Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 09:22 pm GMT

PDB ID	:	6EU0
EMDB ID	:	EMD-3955
Title	:	RNA Polymerase III open pre-initiation complex (OC-PIC)
Authors	:	Abascal-Palacios, G.; Ramsay, E.P.; Beuron, F.; Morris, E.; Vannini, A.
Deposited on	:	2017-10-27
Resolution	:	4.00 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:

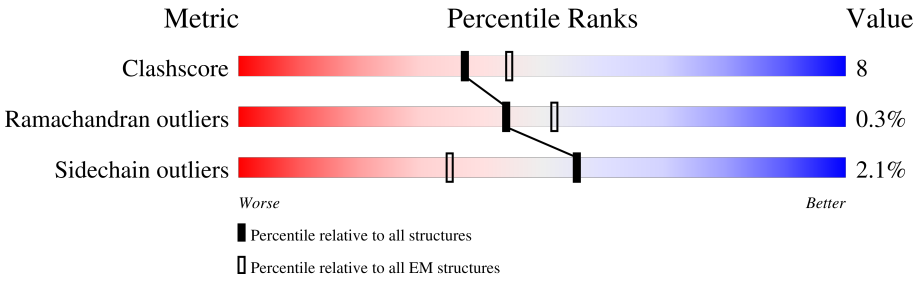
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 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)
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	1460	7% 76% 20%
2	B	1149	7% 70% 26%
3	C	335	82% 18%
4	D	161	20% 63% 21% 13%
5	E	215	9% 77% 23%
6	F	155	46% 7% 46%
7	G	212	25% 83% 17%
8	H	146	13% 81% 18%

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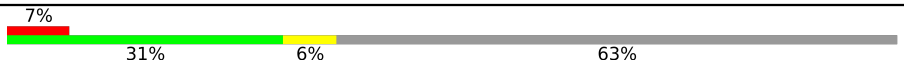
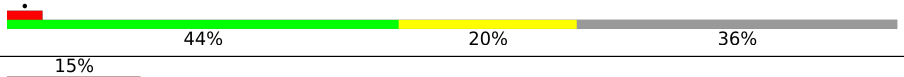
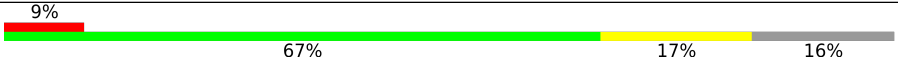
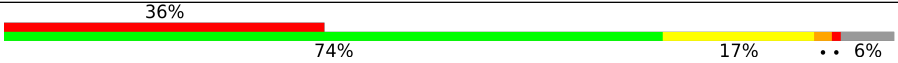
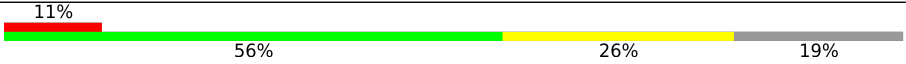
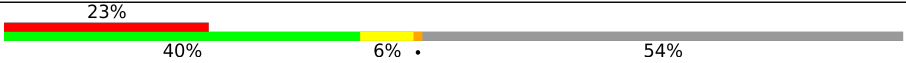
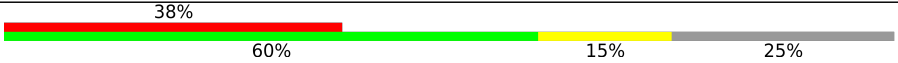
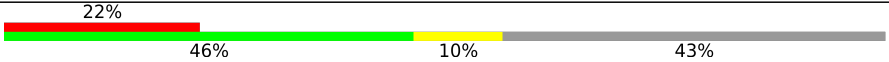
Mol	Chain	Length	Quality of chain
9	I	110	
10	J	70	
11	K	142	
12	L	70	
13	M	282	
14	N	422	
15	O	654	
16	P	317	
17	Q	251	
18	R	70	
19	S	70	
20	V	594	
21	Y	240	
22	Z	596	

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 48918 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 III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1421	11119	7007	1964	2088	60	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1112	8771	5549	1514	1648	60	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	335	2655	1681	454	511	9	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	140	1137	723	193	215	6	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	215	1759	1116	310	321	12	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	83	671	429	114	125	3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	212	Total	C	N	O	S	0	0
			1698	1098	276	317	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	146	Total	C	N	O	S	0	0
			1161	726	195	235	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	41	Total	C	N	O	S	0	0
			313	200	46	61	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			549	350	95	98	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	102	Total	C	N	O	S	0	0
			801	501	131	164	5		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	197	Total	C	N	O	S	0	0
			1589	1003	277	307	2		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	105	Total	C	N	O	S	0	0
			802	508	144	147	3		

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	550	Total	C	N	O	S	0	0
			4421	2812	759	831	19		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	298	Total	C	N	O	S	0	0
			2355	1506	388	450	11		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	88	Total	C	N	O	S	0	0
			589	364	108	116	1		

- Molecule 18 is a DNA chain called Non-Template.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	51	Total	C	N	O	P	0	0
			1038	500	175	312	51		

- Molecule 19 is a DNA chain called Template.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	57	Total	C	N	O	P	0	0
			1174	560	223	334	57		

- Molecule 20 is a protein called Transcription factor TFIIIB component B".

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	273	Total	C	N	O	S	0	0
			1829	1101	354	368	6		

- Molecule 21 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

- Molecule 22 is a protein called Transcription factor IIIB 70 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	339	Total	C	N	O	S	0	0
			2705	1694	492	505	14		

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
23	A	2	Total	Zn	0
			2	2	
23	B	1	Total	Zn	0
			1	1	
23	I	1	Total	Zn	0
			1	1	
23	J	1	Total	Zn	0
			1	1	
23	L	1	Total	Zn	0
			1	1	
23	Z	1	Total	Zn	0
			1	1	

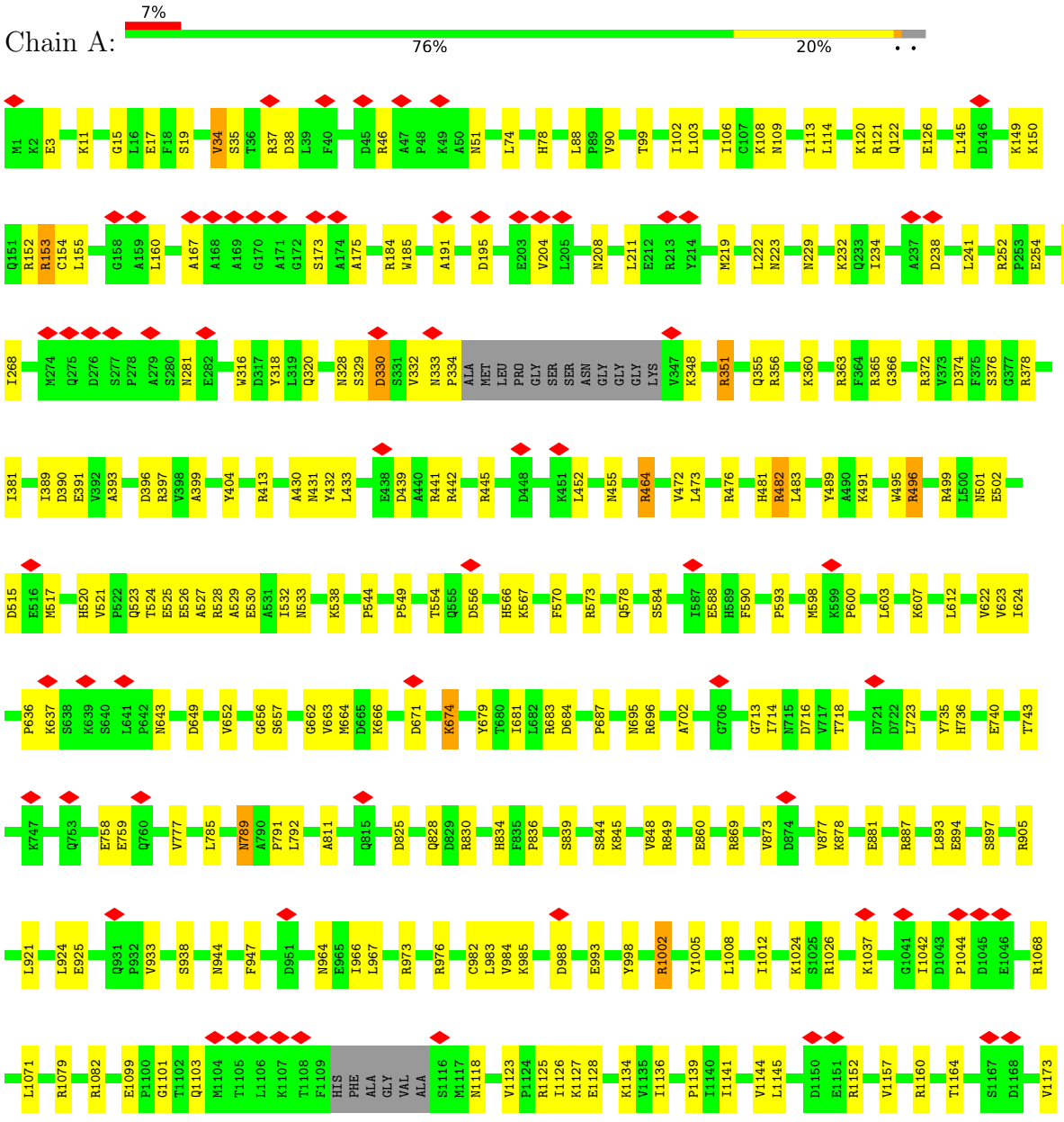
- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

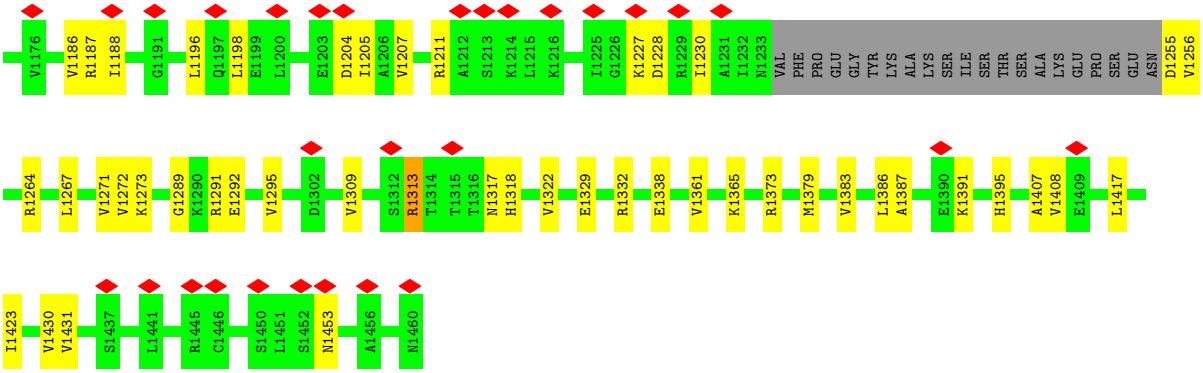
Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

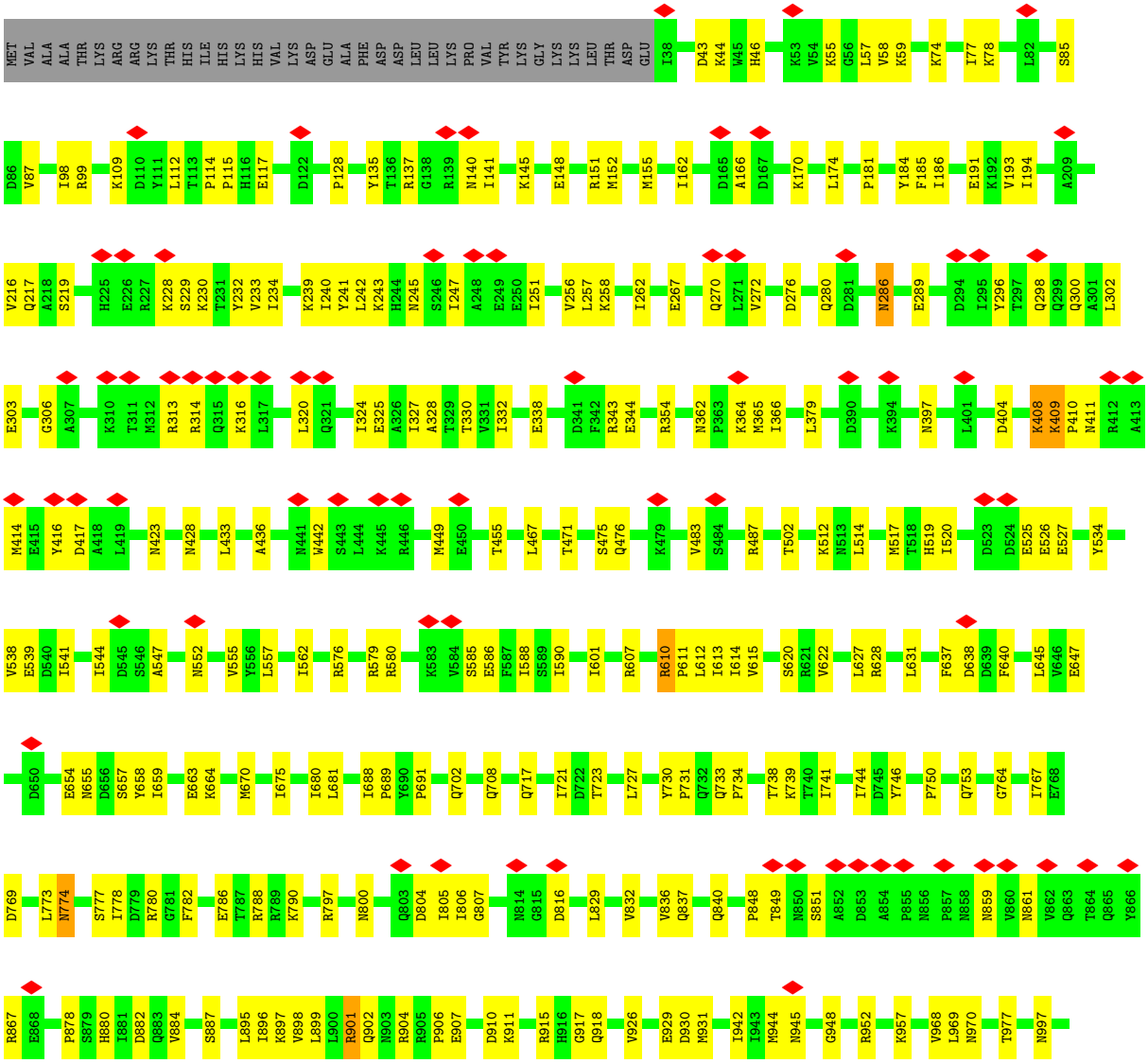
• Molecule 1: DNA-directed RNA polymerase III subunit RPC1

