92:GLU:O	3:C:93:PHE:CG	2.69	0.45
5:E:13:ILE:HD12	5:E:13:ILE:H	1.82	0.45
2:B:908:MET:HE2	12:L:43:ILE:HG23	1.98	0.45
13:M:182:ALA:HB2	17:R:155:PRO:HA	1.99	0.45
19:U:335:VAL:HG22	19:U:358:MET:HB3	1.99	0.45
1:A:477:LEU:HD12	1:A:483:ARG:HD3	1.98	0.45
2:B:773:PRO:CG	10:J:53:VAL:HG21	2.46	0.45
19:U:371:ILE:HD12	20:V:55:ARG:NH1	2.32	0.45
21:a:185:ASP:OD2	21:a:186:HIS:N	2.50	0.45
23:c:89:LEU:HA	23:c:92:VAL:HG12	1.98	0.45
1:A:57:LEU:O	1:A:261:ARG:NH2	2.44	0.45
2:B:218:THR:O	2:B:218:THR:HG23	2.17	0.45
6:F:114:SER:OG	6:F:115:TYR:N	2.50	0.45
15:O:168:ILE:HD12	15:O:226:SER:C	2.42	0.45
17:R:158:ASN:ND2	17:R:163:ILE:CG1	2.80	0.45
22:b:35:PRO:HG3	23:c:121:ASP:OD2	2.17	0.45
1:A:1173:THR:OG1	9:I:56:ASN:OD1	2.32	0.44
2:B:207:VAL:HG11	2:B:375:ALA:CB	2.47	0.44
14:N:-14:DT:H2'	14:N:-13:DA:C8	2.52	0.44
17:R:225:VAL:HG13	17:R:225:VAL:O	2.17	0.44
24:d:14:THR:O	24:d:18:LEU:HG	2.16	0.44
1:A:556:GLU:OE2	1:A:583:ARG:NH1	2.50	0.44
2:B:859:ARG:NH1	2:B:903:ILE:HD11	2.32	0.44
13:M:31:ASP:N	13:M:31:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:206:THR:HG21	17:R:213:LEU:HD13	1.99	0.44
23:c:87:LEU:HD22	24:d:37:GLN:HE22	1.80	0.44
23:c:108:LEU:HB2	24:d:19:LYS:HE3	1.98	0.44
1:A:611:ASP:N	1:A:611:ASP:OD1	2.46	0.44
21:a:190:MET:HA	21:a:193:VAL:HG22	1.99	0.44
22:b:205:LEU:HG	22:b:344:ILE:HG13	1.98	0.44
1:A:668:PHE:CZ	1:A:672:ILE:HD11	2.53	0.44
22:b:175:ILE:CD1	22:b:329:VAL:HG21	2.46	0.44
1:A:533:PRO:HD3	1:A:654:HIS:CG	2.53	0.44
13:M:175:ARG:HB3	13:M:179:GLU:HB2	2.00	0.44
19:U:372:GLY:HA3	20:V:58:PHE:CZ	2.53	0.44
22:b:213:THR:HG22	22:b:293:MET:HE2	1.98	0.44
24:d:4:ARG:O	24:d:8:LEU:HG	2.18	0.44
1:A:1475:LEU:HD21	7:G:22:LEU:HD11	1.99	0.44
5:E:44:PHE:HB3	5:E:52:ARG:HG3	2.00	0.44
14:N:5:DT:H4'	15:O:256:GLN:O	2.18	0.44
2:B:905:ASP:OD2	2:B:922:ARG:NH2	2.41	0.44
2:B:761:THR:HG23	2:B:1000:THR:HA	1.99	0.44
13:M:158:ALA:HA	13:M:186:ILE:HD13	2.00	0.44
14:N:7:DC:H5''	15:O:218:LYS:HB3	2.00	0.44
15:O:172:VAL:HG21	15:O:250:PHE:CE2	2.53	0.44
15:O:208:ARG:HH12	19:U:346:LYS:HB3	1.83	0.44
2:B:647:GLU:O	2:B:648:TYR:CG	2.71	0.44
2:B:910:THR:HG21	12:L:43:ILE:HG12	2.00	0.44
20:V:68:CYS:O	20:V:71:VAL:HG12	2.18	0.44
22:b:213:THR:HA	22:b:216:ARG:HB3	2.00	0.44
22:b:372:ALA:O	23:c:286:ASN:ND2	2.50	0.44
23:c:282:LYS:HD3	23:c:286:ASN:HD21	1.81	0.44
1:A:889:LEU:O	1:A:890:ARG:NH1	2.47	0.43
2:B:941:GLN:NE2	2:B:977:THR:OG1	2.46	0.43
7:G:18:PHE:HA	7:G:22:LEU:HD12	1.99	0.43
17:R:228:ILE:HG23	17:R:229:HIS:ND1	2.33	0.43
21:a:24:VAL:HG13	21:a:76:VAL:HG11	2.00	0.43
21:a:198:LYS:HA	21:a:198:LYS:HD2	1.88	0.43
22:b:356:VAL:O	23:c:335:GLN:HG3	2.18	0.43
1:A:693:ILE:HG22	1:A:694:ALA:N	2.33	0.43
13:M:144:GLN:O	13:M:148:GLN:HG2	2.17	0.43
16:Q:15:VAL:O	16:Q:135:PHE:N	2.51	0.43
22:b:140:ARG:NH2	22:b:144:ILE:HG13	2.33	0.43
22:b:362:ALA:CB	22:b:378:PHE:HB3	2.48	0.43
1:A:469:MET:SD	2:B:1094:GLN:NE2	2.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:GLY:N	1:A:519:ALA:O	2.44	0.43
21:a:63:TRP:HA	21:a:82:LEU:HD11	2.00	0.43
1:A:264:VAL:O	1:A:272:ASN:N	2.40	0.43
2:B:453:TRP:NE1	2:B:466:VAL:HB	2.33	0.43
2:B:909:VAL:CG1	12:L:34:ILE:HD13	2.45	0.43
3:C:190:ASN:ND2	3:C:195:THR:O	2.43	0.43
6:F:84:GLU:O	6:F:84:GLU:HG2	2.17	0.43
23:c:249:PRO:HB2	23:c:251:GLU:OE2	2.19	0.43
1:A:904:GLN:NE2	1:A:981:CYS:O	2.51	0.43
23:c:93:TYR:CD2	24:d:29:LEU:HD11	2.53	0.43
1:A:653:VAL:HG11	1:A:669:TYR:OH	2.19	0.43
13:M:149:LYS:HD2	13:M:149:LYS:HA	1.71	0.43
15:O:257:ASN:OD1	15:O:258:MET:N	2.51	0.43
21:a:143:LEU:H	21:a:143:LEU:HD12	1.83	0.43
22:b:277:TRP:CD2	23:c:159:PRO:HB3	2.53	0.43
23:c:348:GLU:C	23:c:382:ARG:HH22	2.25	0.43
2:B:88:PHE:CE2	2:B:412:LEU:HD11	2.53	0.43
2:B:761:THR:H	2:B:764:MET:HE3	1.84	0.43
19:U:358:MET:HG3	19:U:365:TYR:HB2	2.00	0.43
19:U:360:LEU:HD22	20:V:90:VAL:HG11	2.01	0.43
21:a:228:LYS:HA	21:a:231:LYS:HG2	2.01	0.43
22:b:334:CYS:HB3	22:b:340:TYR:HE1	1.83	0.43
9:I:106:ASP:N	9:I:106:ASP:OD1	2.52	0.43
13:M:263:GLN:HA	13:M:268:LYS:HG3	2.01	0.43
19:U:373:ASP:OD1	19:U:374:ALA:N	2.52	0.43
23:c:111:ASN:O	23:c:115:GLN:HG2	2.18	0.43
1:A:325:LEU:O	1:A:327:ARG:NH2	2.51	0.43
1:A:595:ILE:HD11	1:A:675:VAL:HG11	1.99	0.43
22:b:263:ARG:HB2	22:b:294:GLU:OE2	2.18	0.43
22:b:277:TRP:CE2	22:b:283:ARG:HD3	2.54	0.43
19:U:338:GLN:CG	19:U:355:ASP:OD1	2.64	0.42
23:c:228:ARG:HG2	23:c:232:GLU:OE2	2.18	0.42
1:A:863:ARG:NH2	1:A:1415:THR:HG23	2.34	0.42
1:A:1366:PHE:HB2	1:A:1374:VAL:HG21	2.01	0.42
3:C:154:ARG:HB2	10:J:60:LEU:HD22	2.01	0.42
15:O:231:ARG:HH12	15:O:235:ARG:HH21	1.67	0.42
21:a:173:THR:OG1	21:a:174:SER:N	2.50	0.42
1:A:628:VAL:HA	1:A:638:GLY:HA3	2.02	0.42
8:H:71:ASP:O	8:H:72:ASP:CG	2.62	0.42
15:O:165:LEU:HD12	15:O:318:ARG:HH11	1.84	0.42
19:U:357:ILE:HD11	20:V:48:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:392:GLU:N	22:b:392:GLU:OE2	2.52	0.42
24:d:9:ARG:HD2	24:d:9:ARG:C	2.44	0.42
1:A:404:GLU:OE1	1:A:407:ARG:NE	2.49	0.42
2:B:51:ILE:HD11	2:B:152:ILE:HG21	2.02	0.42
2:B:967:ILE:HG21	2:B:1048:TYR:OH	2.20	0.42
2:B:971:ALA:O	2:B:975:ARG:HD3	2.20	0.42
3:C:149:LEU:CD2	10:J:2:ILE:HD11	2.50	0.42
14:N:-19:DT:H2"	14:N:-18:DG:C8	2.54	0.42
1:A:225:PHE:HA	1:A:228:ILE:HD12	2.02	0.42
1:A:502:ASN:HB3	2:B:1084:LEU:HD13	2.01	0.42
5:E:3:ASP:OD1	5:E:49:SER:OG	2.34	0.42
6:F:69:ARG:NE	6:F:96:GLU:OE1	2.40	0.42
10:J:6:ARG:CD	10:J:13:ILE:HD13	2.49	0.42
20:V:80:GLU:O	20:V:80:GLU:HG3	2.18	0.42
2:B:710:ILE:HA	2:B:764:MET:HE2	2.02	0.42
7:G:34:VAL:HG23	7:G:35:GLU:N	2.34	0.42
16:Q:50:ASP:HA	16:Q:99:LEU:HD12	2.01	0.42
21:a:108:LEU:HD23	21:a:108:LEU:HA	1.86	0.42
21:a:168:VAL:HA	21:a:171:LEU:HD12	2.02	0.42
21:a:191:LYS:HE2	21:a:205:LEU:HG	2.02	0.42
22:b:99:GLU:O	22:b:103:VAL:HG12	2.20	0.42
2:B:635:LEU:HD21	2:B:640:ILE:HD11	2.01	0.42
4:D:87:LEU:HB3	4:D:97:LEU:HD22	2.01	0.42
13:M:143:LYS:O	13:M:147:GLU:HG2	2.20	0.42
22:b:409:THR:HG21	23:c:377:TYR:HD2	1.85	0.42
1:A:141:LEU:HD12	1:A:236:LEU:O	2.20	0.42
2:B:908:MET:HE1	2:B:910:THR:HG21	2.01	0.42
21:a:221:LEU:HA	21:a:224:GLN:HG2	2.02	0.42
1:A:140:ARG:NH1	1:A:234:PHE:O	2.44	0.42
1:A:1261:ILE:HG22	1:A:1262:MET:N	2.35	0.42
18:T:19:DA:N7	23:c:385:MET:HE1	2.35	0.42
19:U:10:VAL:HB	19:U:11:PRO:HD3	2.01	0.42
21:a:125:ILE:HD13	21:a:125:ILE:HA	1.80	0.42
23:c:187:TRP:HE3	23:c:191:LEU:HD13	1.85	0.42
2:B:773:PRO:HG3	10:J:53:VAL:HG21	2.01	0.42
13:M:31:ASP:HB3	13:M:43:ASP:O	2.19	0.42
13:M:186:ILE:HD11	13:M:191:ILE:HG12	2.02	0.42
17:R:25:LYS:O	17:R:29:GLN:N	2.44	0.42
17:R:152:ASN:O	17:R:153:TYR:C	2.63	0.42
24:d:4:ARG:HE	24:d:8:LEU:HG	1.85	0.42
8:H:87:GLN:O	8:H:146:LYS:NZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:199:ALA:HB2	15:O:214:PHE:CE2	2.55	0.41
19:U:358:MET:HE1	20:V:56:VAL:HG11	2.02	0.41
21:a:120:PHE:HB3	22:b:100:LEU:HD11	2.01	0.41
2:B:65:ILE:HD13	2:B:415:VAL:HG23	2.03	0.41
2:B:136:GLY:O	2:B:137:GLU:HG3	2.20	0.41