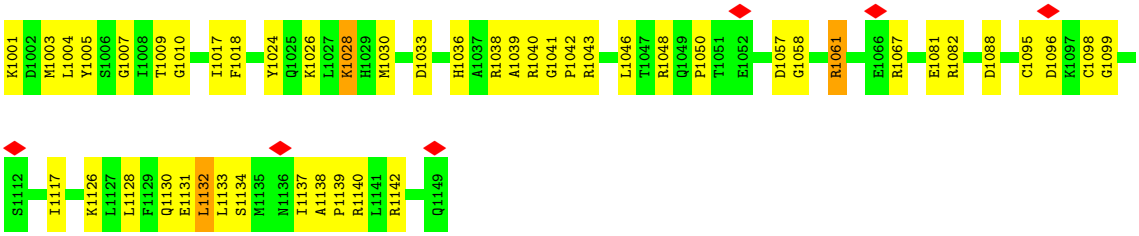




• Molecule 2: DNA-directed RNA polymerase III subunit RPC2

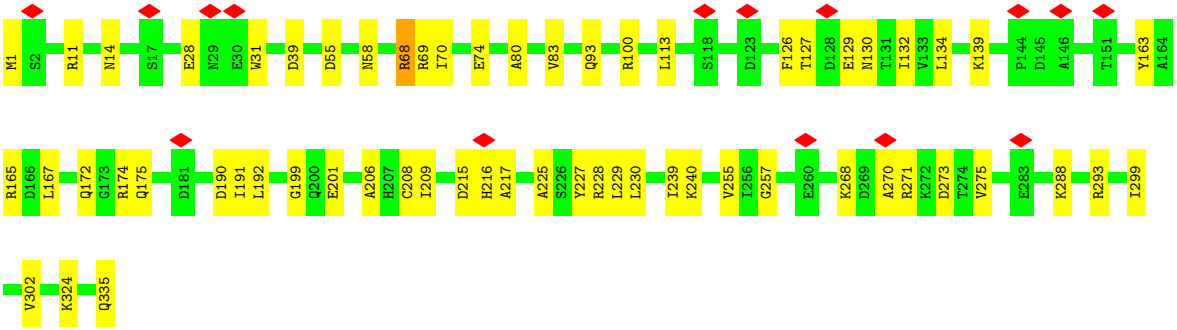
Chain B:





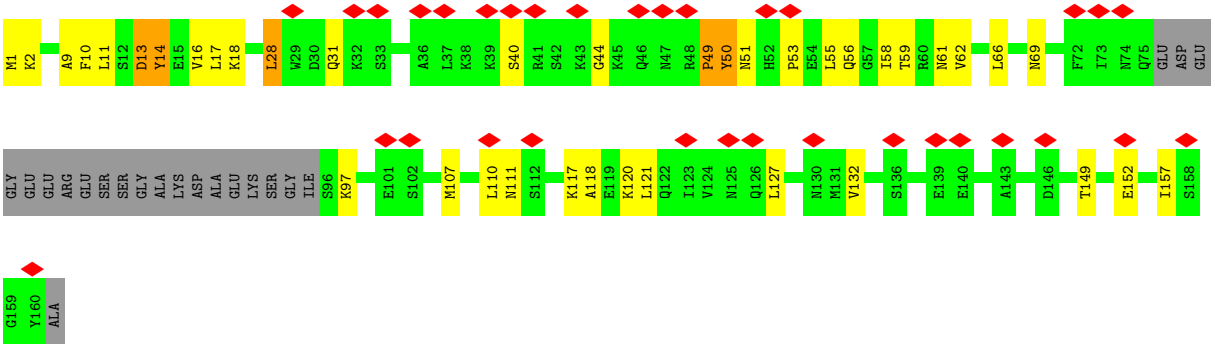
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C:



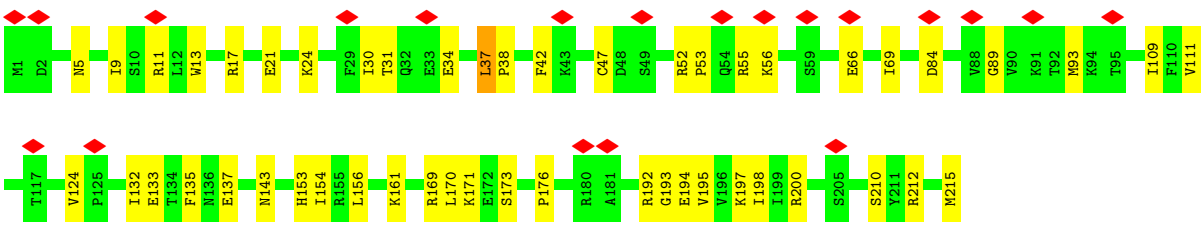
• Molecule 4: DNA-directed RNA polymerase III subunit RPC9

Chain D:



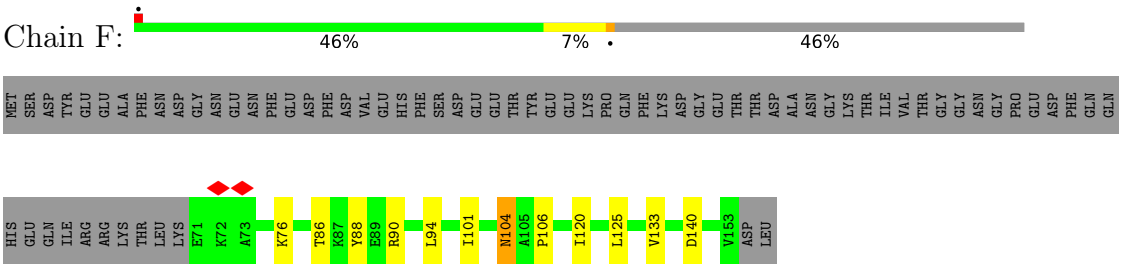
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



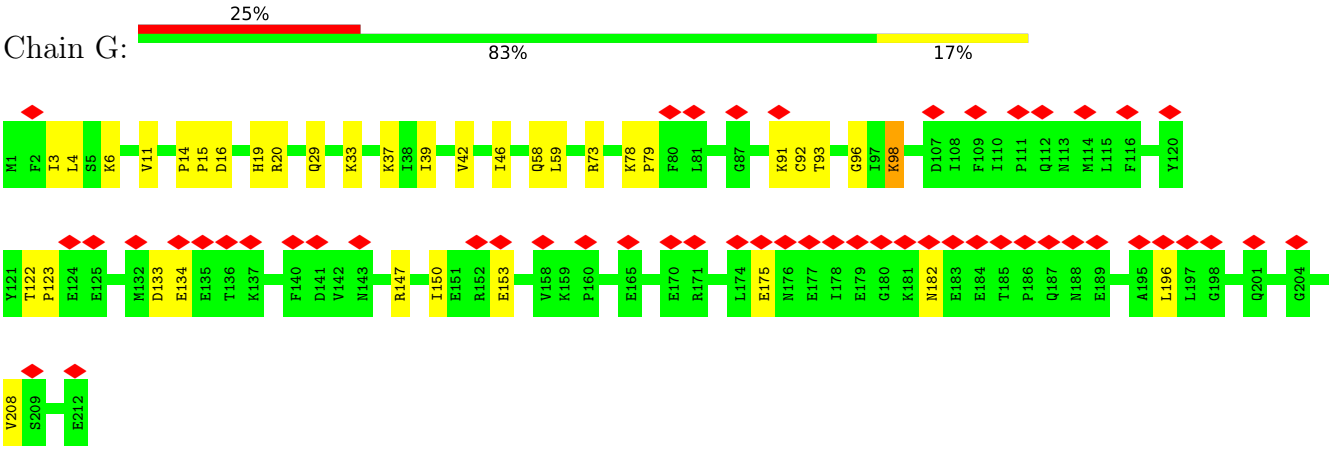
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



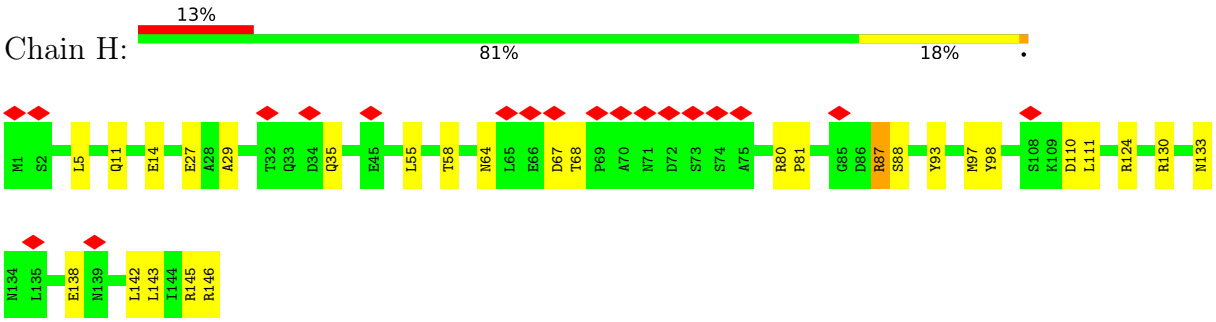
• Molecule 7: DNA-directed RNA polymerase III subunit RPC8

Chain G:



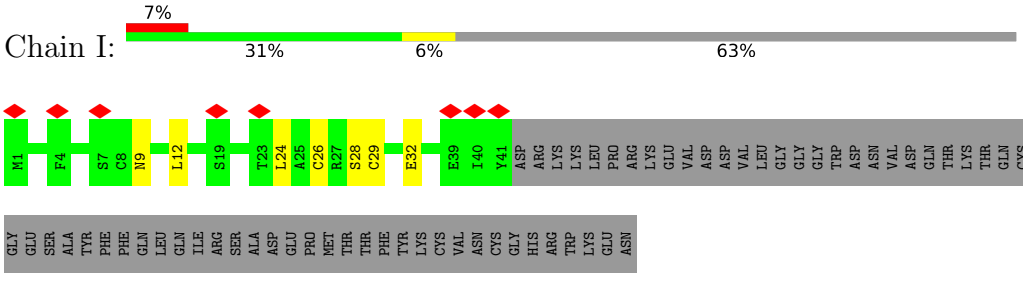
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



• Molecule 9: DNA-directed RNA polymerase III subunit RPC10

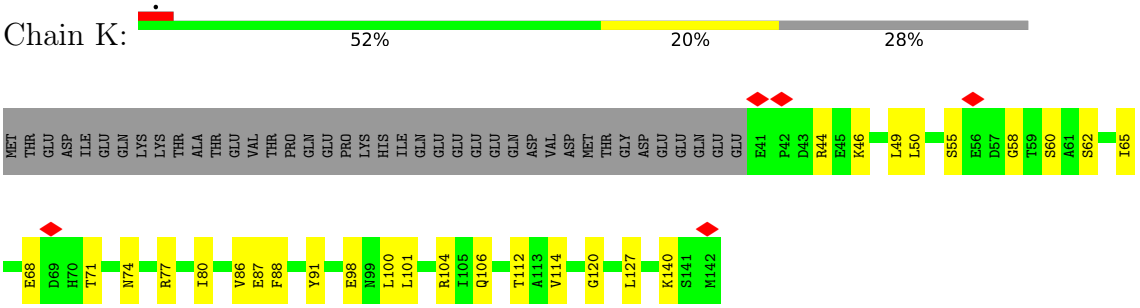
Chain I:



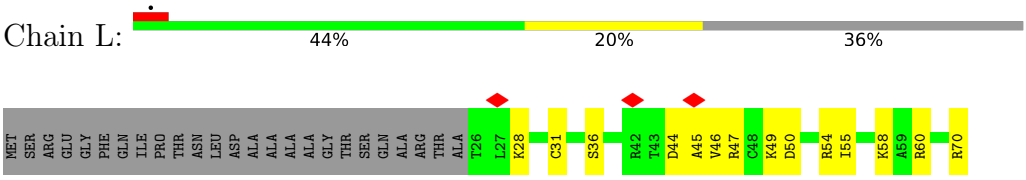
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:

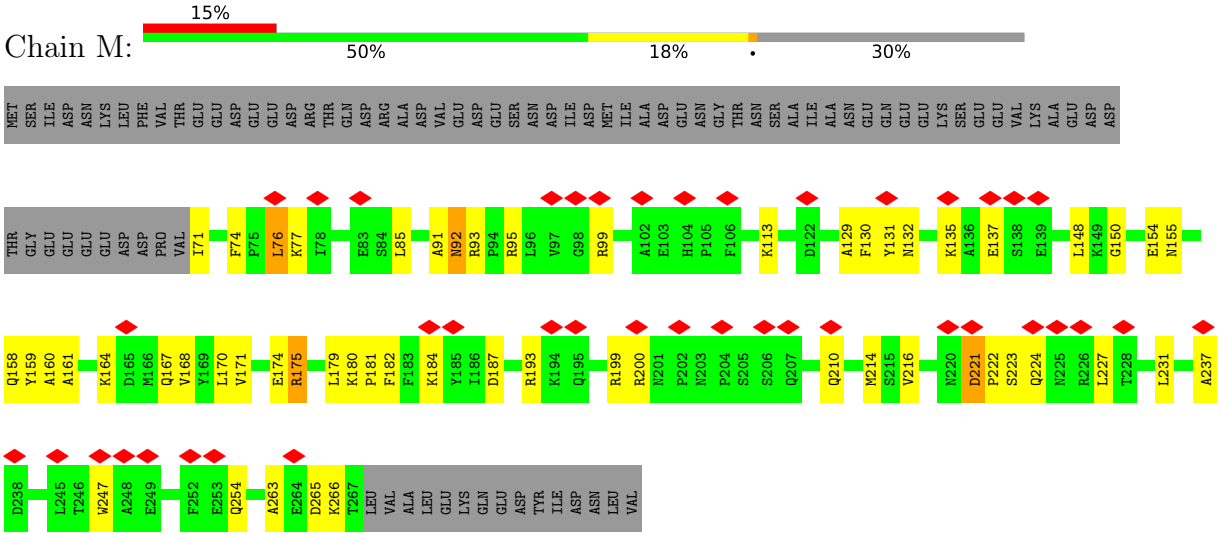
• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2



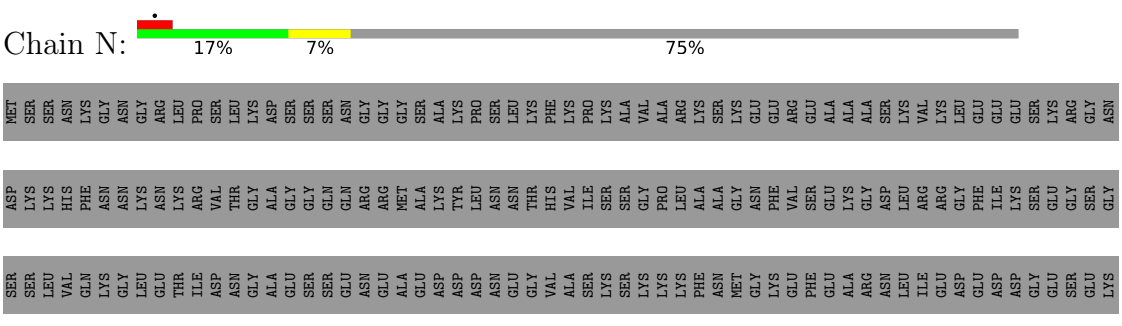
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