11:K:57:LEU:N	11:K:76:GLN:O	2.52	0.41
21:a:23:SER:O	21:a:73:GLN:NE2	2.45	0.41
23:c:101:LEU:HD21	24:d:22:LEU:HB3	2.02	0.41
1:A:823:VAL:CG1	1:A:831:LEU:HD22	2.49	0.41
1:A:1200:PRO:HG2	1:A:1204:VAL:HG22	2.03	0.41
15:O:202:MET:HE3	15:O:202:MET:HB2	1.78	0.41
15:O:272:GLY:O	15:O:276:THR:HG23	2.20	0.41
15:O:295:MET:HE2	15:O:295:MET:HB2	1.91	0.41
16:Q:120:GLU:OE1	16:Q:120:GLU:N	2.44	0.41
21:a:129:LEU:HD23	21:a:129:LEU:HA	1.79	0.41
22:b:373:PRO:HD3	23:c:331:PHE:CG	2.55	0.41
1:A:72:GLN:OE1	1:A:72:GLN:N	2.53	0.41
1:A:1341:VAL:HG23	1:A:1341:VAL:O	2.21	0.41
7:G:52:ASP:N	7:G:71:LYS:O	2.53	0.41
7:G:92:VAL:HG23	7:G:139:GLN:HG2	2.03	0.41
13:M:232:ALA:HA	13:M:235:ILE:HD12	2.03	0.41
13:M:311:ASP:O	24:d:3:SER:N	2.54	0.41
1:A:883:ILE:O	1:A:883:ILE:HG22	2.20	0.41
3:C:68:LEU:HA	3:C:71:ILE:HD12	2.01	0.41
9:I:69:ILE:O	9:I:72:VAL:HG22	2.21	0.41
20:V:31:GLN:O	20:V:34:LEU:HG	2.20	0.41
21:a:205:LEU:HD11	24:d:32:GLU:HB3	2.02	0.41
1:A:495:ASP:OD1	1:A:495:ASP:C	2.63	0.41
2:B:598:VAL:HG23	2:B:601:VAL:HG23	2.01	0.41
9:I:39:CYS:SG	9:I:42:CYS:HB3	2.61	0.41
18:T:-27:DA:H2"	18:T:-26:DG:C8	2.55	0.41
23:c:184:TRP:CE3	23:c:192:LEU:HD11	2.29	0.41
5:E:185:ILE:HD12	5:E:209:VAL:HG21	2.03	0.41
19:U:335:VAL:HG13	19:U:358:MET:HB3	2.03	0.41
1:A:1456:GLU:OE1	1:A:1456:GLU:N	2.43	0.41
1:A:1475:LEU:CD2	7:G:22:LEU:HD11	2.51	0.41
2:B:230:ARG:HG2	2:B:405:ARG:HD2	2.02	0.41
2:B:761:THR:HG22	2:B:763:SER:H	1.86	0.41
4:D:135:GLN:OE1	4:D:138:ARG:NH1	2.54	0.41
13:M:130:LEU:HD13	13:M:134:ILE:HB	2.03	0.41
13:M:309:PRO:HG2	13:M:312:LYS:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:31:TRP:CD1	17:R:62:LEU:HD21	2.56	0.41
22:b:211:LYS:HA	22:b:297:THR:HG22	2.01	0.41
22:b:388:HIS:HB3	22:b:399:PHE:CZ	2.56	0.41
23:c:204:LEU:HD23	23:c:204:LEU:HA	1.83	0.41
1:A:525:ILE:HA	1:A:535:MET:HE3	2.02	0.41
2:B:117:ASN:HA	2:B:189:GLY:HA3	2.03	0.41
2:B:617:ASP:OD1	2:B:617:ASP:N	2.54	0.41
2:B:1109:GLU:OE1	2:B:1150:ARG:NH2	2.54	0.41
3:C:7:PRO:O	11:K:104:ARG:NH1	2.51	0.41
3:C:62:GLU:OE1	3:C:62:GLU:N	2.52	0.41
11:K:63:VAL:O	11:K:63:VAL:CG2	2.69	0.41
15:O:333:LYS:HD2	15:O:333:LYS:HA	1.95	0.41
19:U:333:ASN:HB3	19:U:360:LEU:HD23	2.02	0.41
20:V:82:ARG:HA	20:V:82:ARG:HD2	1.90	0.41
21:a:32:LEU:HD23	21:a:32:LEU:HA	1.88	0.41
21:a:205:LEU:HD12	21:a:205:LEU:HA	1.94	0.41
22:b:205:LEU:HG	22:b:344:ILE:CG1	2.50	0.41
23:c:391:TRP:HA	23:c:395:LEU:HB2	2.01	0.41
1:A:367:ILE:HA	1:A:482:PHE:O	2.21	0.41
1:A:904:GLN:N	1:A:977:VAL:O	2.41	0.41
2:B:88:PHE:CE1	2:B:128:ILE:HG23	2.55	0.41
2:B:101:ARG:NH2	13:M:171:GLU:HB3	2.35	0.41
2:B:736:TYR:CE2	2:B:737:ILE:HG22	2.55	0.41
13:M:244:LEU:HD21	13:M:295:ARG:HB2	2.02	0.41
18:T:-39:DT:H6	18:T:-39:DT:H2'	1.66	0.41
18:T:-32:DA:H2''	18:T:-31:DA:C8	2.56	0.41
19:U:22:ILE:HD13	19:U:22:ILE:HA	1.88	0.41
23:c:185:LYS:HA	23:c:185:LYS:HD3	1.83	0.41
23:c:301:GLU:OE1	23:c:326:THR:HG21	2.20	0.41
1:A:531:ASN:ND2	1:A:531:ASN:O	2.54	0.40
1:A:542:LEU:HD23	1:A:774:ALA:HA	2.02	0.40
1:A:901:VAL:HB	1:A:978:VAL:HG12	2.02	0.40
2:B:438:ARG:NE	13:M:126:ASP:CG	2.63	0.40
8:H:71:ASP:OD1	8:H:72:ASP:N	2.54	0.40
10:J:8:PHE:CE2	10:J:48:MET:HE1	2.57	0.40
1:A:379:GLY:HA2	1:A:475:ARG:O	2.21	0.40
2:B:794:VAL:HG22	2:B:967:ILE:HG22	2.02	0.40
13:M:117:ALA:O	13:M:121:ILE:N	2.42	0.40
13:M:208:LEU:HD12	13:M:209:ILE:H	1.86	0.40
22:b:301:LEU:HG	22:b:303:ILE:HG23	2.03	0.40
23:c:272:GLU:H	23:c:272:GLU:CD	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:d:4:ARG:NH1	24:d:7:GLU:OE2	2.54	0.40
24:d:15:LEU:HD12	24:d:16:LEU:HD22	2.03	0.40
1:A:350:VAL:HA	1:A:354:LEU:HD12	2.03	0.40
1:A:419:ILE:HD12	1:A:429:LEU:HD21	2.03	0.40
1:A:483:ARG:N	1:A:483:ARG:HD2	2.36	0.40
13:M:151:LEU:HB2	13:M:154:ARG:HG2	2.02	0.40
22:b:42:PHE:CE1	22:b:305:LEU:HD13	2.57	0.40
23:c:143:GLY:HA2	23:c:146:MET:HG2	2.02	0.40
23:c:377:TYR:N	23:c:377:TYR:CD1	2.87	0.40
24:d:6:GLN:HA	24:d:9:ARG:CG	2.51	0.40
1:A:1086:MET:SD	1:A:1466:ALA:HB1	2.61	0.40
1:A:1144:LEU:H	1:A:1144:LEU:HD23	1.85	0.40
2:B:718:GLN:HG2	2:B:720:PRO:HD2	2.03	0.40
11:K:42:LEU:HA	11:K:45:ILE:HG22	2.04	0.40
15:O:283:TYR:CZ	15:O:285:PRO:HG3	2.57	0.40
18:T:-3:DC:C5	18:T:-2:DT:H73	2.57	0.40
22:b:181:ILE:HG22	22:b:207:LEU:HD12	2.03	0.40
23:c:108:LEU:HB2	24:d:19:LYS:CE	2.51	0.40
7:G:120:ASP:OD1	7:G:122:ASN:ND2	2.55	0.40
21:a:172:ILE:HD12	21:a:176:VAL:HB	2.02	0.40
21:a:180:MET:HE3	21:a:180:MET:HB3	1.99	0.40
21:a:226:TRP:HA	21:a:229:ASP:OD2	2.21	0.40
21:a:226:TRP:CZ3	24:d:10:LYS:HG2	2.56	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	1413/1970 (72%)	1377 (98%)	36 (2%)	0	100	100
2	B	1130/1174 (96%)	1098 (97%)	32 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	253/275 (92%)	247 (98%)	6 (2%)	0	100	100
4	D	126/142 (89%)	124 (98%)	2 (2%)	0	100	100
5	E	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
6	F	77/127 (61%)	75 (97%)	2 (3%)	0	100	100
7	G	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
8	H	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
9	I	112/125 (90%)	106 (95%)	6 (5%)	0	100	100
10	J	62/67 (92%)	62 (100%)	0	0	100	100
11	K	113/117 (97%)	112 (99%)	1 (1%)	0	100	100
12	L	42/58 (72%)	41 (98%)	1 (2%)	0	100	100
13	M	238/316 (75%)	229 (96%)	9 (4%)	0	100	100
15	O	177/339 (52%)	173 (98%)	4 (2%)	0	100	100
16	Q	134/517 (26%)	129 (96%)	5 (4%)	0	100	100
17	R	218/249 (88%)	212 (97%)	6 (3%)	0	100	100
19	U	84/376 (22%)	79 (94%)	5 (6%)	0	100	100
20	V	95/109 (87%)	87 (92%)	8 (8%)	0	100	100
21	a	211/368 (57%)	201 (95%)	10 (5%)	0	100	100
22	b	359/411 (87%)	332 (92%)	27 (8%)	0	100	100
23	c	299/1469 (20%)	280 (94%)	19 (6%)	0	100	100
24	d	50/98 (51%)	50 (100%)	0	0	100	100
All	All	5715/8839 (65%)	5525 (97%)	190 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	1254/1749 (72%)	1254 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	994/1027 (97%)	994 (100%)	0	100	100
3	C	234/252 (93%)	234 (100%)	0	100	100
4	D	118/126 (94%)	118 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	69/111 (62%)	69 (100%)	0	100	100
7	G	152/153 (99%)	152 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	103/112 (92%)	103 (100%)	0	100	100
10	J	53/56 (95%)	53 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	41/55 (74%)	41 (100%)	0	100	100
13	M	206/268 (77%)	205 (100%)	1 (0%)	81	89
15	O	154/293 (53%)	154 (100%)	0	100	100
16	Q	121/448 (27%)	121 (100%)	0	100	100
17	R	196/218 (90%)	196 (100%)	0	100	100
19	U	82/324 (25%)	82 (100%)	0	100	100
20	V	89/98 (91%)	89 (100%)	0	100	100
21	a	198/334 (59%)	198 (100%)	0	100	100
22	b	323/356 (91%)	323 (100%)	0	100	100
23	c	270/1213 (22%)	270 (100%)	0	100	100
24	d	48/93 (52%)	48 (100%)	0	100	100
All	All	5129/7715 (66%)	5128 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	188	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	387	ASN
1	A	459	ASN
1	A	531	ASN