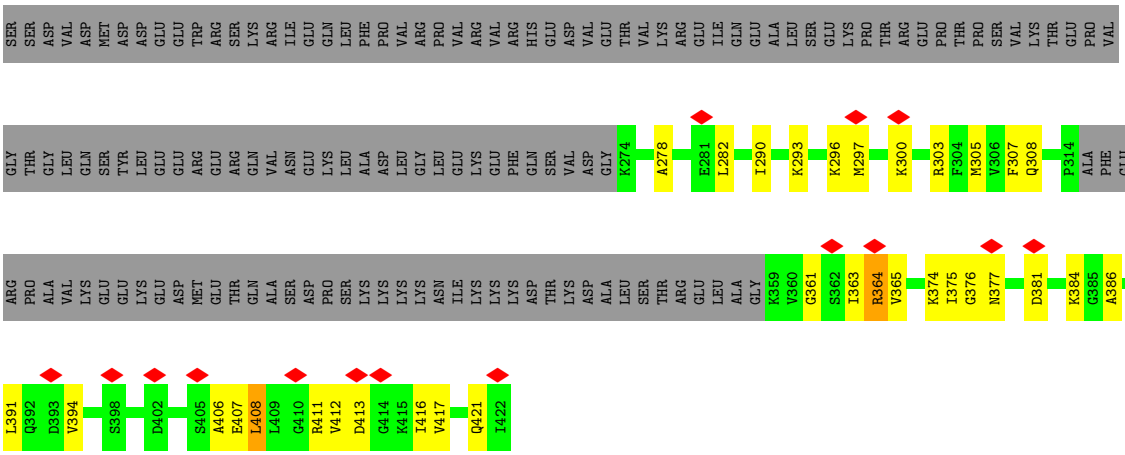


• Molecule 13: DNA-directed RNA polymerase III subunit RPC5



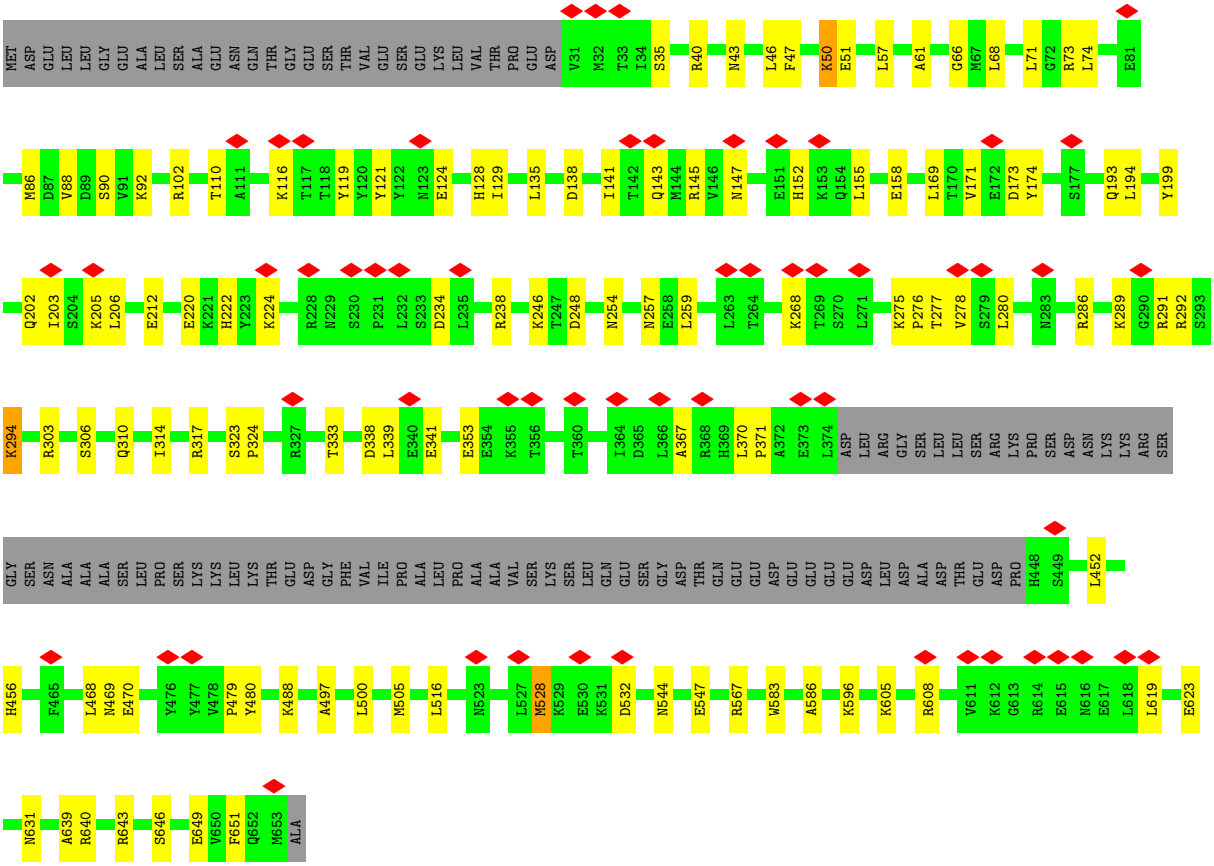
• Molecule 14: DNA-directed RNA polymerase III subunit RPC4





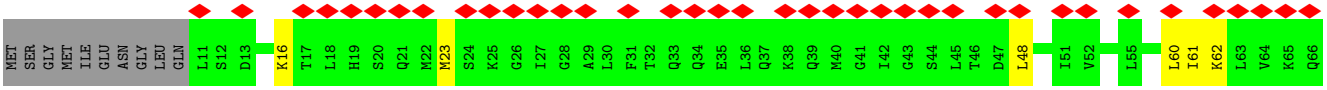
• Molecule 15: DNA-directed RNA polymerase III subunit RPC3

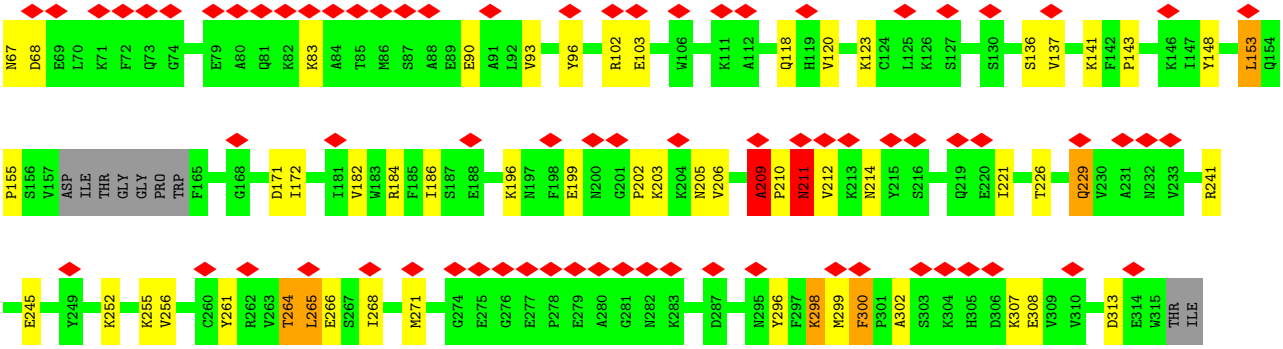
Chain O:



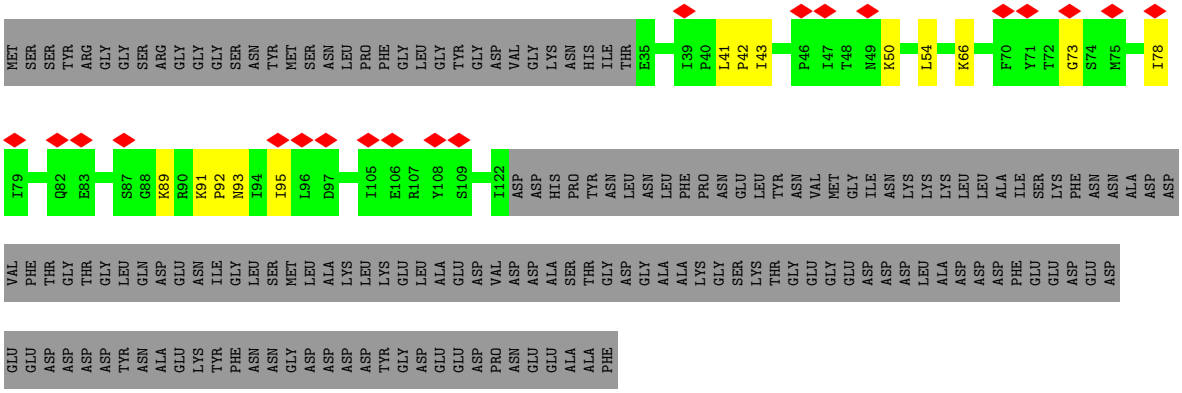
• Molecule 16: DNA-directed RNA polymerase III subunit RPC6

Chain P:

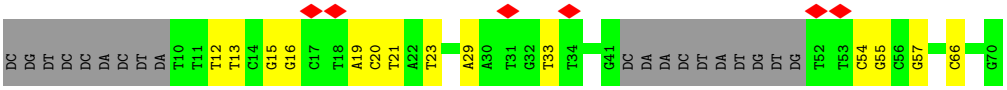




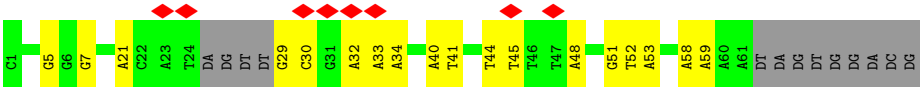
• Molecule 17: DNA-directed RNA polymerase III subunit RPC7



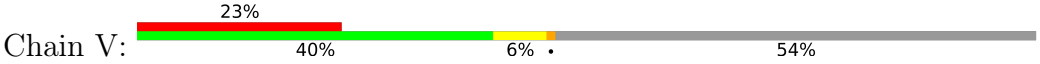
• Molecule 18: Non-Template

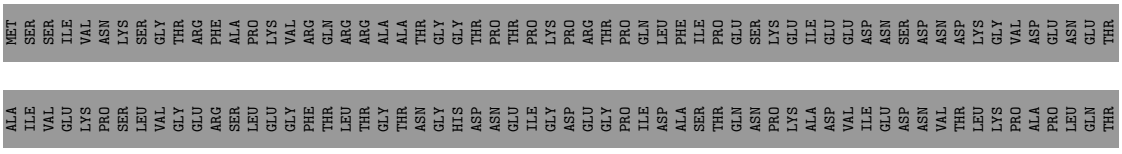


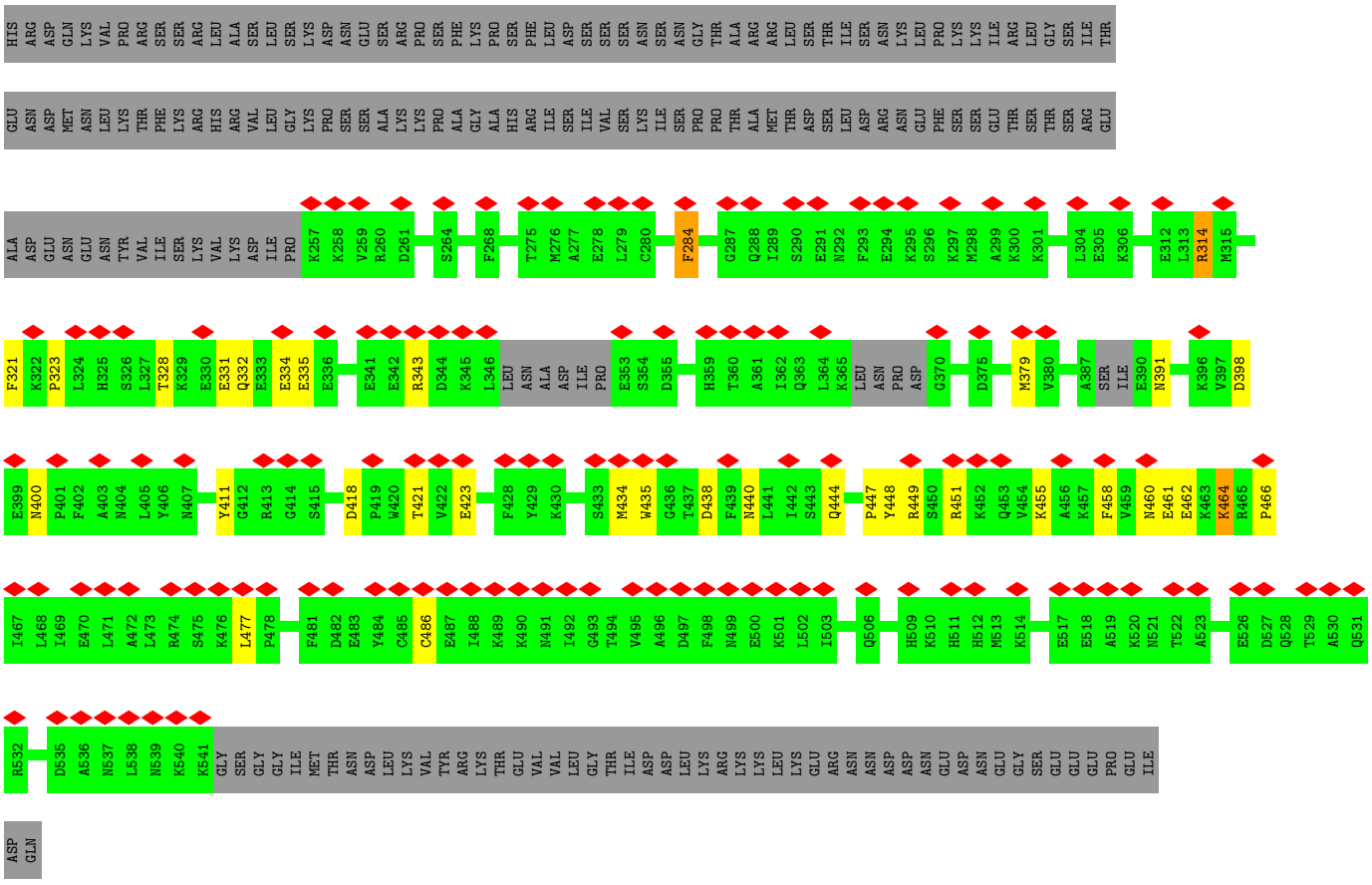
• Molecule 19: Template



• Molecule 20: Transcription factor TFIIIB component B"

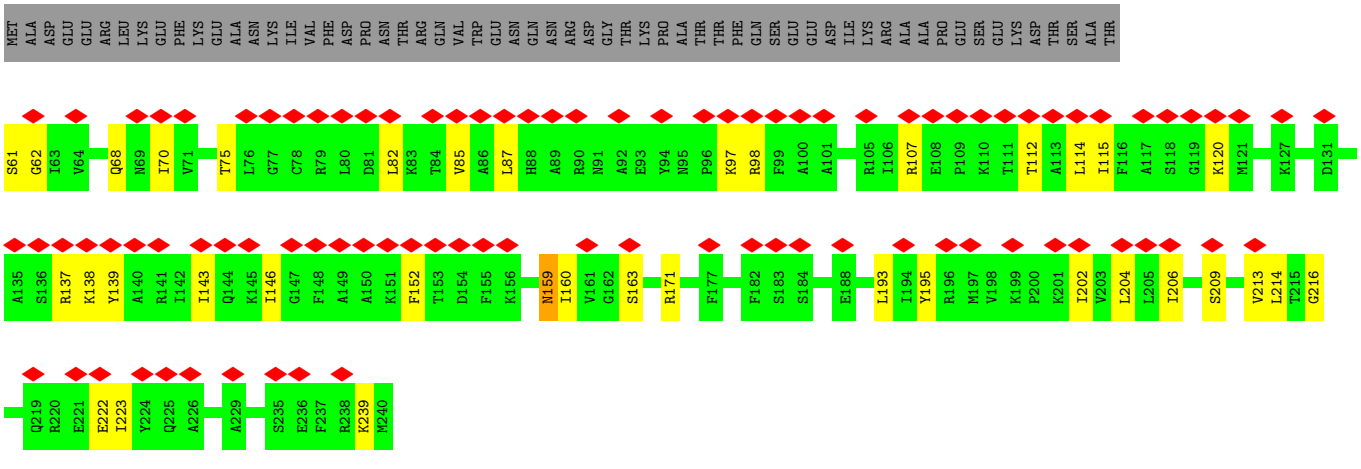






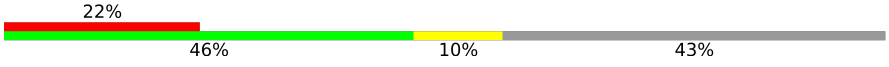
• Molecule 21: TATA-box-binding protein

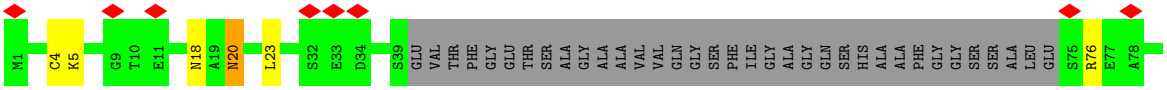
Chain Y:

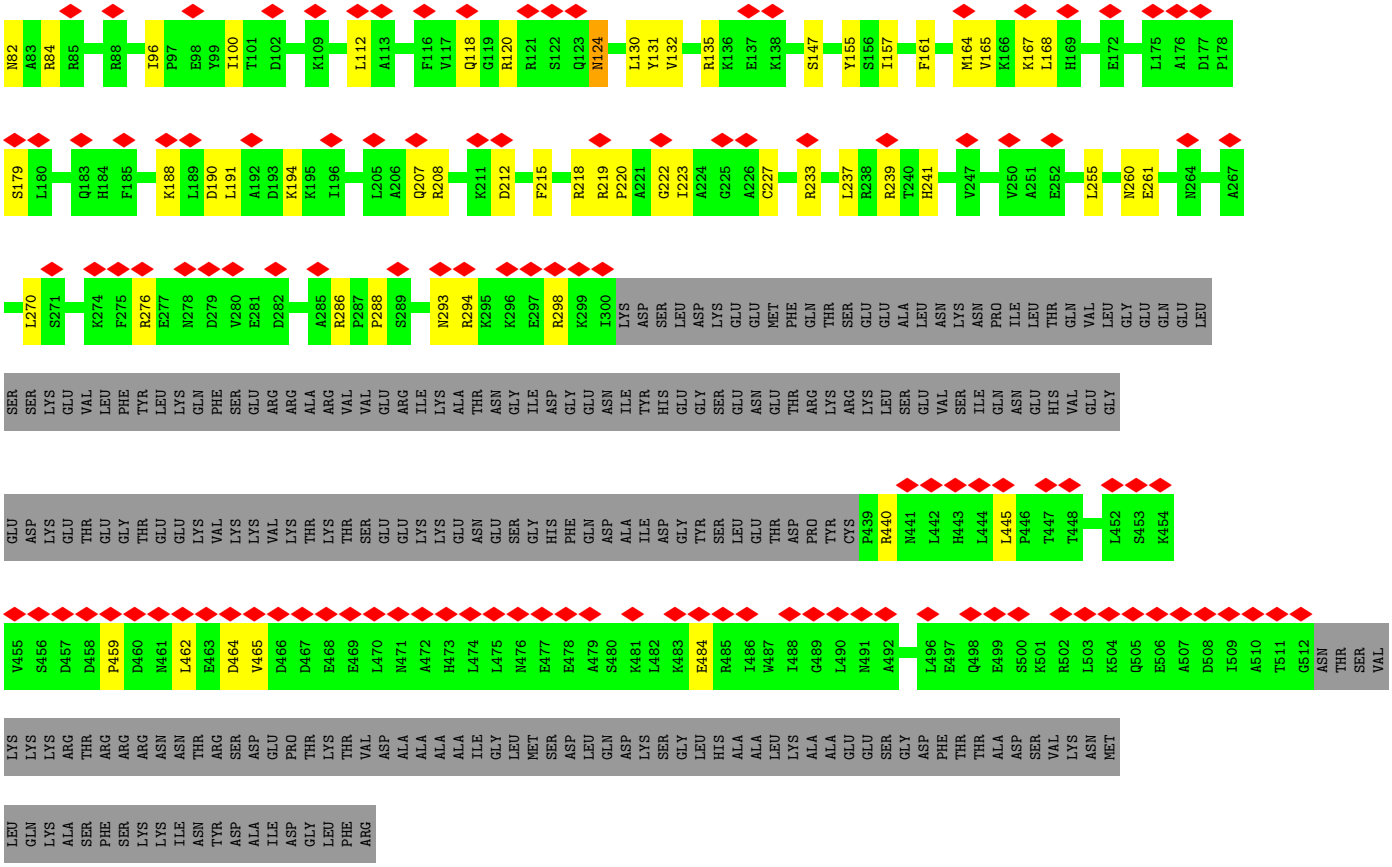


• Molecule 22: Transcription factor IIIB 70 kDa subunit

Chain Z:






N82 A83 R84 R85 R88 I96 P97 E98 Y99 I100 T101 D102 K109 L112 A113 F116 V117 Q118 G119 R120 R121 S122 Q123 N124 L130 Y131 V132 R135 K136 E137 K138 S147 Y155 S156 I157 F161 M164 V165 K166 K167 L168 H169 E172 L175 A176 D177 P178
S179 L180 Q183 H184 F185 K188 L189 D190 L191 A192 D193 K194 K195 I196 L205 A206 Q207 R208 K211 D212 F215 R218 R219 P220 A221 G222 I223 A224 G225 A226 C227 R233 L237 R238 R239 T240 H241 V247 V250 A251 E252 L255 N260 E261 N264 A267
L270 S271 K274 F275 R276 E277 N278 D279 V280 E281 D282 A285 R286 P287 P288 S289 N293 R294 K295 K296 E297 R298 K299 I300 LYS ASP SER LEU ASP LYS GLU GLU MET PHE GLN THR SER GLU GLU ALA LEU ASN LYS ASN PRO ILE LEU THR GLN VAL LEU GLY GLU GLN GLU LEU
SER SER LYS GLU VAL LEU PHE TYR LEU LYS GLN PHE SER GLU ARG ARG ALA ARG VAL VAL GLU ARG ILE LYS ALA THR ASN GLY ILE ASP GLY GLU ASN ILE TYR HIS GLU GLY SER GLU ASN GLU THR ARG LYS ARG LYS LEU SER GLU VAL SER ILE GLN ASN GLU HIS VAL GLU GLY
GLU ASP LYS GLU THR GLU GLY THR GLU GLU LYS VAL LYS LYS VAL LYS THR LYS THR SER GLU GLU LYS LYS GLU ASN GLU GLU SER GLY HIS PHE GLN ASP ALA ILE ASP GLY TYR SER LEU GLU GLU THR ASP PRO TYR CYS P439 R440 N441 L442 H443 L444 L445 P446 T447 T448 L452 S453 K454
V455 S456 D457 D458 P459 D460 N461 L462 E463 D464 V465 D466 D467 E468 E469 L470 N471 A472 H473 L474 L475 N476 E477 E478 A479 S480 K481 L482 K483 E484 R485 I486 W487 I488 G489 L490 N491 A492 L496 E497 Q498 E499 S500 K501 R502 L503 K504 Q505 E506 A507 D508 I509 A510 T511 G512 ASN THR SER VAL
LYS LYS LYS ARG THR ARG ARG ARG ASN ASN THR ARG SER ASP GLU PRO THR LYS THR VAL ASP ALA ALA ALA ALA ILE GLY LEU MET SER ASP LEU GLN ASP LYS SER GLY LEU HIS ALA ALA LEU LYS ALA ALA GLU GLU SER GLY ASP PHE THR THR ALA ASP SER VAL LYS ASN MET
LEU GLN LYS ALA SER PHE SER LYS LYS ILE ASN TYR ASP ALA ILE ASP GLY LEU PHE ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	40847	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	39	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.128	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	328.59998, 328.59998, 328.59998	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.29	1/11315 (0.0%)	0.62	3/15284 (0.0%)
2	B	0.29	0/8926	0.63	3/12045 (0.0%)
3	C	0.29	0/2711	0.58	0/3676
4	D	0.29	0/1154	0.63	1/1546 (0.1%)
5	E	0.27	0/1795	0.56	1/2416 (0.0%)
6	F	0.27	0/683	0.60	0/923
7	G	0.29	0/1740	0.62	0/2362
8	H	0.28	0/1181	0.62	0/1602
9	I	0.29	0/320	0.68	0/434
10	J	0.27	0/558	0.59	0/750
11	K	0.27	0/812	0.58	0/1096
12	L	0.28	0/360	0.69	0/478
13	M	0.32	0/1624	0.65	2/2199 (0.1%)
14	N	0.29	0/810	0.66	1/1088 (0.1%)
15	O	0.28	0/4488	0.63	3/6055 (0.0%)
16	P	0.30	0/2397	0.67	3/3233 (0.1%)
17	Q	0.29	0/599	0.62	0/797
18	R	0.57	0/1159	1.00	0/1783
19	S	0.60	0/1319	0.99	1/2031 (0.0%)
20	V	0.26	0/1854	0.51	0/2433
21	Y	0.27	0/1443	0.55	0/1942
22	Z	0.28	0/2747	0.57	1/3699 (0.0%)
All	All	0.31	1/49995 (0.0%)	0.64	19/67872 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	3
3	C	0	1
4	D	0	2
12	L	0	1
13	M	0	2
14	N	0	1
16	P	0	6
20	V	0	1
22	Z	0	1
All	All	0	25