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Mol	Chain	Res	Type
1	A	673	GLN
1	A	765	ASN
1	A	792	ASN
1	A	861	GLN
1	A	905	ASN
1	A	1462	GLN
2	B	117	ASN
2	B	654	GLN
2	B	906	GLN
2	B	1049	GLN
3	C	6	GLN
3	C	66	HIS
5	E	22	HIS
5	E	71	GLN
5	E	189	GLN
8	H	130	ASN
9	I	91	HIS
11	K	40	HIS
11	K	49	GLN
13	M	139	ASN
15	O	189	ASN
16	Q	53	ASN
17	R	64	ASN
17	R	158	ASN
17	R	194	HIS
19	U	338	GLN
19	U	343	HIS
20	V	16	GLN
21	a	112	GLN
22	b	299	ASN
22	b	331	HIS
23	c	114	GLN
23	c	286	ASN
23	c	340	HIS
24	d	6	GLN
24	d	27	ASN
24	d	37	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

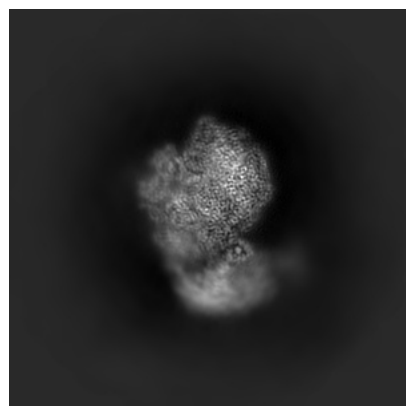
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14997. These allow visual inspection of the internal detail of the map and identification of artifacts.

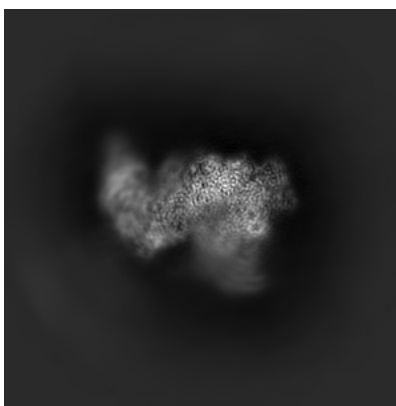
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

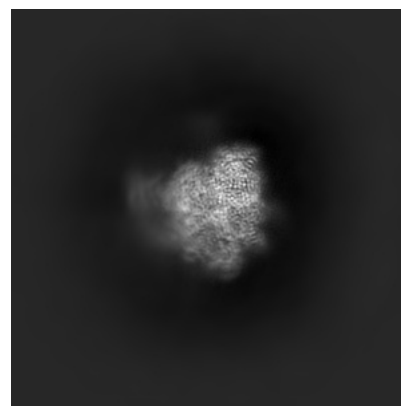
6.1.1 Primary map



X

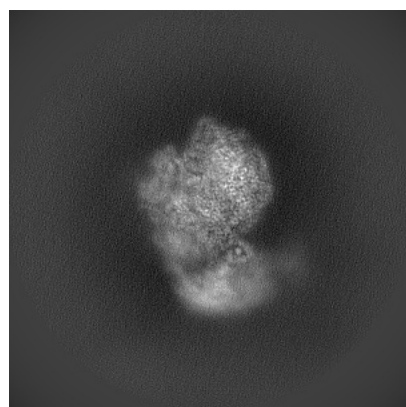


Y

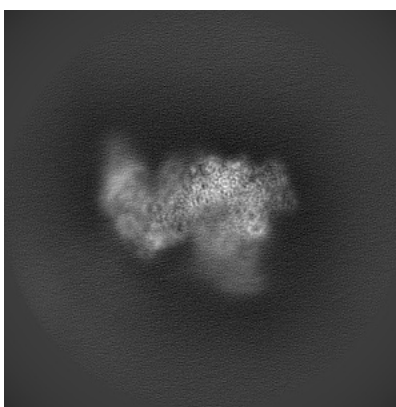


Z

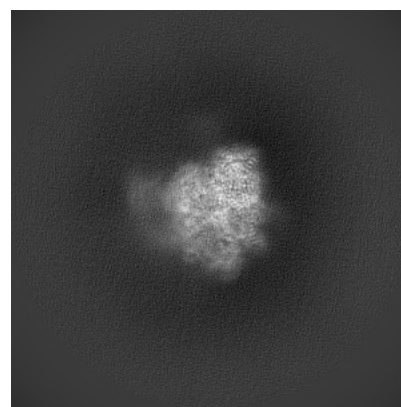
6.1.2 Raw map



X



Y

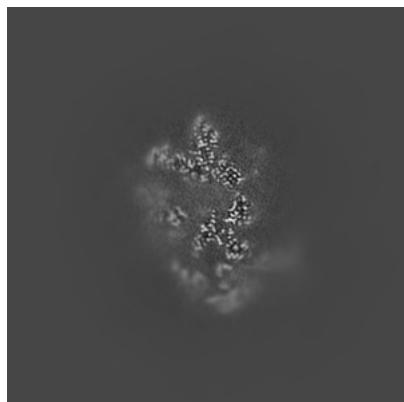


Z

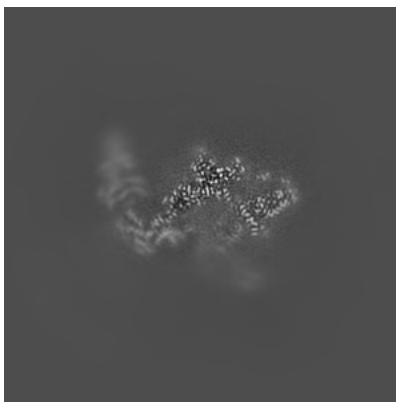
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