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1267	LEU	C-N	5.15	1.44	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	S	30	DC	O4'-C4'-C3'	-8.70	100.78	106.00
1	A	330	ASP	CB-CG-OD1	7.58	125.12	118.30
16	P	153	LEU	CA-CB-CG	7.16	131.78	115.30
16	P	265	LEU	CA-CB-CG	7.11	131.64	115.30
15	O	500	LEU	CA-CB-CG	6.04	129.20	115.30
15	O	206	LEU	CA-CB-CG	5.93	128.94	115.30
2	B	320	LEU	CA-CB-CG	5.87	128.79	115.30
13	M	85	LEU	CA-CB-CG	5.82	128.69	115.30
5	E	37	LEU	CA-CB-CG	5.68	128.35	115.30
2	B	1132	LEU	CA-CB-CG	5.57	128.11	115.30
15	O	135	LEU	CA-CB-CG	5.51	127.98	115.30
1	A	114	LEU	CA-CB-CG	5.45	127.83	115.30
22	Z	23	LEU	CA-CB-CG	5.41	127.75	115.30
4	D	28	LEU	CA-CB-CG	5.36	127.63	115.30
1	A	219	MET	CA-CB-CG	5.35	122.39	113.30
14	N	408	LEU	CA-CB-CG	5.25	127.38	115.30
16	P	264	THR	C-N-CA	5.19	134.69	121.70
2	B	1133	LEU	CA-CB-CG	5.04	126.90	115.30
13	M	76	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1211	ARG	Peptide
1	A	34	VAL	Peptide
1	A	348	LYS	Peptide
1	A	554	THR	Peptide
1	A	584	SER	Peptide
1	A	598	MET	Peptide
1	A	600	PRO	Peptide
2	B	229	SER	Peptide
2	B	552	ASN	Peptide
2	B	816	ASP	Peptide
3	C	28	GLU	Peptide
4	D	13	ASP	Peptide
4	D	49	PRO	Peptide
12	L	45	ALA	Peptide
13	M	130	PHE	Peptide
13	M	221	ASP	Peptide
14	N	300	LYS	Peptide
16	P	205	ASN	Peptide
16	P	209	ALA	Peptide
16	P	211	ASN	Peptide
16	P	229	GLN	Peptide
16	P	256	VAL	Peptide
16	P	300	PHE	Peptide
20	V	284	PHE	Peptide
22	Z	227	CYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11119	0	11260	206	0
2	B	8771	0	8894	219	0
3	C	2655	0	2628	46	0
4	D	1137	0	1145	20	0
5	E	1759	0	1788	28	0
6	F	671	0	692	8	0
7	G	1698	0	1672	30	0
8	H	1161	0	1124	13	0
9	I	313	0	300	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	549	0	561	15	0
11	K	801	0	795	21	0
12	L	358	0	384	12	0
13	M	1589	0	1553	40	0
14	N	802	0	848	24	0
15	O	4421	0	4589	74	0
16	P	2355	0	2325	38	0
17	Q	589	0	535	10	0
18	R	1038	0	583	12	0
19	S	1174	0	643	28	0
20	V	1829	0	1506	25	0
21	Y	1416	0	1493	33	0
22	Z	2705	0	2739	42	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	I	1	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
23	Z	1	0	0	0	0
24	A	1	0	0	0	0
All	All	48918	0	48057	789	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 (789) 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)
19:S:32:DA:H2	19:S:34:DA:N6	1.39	1.19
19:S:32:DA:C2	19:S:34:DA:N6	2.22	1.07
1:A:441:ARG:HH12	2:B:1040:ARG:NH1	1.60	0.99
1:A:1079:ARG:HH11	1:A:1082:ARG:HH12	1.10	0.93
1:A:441:ARG:NH1	2:B:1040:ARG:HH11	1.65	0.93
19:S:32:DA:H2	19:S:34:DA:H61	1.04	0.89
2:B:313:ARG:HH12	13:M:224:GLN:HG2	1.38	0.88
15:O:289:LYS:NZ	15:O:324:PRO:O	2.10	0.84
2:B:137:ARG:HH11	2:B:141:ILE:HG21	1.44	0.83
2:B:576:ARG:NH1	2:B:647:GLU:OE1	2.11	0.82
13:M:263:ALA:O	13:M:266:LYS:NZ	2.12	0.82
5:E:161:LYS:NZ	5:E:193:GLY:O	2.12	0.82
1:A:1079:ARG:HH11	1:A:1082:ARG:NH1	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:640:ARG:NH1	17:Q:42:PRO:O	2.13	0.81
1:A:1173:VAL:O	1:A:1264:ARG:NH1	2.14	0.81
2:B:780:ARG:NH1	10:J:10:CYS:O	2.13	0.80
1:A:1187:ARG:NH1	1:A:1227:LYS:O	2.15	0.80
2:B:968:VAL:O	10:J:47:ARG:NH1	2.15	0.79
16:P:62:LYS:NZ	20:V:379:MET:O	2.15	0.79
15:O:234:ASP:O	15:O:238:ARG:HB2	1.83	0.78
2:B:1007:GLY:O	3:C:69:ARG:NH1	2.16	0.77
7:G:147:ARG:NH1	7:G:208:VAL:O	2.17	0.77
15:O:222:HIS:NE2	15:O:248:ASP:OD2	2.17	0.77
8:H:5:LEU:O	8:H:130:ARG:NH1	2.18	0.77
1:A:351:ARG:HH11	1:A:356:ARG:HG2	1.49	0.77
2:B:786:GLU:OE2	3:C:93:GLN:NE2	2.17	0.77
1:A:439:ASP:OD2	1:A:442:ARG:NH2	2.18	0.76
22:Z:164:MET:O	22:Z:167:LYS:NZ	2.19	0.75
2:B:579:ARG:NE	2:B:647:GLU:OE2	2.19	0.75
15:O:292:ARG:NH1	15:O:480:TYR:OH	2.20	0.75
2:B:1128:LEU:O	2:B:1132:LEU:HB2	1.88	0.74
1:A:318:TYR:OH	19:S:29:DG:P	2.46	0.74
1:A:533:ASN:OD1	6:F:90:ARG:NH1	2.20	0.73
1:A:1125:ARG:NH2	1:A:1338:GLU:OE2	2.22	0.73
1:A:3:GLU:OE1	7:G:37:LYS:NZ	2.22	0.72
15:O:291:ARG:NH1	15:O:646:SER:OG	2.22	0.72
1:A:1157:VAL:HG22	1:A:1160:ARG:HH11	1.53	0.72
1:A:578:GLN:OE1	11:K:77:ARG:NH1	2.23	0.72
1:A:441:ARG:HH12	2:B:1040:ARG:HH11	0.81	0.71
16:P:83:LYS:HZ1	16:P:90:GLU:HG3	1.55	0.71
13:M:164:LYS:H	13:M:167:GLN:HE21	1.36	0.71
2:B:59:LYS:HZ1	2:B:519:HIS:HA	1.54	0.70
11:K:88:PHE:HB3	11:K:106:GLN:HB2	1.73	0.70
15:O:275:LYS:HZ2	15:O:278:VAL:HG23	1.57	0.69
19:S:52:DT:OP2	22:Z:218:ARG:NH1	2.26	0.69
16:P:16:LYS:HZ2	16:P:48:LEU:HB2	1.57	0.69
2:B:727:LEU:HB2	2:B:786:GLU:HB2	1.73	0.69
1:A:502:GLU:HG2	2:B:767:ILE:HG13	1.75	0.68
2:B:1038:ARG:HH11	2:B:1050:PRO:HB3	1.57	0.68
1:A:495:TRP:O	1:A:499:ARG:NH1	2.28	0.67
15:O:73:ARG:HE	15:O:119:TYR:HB3	1.59	0.67
1:A:120:LYS:HG3	1:A:241:LEU:HD11	1.76	0.67
2:B:734:PRO:HB3	2:B:915:ARG:HH12	1.59	0.67
1:A:878:LYS:HD3	1:A:1103:GLN:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:137:ARG:NH1	22:Z:464:ASP:OD2	2.28	0.67
1:A:716:ASP:OD1	1:A:789:ASN:ND2	2.29	0.66
15:O:88:VAL:HG12	15:O:92:LYS:HZ1	1.61	0.65
13:M:148:LEU:HA	13:M:182:PHE:H	1.61	0.65
19:S:45:DT:H4'	21:Y:114:LEU:HD22	1.79	0.65
13:M:210:GLN:HE22	16:P:102:ARG:HH12	1.42	0.65
13:M:74:PHE:HB2	14:N:363:ILE:HB	1.77	0.65
13:M:95:ARG:O	13:M:99:ARG:NH1	2.31	0.64
14:N:303:ARG:HD3	14:N:411:ARG:NH1	2.12	0.64
1:A:777:VAL:HG12	1:A:811:ALA:HB1	1.80	0.64
3:C:100:ARG:HE	10:J:5:VAL:HG13	1.63	0.64
1:A:894:GLU:OE2	2:B:1067:ARG:NH1	2.31	0.64
1:A:476:ARG:NH1	1:A:515:ASP:OD2	2.31	0.63
1:A:404:TYR:HB3	1:A:464:ARG:NH1	2.13	0.63
15:O:50:LYS:HE2	15:O:66:GLY:HA2	1.80	0.63
2:B:1038:ARG:NH1	2:B:1050:PRO:HB3	2.12	0.63
14:N:293:LYS:NZ	14:N:303:ARG:NH1	2.47	0.63
15:O:141:ILE:HG12	15:O:145:ARG:NH1	2.13	0.63
13:M:160:ALA:HB3	13:M:171:VAL:HB	1.81	0.63
15:O:88:VAL:HG12	15:O:92:LYS:NZ	2.14	0.63
1:A:378:ARG:HH12	19:S:21:DA:H2"	1.64	0.62
4:D:14:TYR:OH	4:D:18:LYS:NZ	2.25	0.62
13:M:129:ALA:O	13:M:135:LYS:NZ	2.32	0.62
2:B:270:GLN:HE21	2:B:547:ALA:HB2	1.64	0.62
1:A:360:LYS:H	1:A:365:ARG:HB3	1.65	0.62
1:A:1026:ARG:HH12	8:H:110:ASP:HA	1.64	0.62
15:O:640:ARG:NH1	16:P:308:GLU:HB3	2.14	0.62
9:I:28:SER:HA	13:M:135:LYS:HA	1.81	0.62
1:A:167:ALA:HB3	1:A:175:ALA:HB1	1.82	0.62
1:A:578:GLN:NE2	11:K:91:TYR:O	2.32	0.61
15:O:339:LEU:HD12	15:O:341:GLU:H	1.64	0.61
5:E:171:LYS:HD2	5:E:173:SER:H	1.65	0.61
15:O:35:SER:O	15:O:40:ARG:NH1	2.32	0.61
1:A:154:CYS:SG	1:A:155:LEU:N	2.71	0.61
15:O:47:PHE:O	15:O:51:GLU:HB2	2.00	0.61
15:O:289:LYS:HD3	15:O:323:SER:HB2	1.83	0.61
2:B:837:GLN:HB3	2:B:878:PRO:HB3	1.83	0.61
2:B:313:ARG:NH1	13:M:224:GLN:HG2	2.13	0.61
2:B:880:HIS:HB2	2:B:901:ARG:NH1	2.16	0.61
22:Z:131:TYR:OH	22:Z:135:ARG:NH1	2.34	0.61
1:A:944:ASN:HA	1:A:947:PHE:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1329:GLU:OE2	1:A:1332:ARG:NH2	2.34	0.61
2:B:471:THR:HG22	2:B:514:LEU:HB3	1.82	0.61
4:D:28:LEU:HG	4:D:31:GLN:HB2	1.82	0.61
6:F:94:LEU:HD11	6:F:125:LEU:HD22	1.83	0.61
3:C:132:ILE:H	3:C:208:CYS:HB3	1.66	0.60
10:J:12:LYS:HZ2	10:J:17:LYS:NZ	1.99	0.60
1:A:482:ARG:HH11	1:A:544:PRO:HG3	1.66	0.60
1:A:897:SER:HB2	1:A:1423:ILE:HG22	1.82	0.60
15:O:203:ILE:HD12	15:O:205:LYS:H	1.65	0.60
15:O:147:ASN:ND2	15:O:193:GLN:OE1	2.34	0.60
19:S:40:DA:H4'	22:Z:120:ARG:HH22	1.66	0.60
22:Z:190:ASP:HA	22:Z:239:ARG:HE	1.66	0.60
1:A:839:SER:HB3	1:A:844:SER:HB3	1.84	0.60
1:A:152:ARG:HH11	1:A:185:TRP:HB3	1.67	0.60
2:B:590:ILE:HG22	2:B:601:ILE:HG12	1.84	0.60
1:A:365:ARG:NH1	1:A:887:ARG:NH1	2.50	0.60
15:O:306:SER:O	15:O:310:GLN:NE2	2.35	0.60
4:D:51:ASN:HA	4:D:55:LEU:HB3	1.84	0.60
5:E:109:ILE:HG22	5:E:133:GLU:HB3	1.82	0.60
1:A:1431:VAL:HG23	7:G:58:GLN:HA	1.84	0.59
15:O:275:LYS:HZ1	15:O:277:THR:HB	1.66	0.59
19:S:29:DG:OP2	19:S:29:DG:O3'	2.20	0.59
8:H:58:THR:HB	8:H:143:LEU:HB3	1.82	0.59
16:P:60:LEU:HD22	16:P:67:ASN:HB3	1.84	0.59
2:B:778:ILE:HA	2:B:782:PHE:HB3	1.83	0.59
5:E:171:LYS:HE3	5:E:173:SER:HB3	1.84	0.59
1:A:683:ARG:HH22	1:A:925:GLU:HA	1.67	0.59
13:M:76:LEU:H	14:N:361:GLY:HA3	1.68	0.59
3:C:191:ILE:HG12	10:J:15:GLY:HA3	1.83	0.59
4:D:10:PHE:HA	7:G:3:ILE:HA	1.83	0.59
15:O:289:LYS:HZ1	15:O:324:PRO:C	2.06	0.59
1:A:19:SER:HB2	2:B:1138:ALA:HB3	1.84	0.59
2:B:580:ARG:HH11	2:B:614:ILE:HD13	1.68	0.59
1:A:520:HIS:HB3	2:B:1082:ARG:HH22	1.68	0.59
20:V:451:ARG:NH1	21:Y:97:LYS:NZ	2.51	0.59
1:A:1431:VAL:HG13	6:F:133:VAL:HG13	1.85	0.59
2:B:708:GLN:HE21	2:B:1028:LYS:HE3	1.67	0.58
3:C:39:ASP:O	3:C:58:ASN:ND2	2.35	0.58
19:S:40:DA:H5'	22:Z:118:GLN:HE21	1.68	0.58
3:C:230:LEU:HD21	3:C:270:ALA:HB1	1.85	0.58
2:B:242:LEU:HD12	2:B:256:VAL:HG21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:150:GLY:HA3	13:M:179:LEU:HA	1.85	0.58
15:O:528:MET:HG3	15:O:532:ASP:HB2	1.85	0.58
14:N:303:ARG:NH1	14:N:413:ASP:OD2	2.37	0.58
20:V:323:PRO:HG3	20:V:448:TYR:HA	1.85	0.58
22:Z:208:ARG:O	22:Z:212:ASP:HB2	2.04	0.58
1:A:1373:ARG:HH11	1:A:1391:LYS:NZ	2.01	0.58
1:A:1042:ILE:HG12	1:A:1044:PRO:HD2	1.85	0.58
1:A:1373:ARG:HH11	1:A:1391:LYS:HD3	1.67	0.57
22:Z:219:ARG:HG3	22:Z:222:GLY:H	1.69	0.57
15:O:516:LEU:HD21	15:O:567:ARG:HD2	1.85	0.57
2:B:615:VAL:HG12	2:B:620:SER:HA	1.86	0.57
2:B:1130:GLN:O	2:B:1134:SER:HB2	2.04	0.57
3:C:335:GLN:HG3	11:K:49:LEU:HB3	1.85	0.57
2:B:155:MET:HA	2:B:185:PHE:HB3	1.86	0.57
2:B:1005:TYR:OH	3:C:293:ARG:NH2	2.37	0.57
3:C:80:ALA:HA	3:C:208:CYS:HA	1.86	0.57
21:Y:152:PHE:H	22:Z:459:PRO:HB3	1.69	0.57