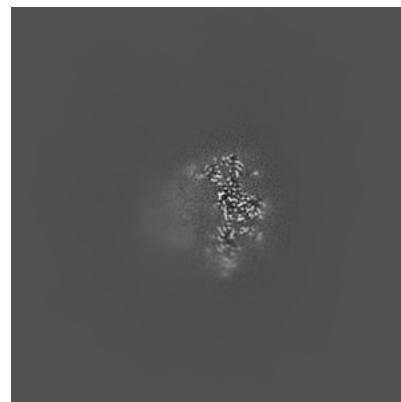
6.2.1 Primary map



X Index: 200

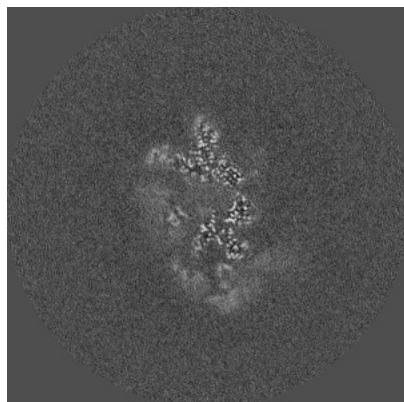


Y Index: 200

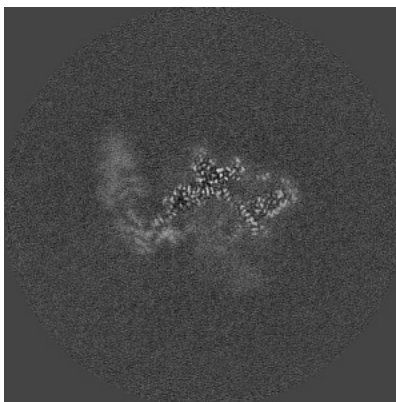


Z Index: 200

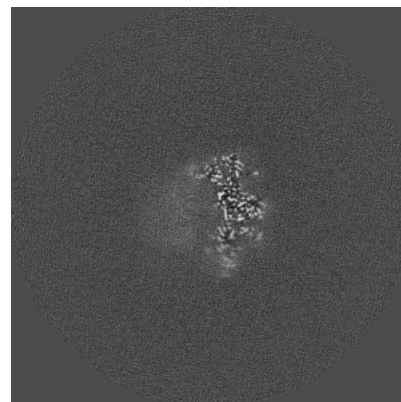
6.2.2 Raw map



X Index: 200



Y Index: 200

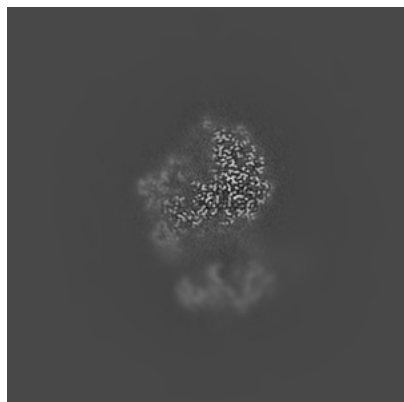


Z Index: 200

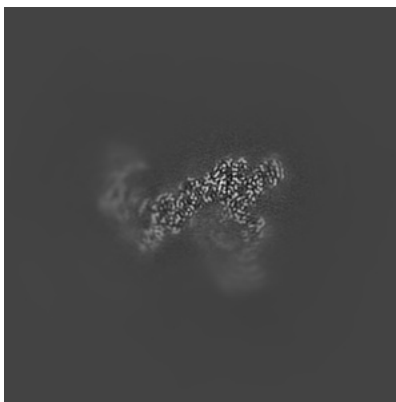
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

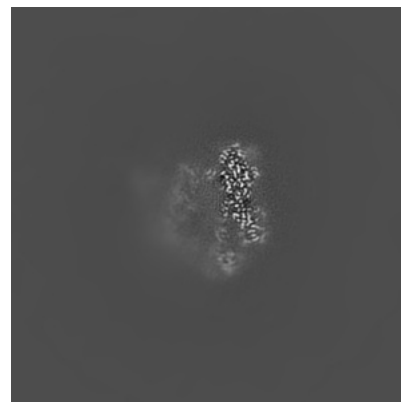
6.3.1 Primary map



X Index: 224

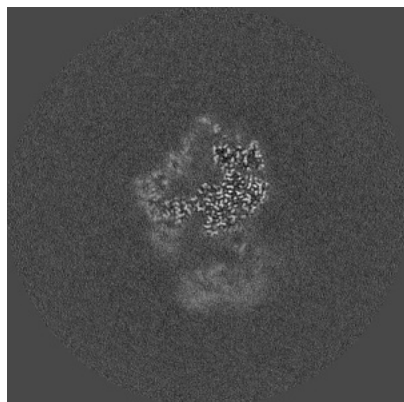


Y Index: 222

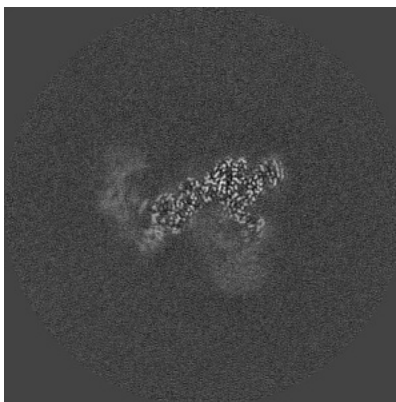


Z Index: 211

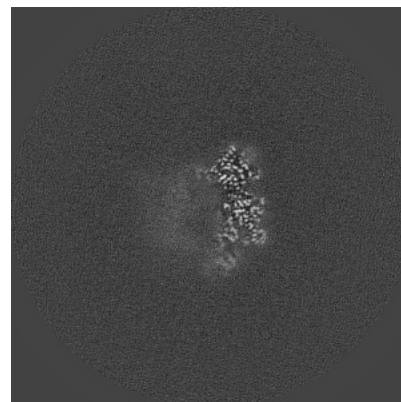
6.3.2 Raw map



X Index: 218



Y Index: 222

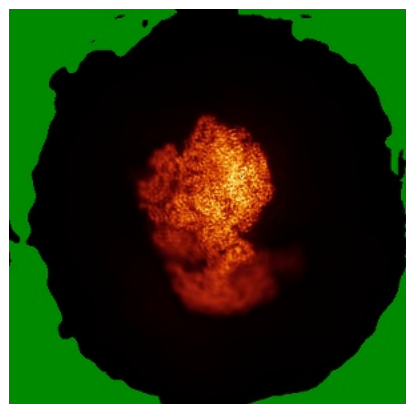


Z Index: 208

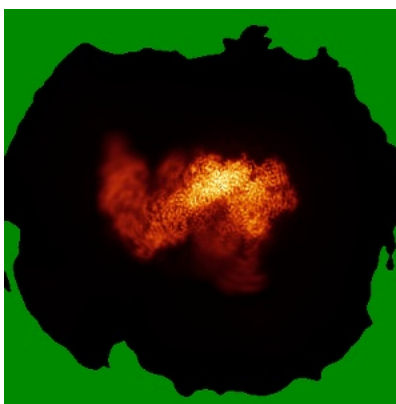
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

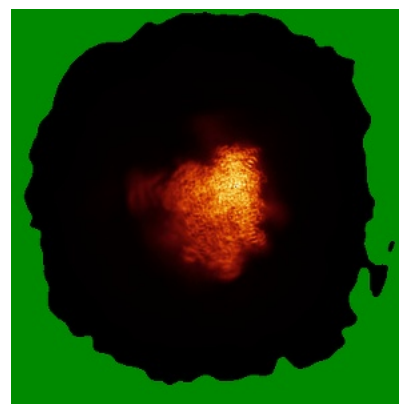
6.4.1 Primary map



X

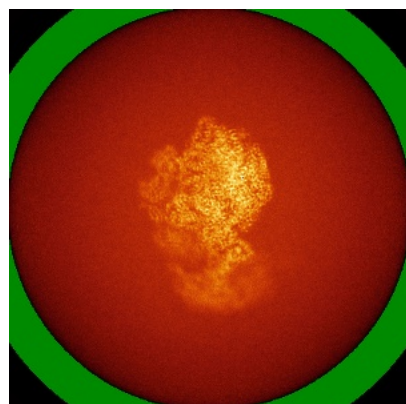


Y

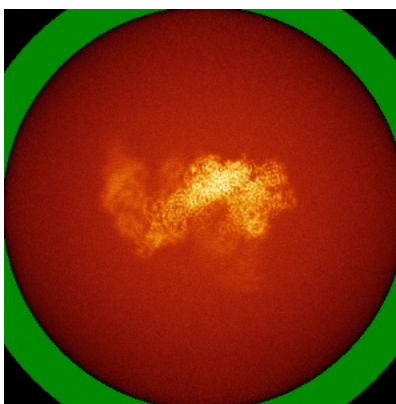


Z

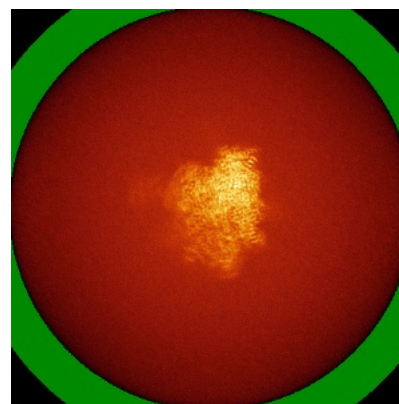
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

This section was not generated.

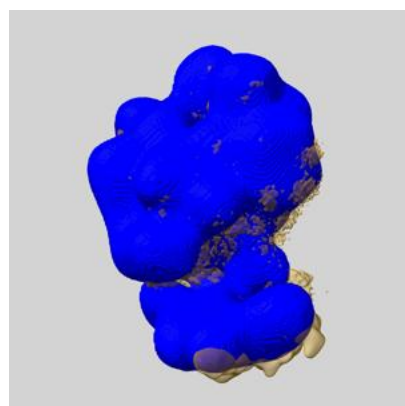
6.6 Mask visualisation [i](#)

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

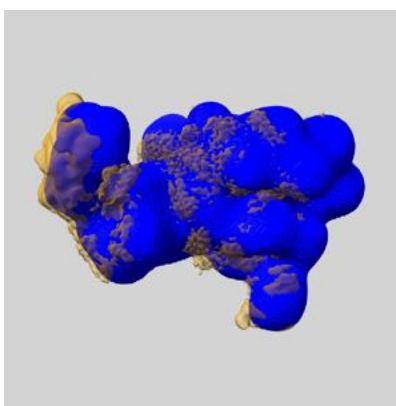
A mask typically either:

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

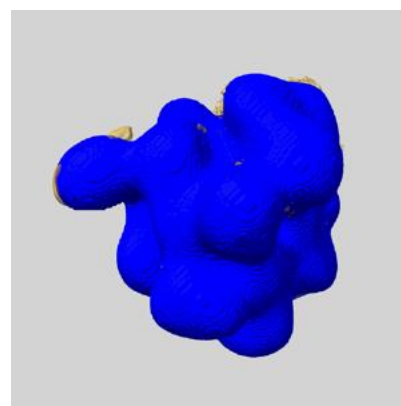
6.6.1 emd_14997_msk_1.map [i](#)



X



Y

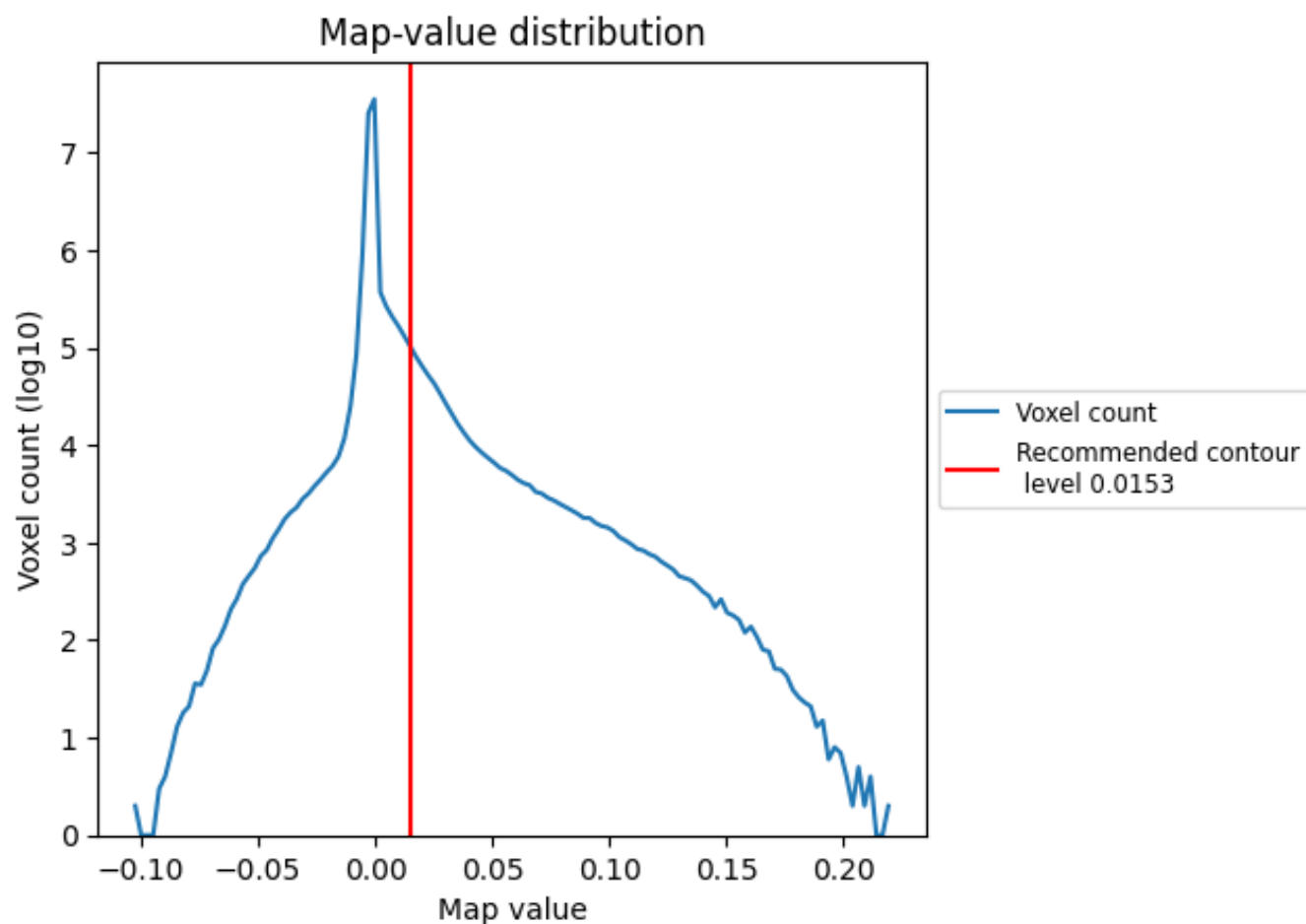


Z

7 Map analysis [i](#)

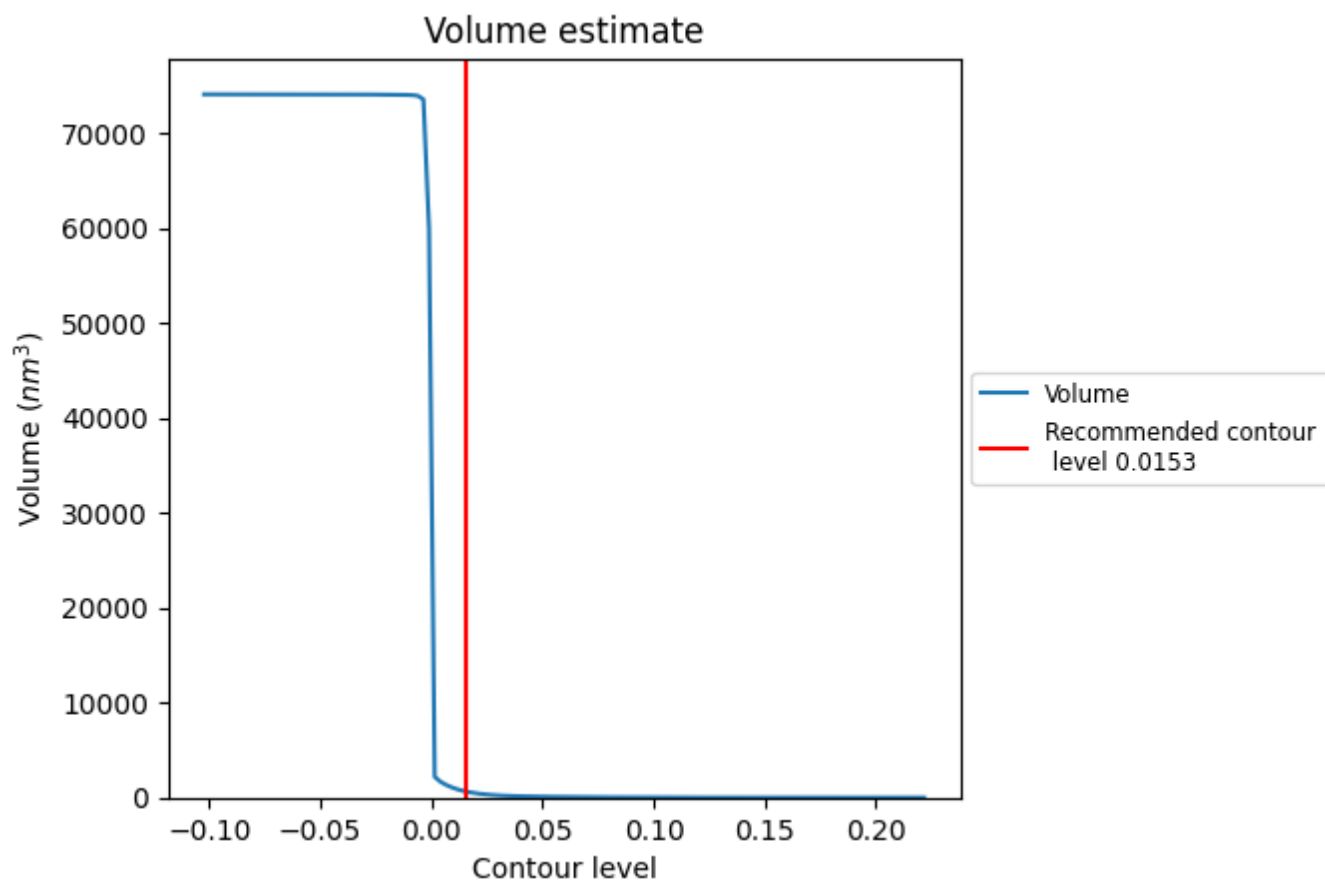
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