1:A:74:LEU:O	2:B:1048:ARG:NH2	2.38	0.57
2:B:59:LYS:NZ	2:B:519:HIS:HA	2.19	0.57
4:D:51:ASN:HB3	4:D:56:GLN:HG2	1.86	0.57
2:B:849:THR:N	2:B:867:ARG:HH12	2.03	0.57
20:V:321:PHE:HB3	20:V:447:PRO:HG2	1.86	0.56
15:O:246:LYS:NZ	15:O:341:GLU:OE2	2.23	0.56
21:Y:209:SER:O	22:Z:293:ASN:ND2	2.38	0.56
6:F:86:THR:HG22	6:F:88:TYR:H	1.70	0.56
15:O:275:LYS:NZ	15:O:278:VAL:HG23	2.20	0.56
9:I:32:GLU:OE2	13:M:132:ASN:ND2	2.38	0.56
11:K:98:GLU:HB3	11:K:100:LEU:HD13	1.86	0.56
2:B:1038:ARG:NH2	2:B:1039:ALA:O	2.39	0.56
3:C:215:ASP:OD2	12:L:70:ARG:NH1	2.34	0.56
1:A:90:VAL:HG23	1:A:320:GLN:HG2	1.87	0.56
1:A:1079:ARG:NH1	1:A:1082:ARG:HH12	1.92	0.56
2:B:836:VAL:HG23	2:B:840:GLN:HB2	1.86	0.56
2:B:1061:ARG:NH2	19:S:21:DA:OP1	2.39	0.56
1:A:229:ASN:HB2	15:O:544:ASN:HD22	1.70	0.56
9:I:12:LEU:HD21	9:I:24:LEU:HB2	1.88	0.56
13:M:199:ARG:NH1	13:M:200:ARG:NH1	2.54	0.56
2:B:721:ILE:HG12	2:B:899:LEU:HD22	1.88	0.56
2:B:911:LYS:HZ3	2:B:911:LYS:HB3	1.70	0.56
22:Z:191:LEU:O	22:Z:239:ARG:NH2	2.39	0.56
1:A:1141:ILE:HB	1:A:1295:VAL:HB	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1137:ILE:HG23	2:B:1139:PRO:HD3	1.87	0.56
15:O:547:GLU:HB2	15:O:567:ARG:HB2	1.87	0.56
20:V:314:ARG:NH2	20:V:449:ARG:HH12	2.04	0.55
1:A:234:ILE:HG22	1:A:252:ARG:HH11	1.72	0.55
11:K:65:ILE:HD11	11:K:101:LEU:HD23	1.87	0.55
15:O:169:LEU:HB3	15:O:280:LEU:HB3	1.87	0.55
20:V:435:TRP:NE1	20:V:438:ASP:OD2	2.39	0.55
1:A:374:ASP:OD2	2:B:1043:ARG:NH1	2.39	0.55
2:B:622:VAL:HG13	2:B:627:LEU:HD13	1.87	0.55
22:Z:237:LEU:HG	22:Z:239:ARG:HH12	1.71	0.55
2:B:408:LYS:O	2:B:408:LYS:HG3	2.07	0.55
2:B:734:PRO:HB3	2:B:915:ARG:NH1	2.21	0.55
8:H:87:ARG:NH2	8:H:88:SER:O	2.39	0.55
1:A:17:GLU:HB2	2:B:1140:ARG:HB2	1.88	0.55
1:A:1012:ILE:HD11	1:A:1071:LEU:HD21	1.88	0.55
5:E:55:ARG:HD2	5:E:84:ASP:HA	1.87	0.55
7:G:3:ILE:HD13	7:G:78:LYS:HE3	1.89	0.55
2:B:379:LEU:HD11	2:B:520:ILE:HG21	1.89	0.55
12:L:50:ASP:HB2	22:Z:194:LYS:NZ	2.22	0.55
21:Y:87:LEU:HD21	22:Z:484:GLU:HB2	1.87	0.55
2:B:409:LYS:HD3	2:B:410:PRO:HD2	1.89	0.55
10:J:59:LYS:NZ	10:J:62:ARG:HH21	2.05	0.55
13:M:113:LYS:NZ	13:M:237:ALA:O	2.40	0.55
1:A:570:PHE:HB3	1:A:603:LEU:HB3	1.89	0.55
1:A:1188:ILE:N	1:A:1228:ASP:OD2	2.39	0.55
13:M:76:LEU:HB3	13:M:168:VAL:HG13	1.90	0.55
1:A:573:ARG:HH21	11:K:87:GLU:HB2	1.72	0.54
1:A:318:TYR:CZ	19:S:29:DG:OP1	2.61	0.54
4:D:107:MET:O	4:D:111:ASN:ND2	2.41	0.54
14:N:290:ILE:HD11	14:N:416:ILE:HD12	1.90	0.54
1:A:590:PHE:H	11:K:106:GLN:HE22	1.54	0.54
4:D:132:VAL:HA	7:G:208:VAL:HG13	1.90	0.54
1:A:1198:LEU:HD12	1:A:1273:LYS:HD3	1.88	0.54
4:D:58:ILE:HB	7:G:46:ILE:HG23	1.90	0.54
1:A:15:GLY:HA2	1:A:1407:ALA:HA	1.88	0.54
15:O:275:LYS:NZ	15:O:277:THR:HB	2.22	0.54
1:A:152:ARG:NH1	1:A:185:TRP:HE3	2.04	0.54
1:A:893:LEU:HD13	1:A:1361:VAL:HG21	1.89	0.54
5:E:111:VAL:HG22	5:E:135:PHE:HB2	1.90	0.54
3:C:228:ARG:NH1	3:C:299:ILE:HG21	2.22	0.54
20:V:466:PRO:HA	21:Y:107:ARG:HH22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LYS:HD2	2:B:1117:ILE:HG13	1.89	0.54
1:A:652:VAL:HG12	1:A:662:GLY:HA3	1.89	0.54
2:B:141:ILE:HA	20:V:400:ASN:HD22	1.72	0.54
2:B:904:ARG:HD3	2:B:1030:MET:HG2	1.89	0.54
4:D:132:VAL:HG13	7:G:208:VAL:HA	1.90	0.54
8:H:93:TYR:HA	8:H:145:ARG:HD3	1.89	0.54
3:C:324:LYS:NZ	11:K:71:THR:OG1	2.28	0.53
14:N:394:VAL:HG12	14:N:412:VAL:H	1.72	0.53
16:P:255:LYS:HG2	16:P:261:TYR:HA	1.90	0.53
21:Y:171:ARG:HH21	21:Y:239:LYS:HG3	1.74	0.53
1:A:413:ARG:NH2	1:A:455:ASN:O	2.41	0.53
1:A:683:ARG:HH12	1:A:925:GLU:HB2	1.74	0.53
2:B:409:LYS:NZ	18:R:33:DT:OP1	2.37	0.53
4:D:132:VAL:HG22	7:G:208:VAL:HG22	1.90	0.53
9:I:26:CYS:HB2	9:I:29:CYS:HB2	1.89	0.53
2:B:944:MET:SD	2:B:1024:TYR:OH	2.66	0.53
14:N:364:ARG:NH1	14:N:376:GLY:HA3	2.22	0.53
15:O:452:LEU:O	15:O:456:HIS:ND1	2.37	0.53
20:V:434:MET:HA	20:V:477:LEU:HB2	1.89	0.53
1:A:1079:ARG:NH1	1:A:1082:ARG:NH1	2.54	0.53
2:B:228:LYS:HD2	2:B:245:ASN:HD21	1.73	0.53
2:B:314:ARG:HG3	2:B:316:LYS:H	1.72	0.53
2:B:1095:CYS:HB3	2:B:1099:GLY:HA2	1.90	0.53
18:R:19:DA:N1	19:S:53:DA:N6	2.56	0.53
21:Y:138:LYS:NZ	22:Z:465:VAL:HB	2.23	0.53
2:B:731:PRO:HB2	2:B:750:PRO:HG2	1.91	0.53
2:B:1001:LYS:HD3	2:B:1018:PHE:HB3	1.90	0.53
15:O:169:LEU:HD22	15:O:280:LEU:HD23	1.91	0.53
1:A:173:SER:HB2	1:A:332:VAL:HB	1.89	0.53
1:A:1128:GLU:OE2	1:A:1136:ILE:HA	2.09	0.53
20:V:314:ARG:NH2	20:V:418:ASP:OD2	2.40	0.53
21:Y:209:SER:HB2	22:Z:293:ASN:HD21	1.73	0.53
1:A:1365:LYS:HG3	1:A:1379:MET:HG2	1.90	0.53
2:B:216:VAL:HB	2:B:233:VAL:HG23	1.91	0.53
4:D:11:LEU:HB2	4:D:16:VAL:HG21	1.91	0.53
5:E:176:PRO:HB2	5:E:212:ARG:HG2	1.90	0.53
13:M:92:ASN:HB3	13:M:93:ARG:HD2	1.89	0.53
2:B:930:ASP:OD1	3:C:69:ARG:NH2	2.34	0.53
3:C:208:CYS:SG	3:C:209:ILE:N	2.82	0.53
1:A:445:ARG:NH1	22:Z:18:ASN:HD21	2.07	0.52
1:A:623:VAL:HG23	1:A:656:GLY:HA2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:993:GLU:O	5:E:197:LYS:NZ	2.36	0.52
2:B:741:ILE:HB	2:B:746:TYR:HB3	1.92	0.52
2:B:170:LYS:O	2:B:174:LEU:HB2	2.09	0.52
2:B:880:HIS:HB2	2:B:901:ARG:HH12	1.73	0.52
12:L:28:LYS:HD2	12:L:58:LYS:NZ	2.24	0.52
13:M:154:GLU:HG2	13:M:175:ARG:HG3	1.91	0.52
16:P:184:ARG:NH1	16:P:271:MET:SD	2.82	0.52
1:A:1205:ILE:HG13	1:A:1272:VAL:HG21	1.90	0.52
2:B:689:PRO:HD3	2:B:915:ARG:HE	1.75	0.52
2:B:234:ILE:HB	2:B:240:ILE:HG23	1.91	0.52
4:D:149:THR:HA	4:D:152:GLU:HG2	1.91	0.52
15:O:152:HIS:HD2	15:O:155:LEU:HD21	1.74	0.52
2:B:114:PRO:HG2	2:B:117:GLU:HB3	1.92	0.52
2:B:848:PRO:C	2:B:867:ARG:HH12	2.12	0.52
2:B:895:LEU:HD21	2:B:897:LYS:HE3	1.92	0.52
11:K:55:SER:OG	11:K:58:GLY:O	2.27	0.52
3:C:228:ARG:HH11	3:C:299:ILE:HD13	1.75	0.52
4:D:9:ALA:O	7:G:4:LEU:N	2.42	0.52
7:G:91:LYS:HZ3	7:G:98:LYS:HZ3	1.57	0.52
14:N:293:LYS:HZ3	14:N:303:ARG:NH1	2.07	0.52
17:Q:92:PRO:HA	17:Q:95:ILE:HG13	1.91	0.52
13:M:91:ALA:HA	14:N:391:LEU:HD22	1.92	0.51
10:J:12:LYS:NZ	10:J:17:LYS:NZ	2.58	0.51
13:M:227:LEU:HD21	13:M:231:LEU:HB2	1.92	0.51
3:C:172:GLN:H	3:C:175:GLN:HB2	1.74	0.51
11:K:112:THR:HG22	11:K:114:VAL:H	1.75	0.51
5:E:31:THR:N	5:E:34:GLU:OE2	2.42	0.51
20:V:461:GLU:HA	20:V:464:LYS:HZ2	1.76	0.51
1:A:905:ARG:HH12	5:E:170:LEU:HD21	1.75	0.51
2:B:1095:CYS:SG	2:B:1096:ASP:N	2.83	0.51
8:H:11:GLN:HE21	8:H:29:ALA:HB3	1.76	0.51
1:A:351:ARG:HA	1:A:355:GLN:HE21	1.75	0.51
1:A:740:GLU:HA	1:A:743:THR:HG22	1.93	0.51
3:C:139:LYS:HB3	3:C:201:GLU:HG2	1.93	0.51
3:C:225:ALA:HA	3:C:302:VAL:HG12	1.93	0.51
19:S:5:DG:H8	19:S:5:DG:OP1	1.93	0.51
20:V:451:ARG:NH1	21:Y:97:LYS:HZ2	2.08	0.51
7:G:92:CYS:SG	7:G:122:THR:OG1	2.66	0.51
16:P:186:ILE:HD11	16:P:221:ILE:HD13	1.93	0.51
22:Z:4:CYS:SG	22:Z:5:LYS:N	2.84	0.51
22:Z:270:LEU:HD22	22:Z:276:ARG:HH21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:TYR:HD2	1:A:441:ARG:HH21	1.58	0.51
3:C:257:GLY:HA3	3:C:268:LYS:HE2	1.91	0.51
1:A:828:GLN:H	2:B:655:ASN:HD21	1.57	0.51
2:B:780:ARG:HE	3:C:217:ALA:HB1	1.75	0.51
15:O:367:ALA:HA	15:O:370:LEU:HD23	1.92	0.51
15:O:158:GLU:O	15:O:174:TYR:OH	2.28	0.51
1:A:103:LEU:HD21	1:A:222:LEU:HD22	1.93	0.50
1:A:363:ARG:HH12	2:B:1046:LEU:HD21	1.75	0.50
1:A:473:LEU:HB2	1:A:520:HIS:HB2	1.92	0.50
2:B:43:ASP:OD2	2:B:46:HIS:ND1	2.43	0.50
2:B:276:ASP:O	2:B:280:GLN:NE2	2.44	0.50
2:B:733:GLN:HE21	10:J:54:VAL:HG13	1.76	0.50
2:B:929:GLU:HB2	3:C:68:ARG:HH12	1.76	0.50
7:G:6:LYS:HA	7:G:73:ARG:HA	1.92	0.50
13:M:77:LYS:HD3	13:M:265:ASP:OD2	2.10	0.50
1:A:869:ARG:HH12	2:B:502:THR:CB	2.24	0.50
1:A:1144:VAL:HG21	1:A:1313:ARG:HE	1.76	0.50
2:B:688:ILE:HB	2:B:691:PRO:HG3	1.93	0.50
2:B:948:GLY:HA2	2:B:952:ARG:HH11	1.77	0.50
10:J:9:SER:OG	10:J:45:CYS:SG	2.68	0.50
10:J:10:CYS:SG	10:J:11:GLY:N	2.82	0.50
2:B:217:GLN:HB3	2:B:232:TYR:HD2	1.75	0.50
2:B:680:ILE:HG23	2:B:681:LEU:HD12	1.92	0.50
5:E:21:GLU:OE2	5:E:143:ASN:HB3	2.11	0.50
5:E:200:ARG:NH2	5:E:210:SER:OG	2.44	0.50
13:M:247:TRP:HB3	14:N:406:ALA:HB3	1.93	0.50
21:Y:137:ARG:HD3	22:Z:462:LEU:HD23	1.94	0.50
1:A:1005:TYR:OH	1:A:1079:ARG:NH2	2.44	0.50
2:B:241:TYR:HB2	2:B:243:LYS:NZ	2.27	0.50
2:B:408:LYS:NZ	2:B:408:LYS:CB	2.73	0.50
2:B:773:LEU:HD23	2:B:942:ILE:HG12	1.93	0.50
13:M:76:LEU:HD13	13:M:170:LEU:HD13	1.93	0.50
13:M:148:LEU:HD13	13:M:179:LEU:HD13	1.92	0.50
15:O:220:GLU:OE2	15:O:224:LYS:HD2	2.12	0.50
2:B:517:MET:HB3	2:B:611:PRO:HD2	1.94	0.50
15:O:353:GLU:OE2	15:O:480:TYR:N	2.39	0.50
1:A:223:ASN:HB2	1:A:316:TRP:HH2	1.76	0.50
7:G:150:ILE:HG22	7:G:196:LEU:HD21	1.94	0.50
16:P:264:THR:OG1	16:P:265:LEU:N	2.44	0.50
1:A:152:ARG:HB2	1:A:153:ARG:NH1	2.26	0.50
2:B:730:TYR:O	2:B:753:GLN:NE2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:800:ASN:ND2	2:B:851:SER:O	2.45	0.50
2:B:702:GLN:HB2	2:B:917:GLY:HA2	1.93	0.50
2:B:907:GLU:N	2:B:910:ASP:OD2	2.45	0.50
2:B:926:VAL:HG11	2:B:931:MET:HG3	1.94	0.50
15:O:303:ARG:NH1	15:O:468:LEU:HD13	2.26	0.50
16:P:120:VAL:HA	16:P:123:LYS:HG2	1.94	0.49
16:P:209:ALA:O	16:P:211:ASN:N	2.39	0.49
21:Y:68:GLN:NE2	21:Y:163:SER:OG	2.44	0.49
2:B:219:SER:HB3	2:B:230:LYS:HG2	1.94	0.49
7:G:29:GLN:O	7:G:33:LYS:HB2	2.12	0.49
14:N:381:ASP:HA	14:N:421:GLN:HG2	1.93	0.49
2:B:1040:ARG:O	22:Z:20:ASN:ND2	2.44	0.49
4:D:17:LEU:HD13	4:D:66:LEU:HD22	1.93	0.49
13:M:221:ASP:O	13:M:223:SER:N	2.45	0.49
16:P:226:THR:HA	16:P:229:GLN:HE22	1.77	0.49
1:A:549:PRO:HG3	1:A:679:TYR:HB2	1.93	0.49
1:A:967:LEU:HD21	1:A:1008:LEU:HD23	1.93	0.49
5:E:66:GLU:HA	5:E:69:ILE:HG22	1.95	0.49
11:K:91:TYR:HB2	11:K:101:LEU:HD11	1.94	0.49
15:O:497:ALA:HB2	15:O:505:MET:HG3	1.94	0.49
20:V:462:GLU:HG3	21:Y:107:ARG:HG2	1.94	0.49
21:Y:70:ILE:HG22	21:Y:160:ILE:HA	1.95	0.49
1:A:849:ARG:HG2	1:A:860:GLU:OE2	2.13	0.49
2:B:267:GLU:HA	2:B:270:GLN:HB3	1.93	0.49
1:A:736:HIS:NE2	1:A:740:GLU:OE2	2.44	0.49
1:A:921:LEU:HA	1:A:1082:ARG:HA	1.94	0.49
14:N:374:LYS:HE3	14:N:375:ILE:HG22	1.94	0.49
20:V:444:GLN:NE2	20:V:486:CYS:SG	2.80	0.49
2:B:1004:LEU:HD13	2:B:1017:ILE:HB	1.94	0.49
2:B:286:ASN:ND2	2:B:289:GLU:OE1	2.45	0.49
2:B:904:ARG:NH1	2:B:1033:ASP:OD2	2.26	0.49
1:A:1373:ARG:HH11	1:A:1391:LYS:HZ2	1.59	0.49
2:B:85:SER:OG	2:B:404:ASP:OD1	2.29	0.49
1:A:34:VAL:HA	1:A:51:ASN:HB3	1.95	0.49
1:A:529:ALA:HA	1:A:532:ILE:HG22	1.94	0.49
2:B:832:VAL:HB	12:L:60:ARG:HA	1.95	0.49
3:C:134:LEU:HD23	3:C:167:LEU:HB3	1.95	0.49
4:D:118:ALA:HA	4:D:121:LEU:HB2	1.95	0.49
5:E:161:LYS:HE2	5:E:195:VAL:HG23	1.95	0.49
15:O:488:LYS:NZ	15:O:651:PHE:HA	2.28	0.49
16:P:16:LYS:HZ2	16:P:48:LEU:CB	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:HIS:O	2:B:1126:LYS:NZ	2.33	0.48
1:A:229:ASN:HD22	15:O:544:ASN:HB2	1.78	0.48
1:A:389:ILE:HG12	1:A:695:ASN:HD21	1.78	0.48
1:A:649:ASP:OD2	1:A:663:VAL:HG13	2.12	0.48
1:A:758:GLU:HG3	1:A:759:GLU:HG2	1.95	0.48
15:O:68:LEU:HD12	15:O:74:LEU:HD23	1.95	0.48
20:V:328:THR:HA	20:V:331:GLU:HG2	1.95	0.48
1:A:365:ARG:NH1	1:A:887:ARG:HH12	2.10	0.48
1:A:544:PRO:HB3	1:A:924:LEU:HD12	1.95	0.48
2:B:997:ASN:HD22	2:B:1001:LYS:HB2	1.78	0.48
4:D:40:SER:O	4:D:44:GLY:N	2.41	0.48
21:Y:214:LEU:HD22	21:Y:223:ILE:HG12	1.95	0.48
2:B:723:THR:HB	2:B:790:LYS:HE3	1.96	0.48
21:Y:75:THR:HA	21:Y:120:LYS:HG2	1.95	0.48
2:B:140:ASN:HA	20:V:398:ASP:OD2	2.13	0.48
5:E:154:ILE:HB	5:E:197:LYS:HB3	1.96	0.48
6:F:101:ILE:HG21	6:F:120:ILE:HD11	1.95	0.48
7:G:133:ASP:HA	7:G:134:GLU:HA	1.54	0.48
8:H:35:GLN:HE21	8:H:111:LEU:HD21	1.78	0.48
11:K:80:ILE:HG22	11:K:86:VAL:HG11	1.94	0.48
20:V:411:TYR:OH	22:Z:147:SER:O	2.31	0.48
2:B:929:GLU:HB2	3:C:68:ARG:NH1	2.28	0.48
15:O:102:ARG:HH21	15:O:129:ILE:HD11	1.78	0.48
15:O:138:ASP:OD2	17:Q:54:LEU:HA	2.13	0.48
16:P:141:LYS:HG3	16:P:143:PRO:HD3	1.95	0.48
16:P:302:ALA:HB1	16:P:307:LYS:NZ	2.28	0.48
1:A:160:LEU:HB3	15:O:338:ASP:OD2	2.13	0.48
4:D:50:TYR:OH	7:G:20:ARG:NH1	2.46	0.48
8:H:97:MET:HB2	8:H:142:LEU:HB3	1.95	0.48
2:B:77:ILE:HG13	2:B:98:ILE:HD13	1.94	0.48
2:B:906:PRO:HB3	2:B:1026:LYS:HE3	1.95	0.48
7:G:91:LYS:NZ	7:G:98:LYS:NZ	2.61	0.48
11:K:80:ILE:HG12	11:K:120:GLY:HA3	1.95	0.48
19:S:5:DG:OP1	19:S:5:DG:H2'	2.14	0.48
19:S:48:DA:H2"	21:Y:213:VAL:HG21	1.96	0.48
2:B:109:LYS:NZ	2:B:128:PRO:HG3	2.28	0.48
2:B:640:PHE:HB3	2:B:645:LEU:HB2	1.95	0.48
2:B:738:THR:HG23	2:B:977:THR:HA	1.96	0.48
6:F:106:PRO:HG3	7:G:19:HIS:HB3	1.96	0.48
7:G:93:THR:OG1	7:G:96:GLY:O	2.30	0.48
1:A:332:VAL:HG22	1:A:334:PRO:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ASP:O	1:A:489:TYR:N	2.37	0.48
2:B:723:THR:HA	2:B:790:LYS:HG2	1.96	0.48
13:M:71:ILE:N	14:N:365:VAL:O	2.47	0.48
22:Z:440:ARG:HH11	22:Z:445:LEU:HD21	1.78	0.48
1:A:674:LYS:HD2	1:A:674:LYS:H	1.79	0.47
7:G:91:LYS:HZ2	7:G:98:LYS:HZ1	1.61	0.47
13:M:161:ALA:HB3	14:N:305:MET:HB3	1.94	0.47
21:Y:193:LEU:N	21:Y:206:ILE:O	2.47	0.47
21:Y:195:TYR:HB3	21:Y:204:LEU:HB2	1.96	0.47
1:A:145:LEU:HG	1:A:149:LYS:HE2	1.96	0.47
1:A:785:LEU:HD23	1:A:792:LEU:HB2	1.96	0.47
1:A:1152:ARG:HH22	1:A:1196:LEU:HD23	1.80	0.47
2:B:112:LEU:HB3	2:B:162:ILE:HD11	1.96	0.47
2:B:805:ILE:HG22	2:B:807:GLY:H	1.79	0.47
15:O:370:LEU:HD22	15:O:371:PRO:HD2	1.96	0.47
20:V:284:PHE:CA	22:Z:233:ARG:HH12	2.27	0.47
1:A:376:SER:H	2:B:1038:ARG:HB3	1.79	0.47
1:A:556:ASP:OD2	2:B:767:ILE:HD13	2.14	0.47
2:B:58:VAL:HG21	2:B:181:PRO:HB3	1.95	0.47
5:E:192:ARG:HH11	5:E:215:MET:C	2.18	0.47
13:M:158:GLN:HA	14:N:308:GLN:HA	1.95	0.47
13:M:247:TRP:HD1	14:N:408:LEU:HD22	1.78	0.47
1:A:521:VAL:O	2:B:1082:ARG:NH2	2.48	0.47
1:A:622:VAL:O	1:A:657:SER:OG	2.30	0.47
2:B:1010:GLY:O	3:C:227:TYR:OH	2.32	0.47
3:C:113:LEU:HA	3:C:129:GLU:HB2	1.95	0.47
19:S:44:DT:OP1	21:Y:97:LYS:HG2	2.15	0.47
1:A:378:ARG:NH1	19:S:21:DA:H2"	2.28	0.47
2:B:767:ILE:O	2:B:945:ASN:ND2	2.47	0.47
5:E:52:ARG:HD3	5:E:53:PRO:HD2	1.97	0.47
15:O:605:LYS:HA	15:O:608:ARG:HH11	1.78	0.47
1:A:476:ARG:HH12	1:A:515:ASP:CG	2.16	0.47
2:B:324:ILE:HA	2:B:327:ILE:HG22	1.96	0.47
2:B:774:ASN:HB3	2:B:777:SER:HB2	1.95	0.47
3:C:31:TRP:HH2	11:K:127:LEU:HD12	1.79	0.47
5:E:9:ILE:HB	5:E:42:PHE:HE2	1.79	0.47
8:H:14:GLU:HB2	8:H:27:GLU:OE2	2.15	0.47
8:H:64:ASN:ND2	8:H:67:ASP:O	2.47	0.47
11:K:50:LEU:HB2	11:K:62:SER:HB2	1.97	0.47
15:O:202:GLN:HB2	15:O:259:LEU:HD12	1.97	0.47
15:O:470:GLU:HB3	15:O:479:PRO:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:LYS:HE3	2:B:366:ILE:HD11	1.97	0.47
4:D:127:LEU:HB3	4:D:157:ILE:HD11	1.96	0.47
5:E:47:CYS:HA	5:E:53:PRO:HA	1.96	0.47
5:E:169:ARG:HG2	6:F:140:ASP:OD2	2.15	0.47
18:R:54:DC:H2"	18:R:55:DG:OP2	2.15	0.47
1:A:88:LEU:O	1:A:316:TRP:NE1	2.42	0.47
15:O:171:VAL:HB	15:O:276:PRO:HB3	1.96	0.47
20:V:331:GLU:HA	20:V:334:GLU:HG2	1.96	0.47
2:B:112:LEU:HD22	2:B:162:ILE:HG12	1.97	0.47
2:B:148:GLU:OE2	2:B:423:ASN:ND2	2.48	0.47
2:B:436:ALA:O	2:B:442:TRP:NE1	2.42	0.47
1:A:34:VAL:HB	1:A:38:ASP:OD2	2.15	0.46
1:A:525:GLU:OE1	1:A:528:ARG:NH2	2.48	0.46
1:A:714:ILE:O	1:A:718:THR:OG1	2.25	0.46
1:A:366:GLY:HA2	2:B:1061:ARG:HH12	1.81	0.46
2:B:262:ILE:HB	13:M:180:LYS:HE2	1.97	0.46
12:L:28:LYS:HD2	12:L:58:LYS:HZ1	1.79	0.46
16:P:296:TYR:HA	17:Q:43:ILE:HD13	1.96	0.46
1:A:396:ASP:HA	1:A:399:ALA:HB3	1.97	0.46
2:B:87:VAL:HG12	16:P:120:VAL:HG13	1.97	0.46
13:M:159:TYR:O	14:N:307:PHE:N	2.44	0.46
15:O:619:LEU:HB3	15:O:623:GLU:OE2	2.14	0.46
21:Y:202:ILE:HD11	21:Y:222:GLU:HB3	1.98	0.46
1:A:933:VAL:O	1:A:938:SER:OG	2.33	0.46
12:L:31:CYS:SG	12:L:36:SER:OG	2.72	0.46
21:Y:61:SER:OG	21:Y:62:GLY:N	2.49	0.46
1:A:430:ALA:HA	1:A:464:ARG:HA	1.98	0.46
1:A:588:GLU:OE2	1:A:696:ARG:NH1	2.49	0.46
1:A:1289:GLY:O	1:A:1291:ARG:NH1	2.49	0.46
2:B:55:LYS:HZ2	2:B:637:PHE:HE2	1.61	0.46
2:B:257:LEU:HD21	2:B:272:VAL:HG11	1.96	0.46
1:A:393:ALA:HB3	1:A:499:ARG:HB2	1.96	0.46
16:P:118:GLN:HG2	19:S:33:DA:H4'	1.97	0.46
1:A:445:ARG:HH12	22:Z:18:ASN:HD21	1.63	0.46
2:B:140:ASN:O	20:V:400:ASN:ND2	2.49	0.46
2:B:576:ARG:O	2:B:580:ARG:NE	2.43	0.46
2:B:790:LYS:HA	2:B:899:LEU:HA	1.96	0.46
5:E:24:LYS:HB2	5:E:30:ILE:HD11	1.97	0.46
16:P:245:GLU:OE2	16:P:255:LYS:HE2	2.15	0.46
19:S:41:DT:OP1	22:Z:120:ARG:NH1	2.49	0.46
1:A:624:ILE:HG21	1:A:681:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:613:ILE:HG13	2:B:675:ILE:HG12	1.97	0.46
3:C:100:ARG:NH2	3:C:192:LEU:O	2.48	0.46
1:A:372:ARG:HG2	2:B:1061:ARG:HB3	1.98	0.46
1:A:567:LYS:HA	1:A:607:LYS:NZ	2.29	0.46
8:H:64:ASN:HD21	8:H:68:THR:HB	1.81	0.46
14:N:278:ALA:O	14:N:282:LEU:HB2	2.16	0.46
1:A:381:ILE:HD11	1:A:517:MET:HB3	1.98	0.46
2:B:475:SER:OG	2:B:476:GLN:N	2.48	0.46
2:B:717:GLN:HE21	2:B:727:LEU:HD13	1.81	0.46
13:M:137:GLU:OE1	13:M:193:ARG:NH2	2.47	0.46
18:R:12:DT:H3	19:S:59:DA:H2	1.64	0.46
1:A:90:VAL:HG13	1:A:258:TRP:HB2	1.98	0.45
2:B:408:LYS:HE3	2:B:408:LYS:HB2	1.68	0.45
2:B:414:MET:HG3	2:B:417:ASP:HB3	1.98	0.45
3:C:255:VAL:HG11	3:C:273:ASP:OD2	2.16	0.45
13:M:210:GLN:HE22	16:P:102:ARG:NH1	2.11	0.45
1:A:966:ILE:HG12	1:A:1068:ARG:NH1	2.30	0.45
2:B:137:ARG:HH21	2:B:416:TYR:HE1	1.62	0.45
13:M:199:ARG:NH1	13:M:200:ARG:HH12	2.15	0.45
19:S:29:DG:OP2	19:S:29:DG:H4'	2.08	0.45
1:A:329:SER:OG	1:A:330:ASP:N	2.48	0.45
1:A:877:VAL:HG11	2:B:483:VAL:HB	1.97	0.45
1:A:1134:LYS:NZ	18:R:57:DG:OP1	2.45	0.45
2:B:654:GLU:HA	2:B:657:SER:HB3	1.98	0.45
12:L:47:ARG:HG2	12:L:54:ARG:NH1	2.31	0.45
12:L:49:LYS:HG3	12:L:50:ASP:H	1.80	0.45
1:A:495:TRP:HB2	1:A:499:ARG:HH22	1.81	0.45
1:A:1204:ASP:HA	1:A:1207:VAL:HG12	1.98	0.45
20:V:314:ARG:HH22	20:V:449:ARG:HH12	1.63	0.45
21:Y:85:VAL:HG21	21:Y:146:ILE:HA	1.98	0.45
1:A:1318:HIS:HB2	1:A:1322:VAL:HG23	1.99	0.45
2:B:948:GLY:HA2	2:B:952:ARG:NH1	2.32	0.45
3:C:199:GLY:HA3	10:J:67:GLU:HG3	1.99	0.45
13:M:174:GLU:HB2	13:M:175:ARG:NH1	2.31	0.45
15:O:254:ASN:HA	15:O:257:ASN:HD22	1.82	0.45
1:A:702:ALA:HB1	2:B:764:GLY:HA3	1.99	0.45
1:A:836:PRO:O	1:A:839:SER:OG	2.33	0.45
2:B:114:PRO:HA	2:B:115:PRO:HD3	1.85	0.45
2:B:1038:ARG:HH22	2:B:1041:GLY:H	1.63	0.45
1:A:1144:VAL:HG23	1:A:1292:GLU:OE2	2.17	0.45
1:A:1373:ARG:NH1	1:A:1391:LYS:NZ	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:882:ASP:OD2	2:B:901:ARG:HG2	2.17	0.45
2:B:902:GLN:HE21	2:B:904:ARG:HE	1.64	0.45
14:N:293:LYS:HZ1	14:N:303:ARG:NH1	2.14	0.45
22:Z:241:HIS:HE1	22:Z:255:LEU:HD22	1.82	0.45
1:A:191:ALA:HB1	1:A:195:ASP:OD2	2.16	0.45
1:A:524:THR:HG23	1:A:526:GLU:H	1.82	0.45
2:B:1036:HIS:HE1	2:B:1058:GLY:HA3	1.81	0.45
7:G:175:GLU:O	7:G:182:ASN:ND2	2.41	0.45
15:O:86:MET:HG2	15:O:90:SER:HB2	1.98	0.45
16:P:136:SER:HB3	16:P:148:TYR:HD1	1.81	0.45
22:Z:220:PRO:HA	22:Z:223:ILE:HG22	1.97	0.45
1:A:520:HIS:HB3	2:B:1082:ARG:HH12	1.82	0.45
14:N:375:ILE:HG13	14:N:377:ASN:H	1.82	0.45
1:A:208:ASN:HA	1:A:211:LEU:HB2	1.98	0.45
3:C:163:TYR:HD2	3:C:165:ARG:NH1	2.14	0.45
3:C:239:ILE:HG22	3:C:288:LYS:HD3	1.99	0.45
15:O:110:THR:HB	15:O:116:LYS:HD3	1.98	0.45
16:P:182:VAL:HG11	16:P:241:ARG:HH12	1.82	0.45