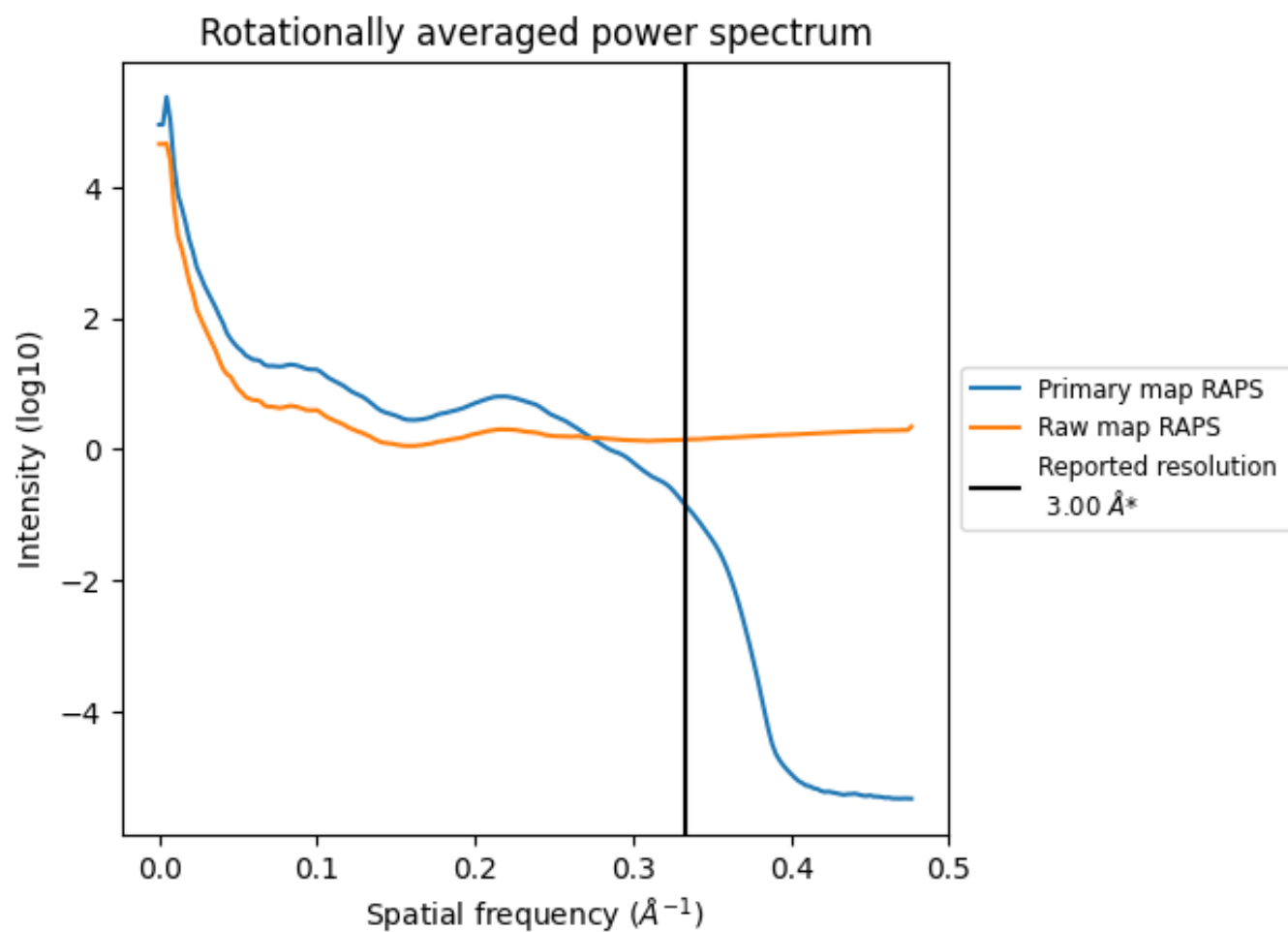
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 651 nm^3 ; this corresponds to an approximate mass of 588 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 ⓘ

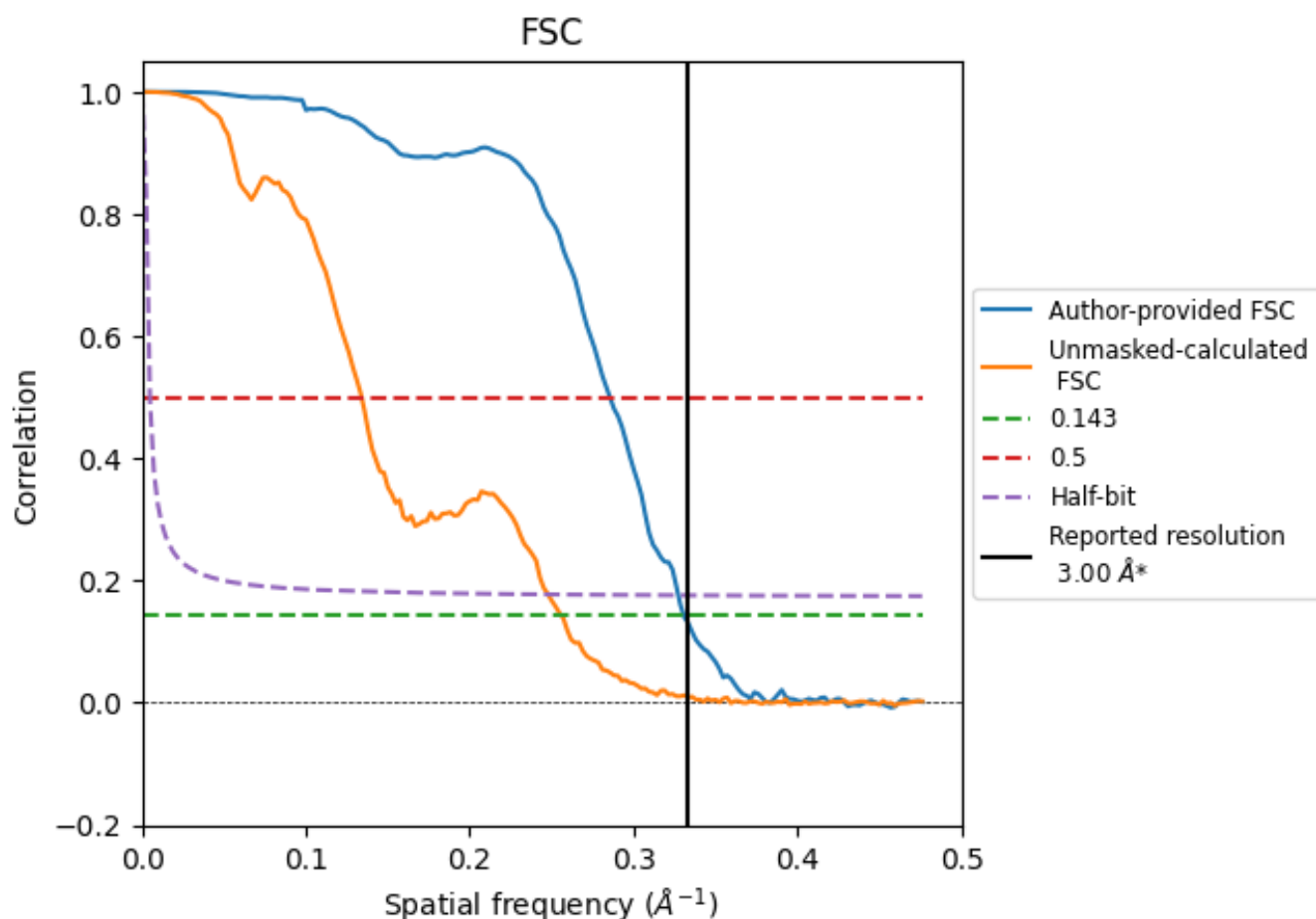


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.02	3.50	3.06
Unmasked-calculated*	3.91	7.47	4.04

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 3.0 by more than 10 %

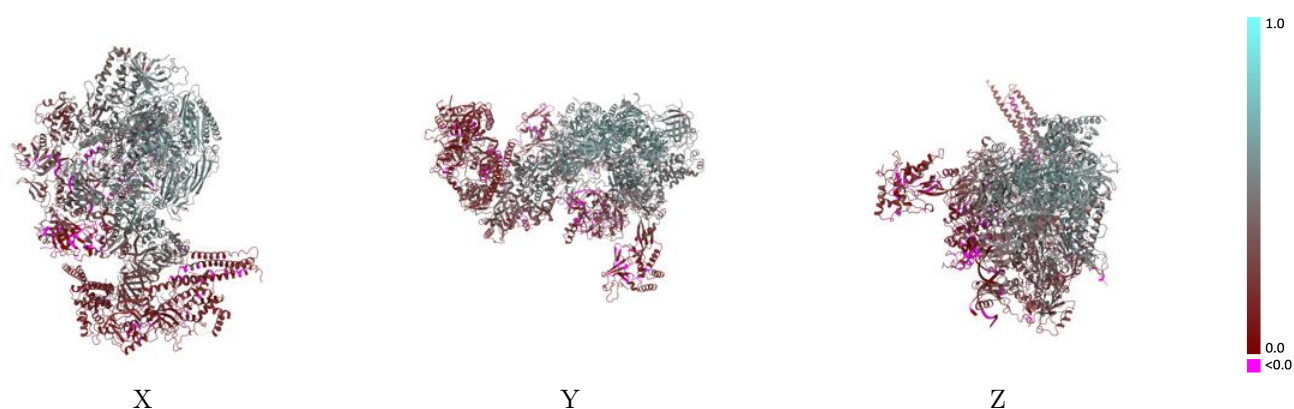
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14997 and PDB model 7ZWD. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)

This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)

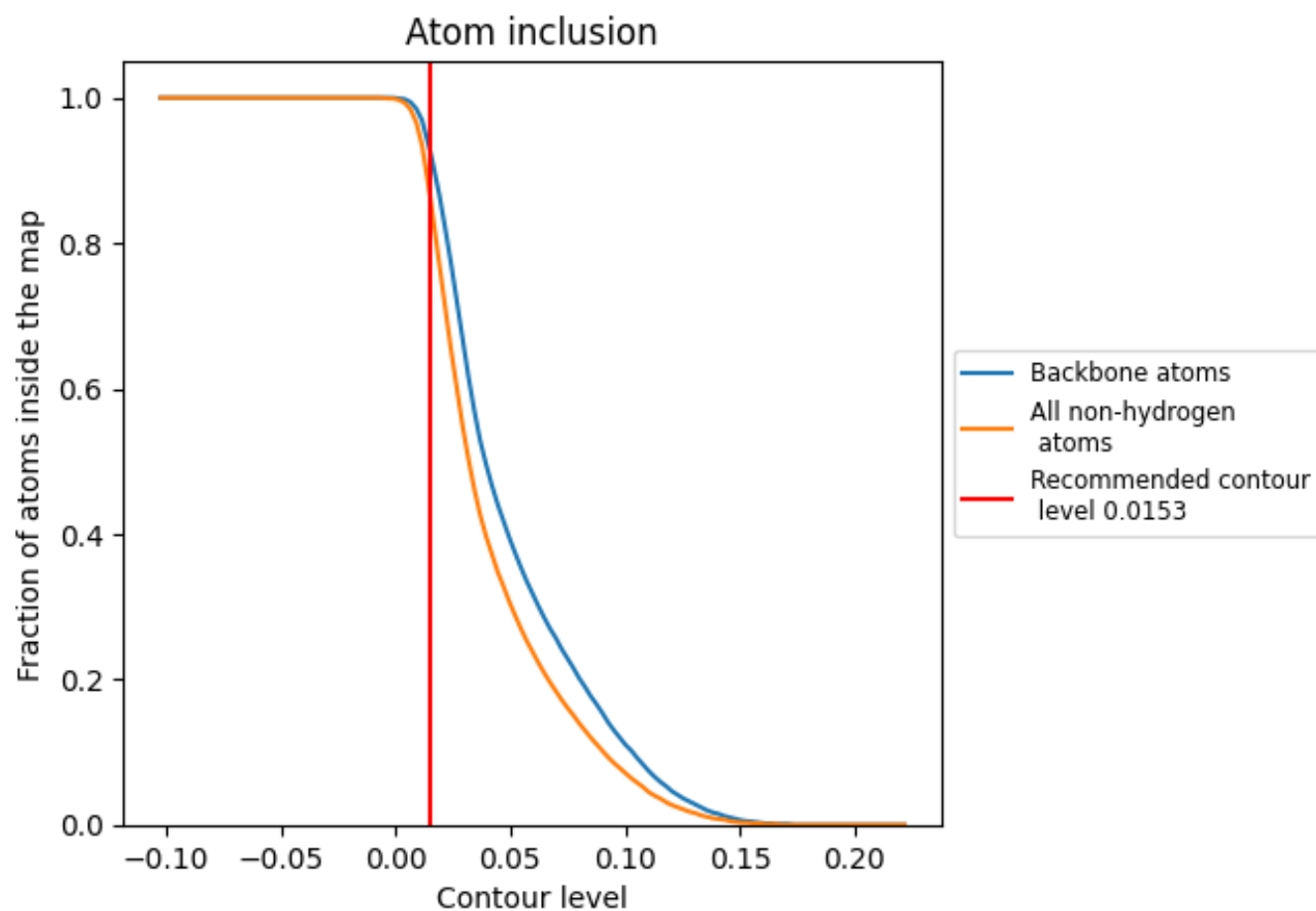


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.0153) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8600	 0.3420
A	 0.8640	 0.3870
B	 0.9230	 0.4770
C	 0.9680	 0.5490
D	 0.5330	 0.1320
E	 0.9180	 0.3300
F	 0.9480	 0.4740
G	 0.5790	 0.1600
H	 0.9620	 0.4950
I	 0.9420	 0.4110
J	 0.9820	 0.5810
K	 0.9700	 0.5490
L	 0.9240	 0.4470
M	 0.9020	 0.4320
N	 0.7800	 0.2180
O	 0.9260	 0.3410
Q	 0.8370	 0.1980
R	 0.7870	 0.1470
T	 0.7730	 0.2070
U	 0.8930	 0.2310
V	 0.9100	 0.2520
a	 0.7060	 0.1490
b	 0.9110	 0.1530
c	 0.8150	 0.1530
d	 0.2820	 0.1210