22:Z:96:ILE:HD13	22:Z:130:LEU:HD21	1.99	0.45
22:Z:132:VAL:HB	22:Z:161:PHE:HE1	1.81	0.45
1:A:735:TYR:HE2	1:A:849:ARG:NH1	2.14	0.44
1:A:976:ARG:HB2	1:A:984:VAL:HG11	1.98	0.44
2:B:298:GLN:NE2	13:M:187:ASP:O	2.50	0.44
2:B:1005:TYR:HH	3:C:293:ARG:HH21	1.62	0.44
16:P:252:LYS:HE3	16:P:266:GLU:OE2	2.18	0.44
1:A:1157:VAL:HG22	1:A:1160:ARG:NH1	2.28	0.44
2:B:300:GLN:HA	2:B:303:GLU:HB2	2.00	0.44
2:B:918:GLN:HB3	2:B:957:LYS:NZ	2.32	0.44
3:C:126:PHE:HA	3:C:130:ASN:HD22	1.81	0.44
7:G:79:PRO:HD2	7:G:153:GLU:OE2	2.16	0.44
15:O:596:LYS:HD3	17:Q:66:LYS:HZ1	1.82	0.44
16:P:308:GLU:HB2	17:Q:42:PRO:HD2	1.99	0.44
2:B:184:TYR:HB3	2:B:193:VAL:HG22	1.99	0.44
10:J:59:LYS:HZ1	10:J:62:ARG:HH21	1.65	0.44
1:A:389:ILE:HG23	1:A:501:ASN:HD22	1.82	0.44
2:B:330:THR:HG22	2:B:338:GLU:HG3	1.99	0.44
2:B:585:SER:HB2	2:B:588:ILE:HD12	1.99	0.44
2:B:1088:ASP:OD1	2:B:1088:ASP:N	2.51	0.44
1:A:825:ASP:OD1	1:A:845:LYS:NZ	2.50	0.44
1:A:1164:THR:H	1:A:1271:VAL:HG23	1.83	0.44
1:A:1186:VAL:HB	1:A:1230:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:46:LYS:NZ	11:K:68:GLU:HG3	2.32	0.44
22:Z:237:LEU:CD2	22:Z:239:ARG:HH12	2.30	0.44
2:B:741:ILE:HA	2:B:744:ILE:HG12	1.99	0.44
2:B:887:SER:HB2	12:L:55:ILE:HG22	2.00	0.44
5:E:11:ARG:HG2	5:E:137:GLU:OE2	2.18	0.44
5:E:89:GLY:O	5:E:93:MET:N	2.46	0.44
15:O:528:MET:SD	15:O:528:MET:N	2.81	0.44
16:P:298:LYS:HD2	16:P:308:GLU:OE2	2.17	0.44
1:A:593:PRO:HD3	1:A:612:LEU:HD21	1.99	0.44
1:A:1173:VAL:HB	1:A:1264:ARG:NH1	2.32	0.44
1:A:1408:VAL:HG21	1:A:1417:LEU:HD12	1.99	0.44
2:B:788:ARG:HG2	2:B:901:ARG:HB3	1.99	0.44
2:B:1128:LEU:O	2:B:1132:LEU:CB	2.62	0.44
3:C:70:ILE:HG23	3:C:74:GLU:HB2	1.99	0.44
2:B:734:PRO:CB	2:B:915:ARG:HH12	2.28	0.44
2:B:849:THR:HB	2:B:867:ARG:NH1	2.33	0.44
3:C:230:LEU:HD12	3:C:299:ILE:HD11	2.00	0.44
20:V:455:LYS:HA	20:V:458:PHE:HD2	1.83	0.44
2:B:247:ILE:HG12	2:B:251:ILE:HD11	1.99	0.44
2:B:1132:LEU:HD13	2:B:1137:ILE:HG21	1.99	0.44
3:C:83:VAL:HA	3:C:206:ALA:HA	2.00	0.44
3:C:275:VAL:HG23	3:C:293:ARG:HH11	1.83	0.44
5:E:124:VAL:HG23	5:E:132:ILE:HG13	2.00	0.44
1:A:481:HIS:CE1	1:A:483:LEU:HB2	2.53	0.43
1:A:982:CYS:SG	1:A:983:LEU:N	2.91	0.43
2:B:539:GLU:HG3	2:B:544:ILE:HD13	1.99	0.43
7:G:39:ILE:HB	7:G:42:VAL:HB	2.00	0.43
15:O:212:GLU:HG3	15:O:333:THR:HA	2.00	0.43
1:A:538:LYS:HB3	1:A:687:PRO:HB2	2.00	0.43
2:B:302:LEU:HB3	2:B:325:GLU:HG3	1.99	0.43
5:E:153:HIS:CD2	5:E:198:ILE:HG12	2.53	0.43
18:R:29:DA:H2	21:Y:98:ARG:HD3	1.83	0.43
21:Y:114:LEU:HB3	21:Y:115:ILE:H	1.61	0.43
1:A:106:ILE:HG12	1:A:113:ILE:HG13	2.00	0.43
2:B:837:GLN:H	2:B:840:GLN:NE2	2.17	0.43
13:M:216:VAL:O	16:P:96:TYR:OH	2.35	0.43
15:O:639:ALA:O	15:O:643:ARG:NH1	2.51	0.43
16:P:61:ILE:HB	16:P:68:ASP:HB2	2.00	0.43
16:P:203:LYS:HB2	16:P:206:VAL:HG22	1.99	0.43
17:Q:89:LYS:O	17:Q:93:ASN:ND2	2.51	0.43
19:S:44:DT:H2"	19:S:45:DT:H5'	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:GLY:HA3	2:B:1001:LYS:HE3	1.99	0.43
2:B:166:ALA:HB1	2:B:170:LYS:HB3	1.99	0.43
2:B:258:LYS:HE3	2:B:296:TYR:HA	1.99	0.43
2:B:1009:THR:HA	11:K:74:ASN:HD22	1.83	0.43
14:N:386:ALA:HB2	14:N:417:VAL:HG22	2.00	0.43
1:A:99:THR:HA	1:A:102:ILE:HG22	2.00	0.43
2:B:77:ILE:HG13	2:B:98:ILE:HG21	1.99	0.43
2:B:969:LEU:HA	10:J:47:ARG:HH12	1.83	0.43
1:A:318:TYR:HH	19:S:29:DG:P	2.39	0.43
2:B:1098:CYS:HB2	2:B:1140:ARG:HH12	1.84	0.43
15:O:199:TYR:OH	15:O:286:ARG:NH1	2.44	0.43
1:A:523:GLN:HB2	2:B:1081:GLU:OE2	2.18	0.43
1:A:789:ASN:HD22	1:A:791:PRO:HD2	1.83	0.43
15:O:43:ASN:HB3	15:O:46:LEU:HG	2.00	0.43
1:A:723:LEU:HD11	1:A:811:ALA:HA	2.00	0.43
2:B:804:ASP:OD1	2:B:804:ASP:N	2.52	0.43
3:C:55:ASP:OD2	3:C:271:ARG:NE	2.52	0.43
3:C:324:LYS:HZ3	11:K:71:THR:HG1	1.55	0.43
5:E:156:LEU:HD11	5:E:195:VAL:HB	1.99	0.43
16:P:137:VAL:HB	16:P:153:LEU:HA	2.01	0.43
18:R:66:DC:OP2	18:R:66:DC:H2'	2.19	0.43
1:A:121:ARG:HD2	15:O:73:ARG:NH1	2.34	0.43
2:B:74:LYS:NZ	2:B:78:LYS:NZ	2.67	0.43
2:B:234:ILE:HA	2:B:240:ILE:HA	2.00	0.43
2:B:769:ASP:OD2	2:B:952:ARG:NH2	2.52	0.42
15:O:73:ARG:HD3	15:O:121:TYR:CE1	2.54	0.42
20:V:332:GLN:HA	20:V:335:GLU:HG2	2.01	0.42
1:A:268:ILE:HD11	2:B:1131:GLU:HB3	2.00	0.42
1:A:527:ALA:HA	1:A:530:GLU:HB3	2.01	0.42
2:B:152:MET:HG3	2:B:433:LEU:HD21	2.01	0.42
2:B:534:TYR:HA	2:B:538:VAL:HG22	2.00	0.42
3:C:165:ARG:NH2	3:C:190:ASP:OD1	2.46	0.42
15:O:124:GLU:HG2	15:O:128:HIS:CD2	2.54	0.42
1:A:433:LEU:HD13	1:A:452:LEU:HD21	2.01	0.42
2:B:525:GLU:HG2	2:B:527:GLU:H	1.84	0.42
3:C:216:HIS:CE1	12:L:70:ARG:HA	2.54	0.42
7:G:29:GLN:O	7:G:33:LYS:CB	2.67	0.42
12:L:50:ASP:HB2	22:Z:194:LYS:HZ2	1.84	0.42
18:R:21:DT:H4'	22:Z:155:TYR:HB3	2.01	0.42
20:V:451:ARG:HH11	21:Y:97:LYS:HZ1	1.67	0.42
21:Y:143:ILE:HA	21:Y:146:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:VAL:HG21	2:B:487:ARG:HB3	2.01	0.42
15:O:47:PHE:O	15:O:51:GLU:CB	2.66	0.42
1:A:391:GLU:HG2	1:A:489:TYR:HB2	2.01	0.42
1:A:1139:PRO:HA	1:A:1317:ASN:HD22	1.85	0.42
2:B:239:LYS:HB3	2:B:241:TYR:CE2	2.55	0.42
2:B:778:ILE:HD11	2:B:906:PRO:HG2	2.01	0.42
5:E:161:LYS:NZ	5:E:194:GLU:HA	2.34	0.42
8:H:80:ARG:HD2	8:H:81:PRO:HD2	2.00	0.42
15:O:291:ARG:HG2	15:O:649:GLU:OE2	2.19	0.42
1:A:397:ARG:HG2	1:A:496:ARG:HH12	1.85	0.42
2:B:555:VAL:HG13	2:B:562:ILE:HB	2.01	0.42
10:J:21:TYR:OH	10:J:32:GLU:OE2	2.38	0.42
15:O:143:GLN:HG3	15:O:294:LYS:NZ	2.35	0.42
16:P:296:TYR:CG	17:Q:41:LEU:HD22	2.54	0.42
21:Y:82:LEU:HD13	21:Y:146:ILE:HD11	2.02	0.42
1:A:150:LYS:NZ	19:S:7:DG:OP2	2.39	0.42
1:A:372:ARG:HA	2:B:1061:ARG:HA	2.02	0.42
2:B:610:ARG:HE	2:B:612:LEU:HD23	1.83	0.42
2:B:773:LEU:HD13	2:B:778:ILE:HD12	2.00	0.42
15:O:314:ILE:HG23	15:O:317:ARG:NH1	2.34	0.42
22:Z:96:ILE:HD12	22:Z:100:ILE:HG23	2.02	0.42
2:B:806:ILE:H	2:B:806:ILE:HG13	1.71	0.42
2:B:884:VAL:HG23	2:B:898:VAL:HB	2.02	0.42
17:Q:78:ILE:HG23	17:Q:91:LYS:HB3	2.02	0.42
1:A:1125:ARG:NH1	1:A:1136:ILE:HD11	2.34	0.42
2:B:57:LEU:HD22	2:B:467:LEU:HD11	2.02	0.42
2:B:918:GLN:HB3	2:B:957:LYS:HZ1	1.84	0.42
3:C:127:THR:H	3:C:130:ASN:HD22	1.68	0.42
15:O:47:PHE:HD2	15:O:586:ALA:HB1	1.85	0.42
1:A:122:GLN:NE2	1:A:126:GLU:OE1	2.47	0.42
1:A:624:ILE:HG22	1:A:684:ASP:OD2	2.20	0.42
2:B:306:GLY:HA3	2:B:325:GLU:OE2	2.20	0.42
2:B:1061:ARG:HD2	19:S:21:DA:H5'	2.01	0.42
11:K:60:SER:HB3	11:K:104:ARG:HH21	1.85	0.42
1:A:113:ILE:HB	1:A:238:ASP:OD2	2.20	0.41
1:A:1383:VAL:HA	1:A:1386:LEU:HB2	2.00	0.41
2:B:128:PRO:HB3	2:B:151:ARG:HD2	2.02	0.41
6:F:104:ASN:HB3	7:G:16:ASP:HB3	2.02	0.41
7:G:14:PRO:HA	7:G:15:PRO:HD3	1.92	0.41
22:Z:261:GLU:OE2	22:Z:288:PRO:HG3	2.20	0.41
1:A:1145:LEU:HG	1:A:1309:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:ILE:HA	2:B:455:THR:HG22	2.01	0.41
2:B:409:LYS:HD3	2:B:409:LYS:HA	1.68	0.41
2:B:526:GLU:HB2	2:B:557:LEU:HD21	2.01	0.41
2:B:580:ARG:NH1	2:B:614:ILE:HG21	2.35	0.41
2:B:829:LEU:HD11	2:B:896:ILE:HG21	2.01	0.41
9:I:9:ASN:HB3	13:M:181:PRO:HG2	2.01	0.41
13:M:254:GLN:HB2	14:N:407:GLU:HG2	2.01	0.41
14:N:293:LYS:HA	14:N:296:LYS:NZ	2.34	0.41
21:Y:112:THR:HA	21:Y:139:TYR:HE1	1.84	0.41
1:A:431:ASN:HD22	1:A:445:ARG:HH11	1.68	0.41
1:A:985:LYS:HG3	1:A:988:ASP:H	1.85	0.41
1:A:1099:GLU:O	1:A:1101:GLY:N	2.52	0.41
1:A:1255:ASP:HB3	1:A:1256:VAL:H	1.71	0.41
2:B:55:LYS:NZ	2:B:638:ASP:OD1	2.52	0.41
16:P:171:ASP:HA	16:P:172:ILE:HA	1.70	0.41
21:Y:138:LYS:HZ3	22:Z:465:VAL:HB	1.85	0.41
1:A:232:LYS:HG3	1:A:254:GLU:OE2	2.19	0.41
1:A:476:ARG:HH11	1:A:517:MET:CE	2.33	0.41
2:B:628:ARG:HH21	2:B:631:LEU:HD12	1.85	0.41
16:P:93:VAL:HA	16:P:96:TYR:HD2	1.84	0.41
1:A:578:GLN:HE22	11:K:91:TYR:H	1.67	0.41
2:B:186:ILE:HG13	2:B:191:GLU:HB3	2.01	0.41
4:D:59:THR:HA	4:D:62:VAL:HG12	2.01	0.41
1:A:204:VAL:HB	1:A:208:ASN:HD22	1.86	0.41
7:G:11:VAL:HG13	7:G:29:GLN:HG2	2.02	0.41
15:O:173:ASP:OD2	17:Q:73:GLY:HA2	2.21	0.41
16:P:196:LYS:HD3	16:P:268:ILE:HG13	2.03	0.41
18:R:20:DC:H6	18:R:20:DC:H2'	1.71	0.41
2:B:658:TYR:HD2	2:B:670:MET:HG2	1.85	0.41
2:B:739:LYS:H	2:B:977:THR:HB	1.85	0.41
2:B:1096:ASP:O	2:B:1142:ARG:NH2	2.54	0.41
15:O:40:ARG:HA	15:O:583:TRP:HZ2	1.85	0.41
16:P:255:LYS:HE3	16:P:255:LYS:HB3	1.93	0.41
22:Z:76:ARG:HD2	22:Z:112:LEU:HD21	2.03	0.41
22:Z:215:PHE:HZ	22:Z:220:PRO:HG3	1.86	0.41
2:B:328:ALA:HA	2:B:332:ILE:HG12	2.02	0.41
5:E:13:TRP:HE1	5:E:37:LEU:HG	1.85	0.41
10:J:1:MET:HB3	10:J:2:ILE:HD12	2.03	0.41
18:R:13:DT:H3	19:S:58:DA:H2	1.69	0.41
1:A:666:LYS:HE3	1:A:671:ASP:HB3	2.02	0.41
1:A:1123:VAL:HA	1:A:1126:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1:MET:HB2	3:C:14:ASN:HD21	1.86	0.41
3:C:229:LEU:O	3:C:293:ARG:NH2	2.54	0.41
8:H:98:TYR:OH	8:H:138:GLU:O	2.36	0.41
21:Y:97:LYS:HB3	21:Y:98:ARG:H	1.78	0.41
21:Y:159:ASN:HD21	21:Y:216:GLY:H	1.68	0.41
22:Z:179:SER:OG	22:Z:207:GLN:NE2	2.54	0.41
1:A:472:VAL:HG12	1:A:521:VAL:HG12	2.03	0.41
1:A:636:PRO:HG3	1:A:643:ASN:HA	2.03	0.41
1:A:1430:VAL:HG13	7:G:59:LEU:HD23	2.03	0.41
2:B:44:LYS:HD2	2:B:663:GLU:OE2	2.21	0.41
2:B:135:TYR:HE2	2:B:145:LYS:HB3	1.86	0.41
2:B:344:GLU:OE2	2:B:541:ILE:HB	2.21	0.41
2:B:1042:PRO:HD2	2:B:1057:ASP:OD2	2.20	0.41
15:O:57:LEU:HB3	15:O:61:ALA:HB3	2.03	0.41
1:A:393:ALA:HA	1:A:491:LYS:HB3	2.03	0.40
1:A:976:ARG:NH1	1:A:1002:ARG:HH22	2.19	0.40
1:A:1387:ALA:HA	1:A:1395:HIS:HD1	1.86	0.40
12:L:44:ASP:OD2	12:L:46:VAL:HA	2.21	0.40
15:O:71:LEU:HB2	15:O:74:LEU:HD21	2.03	0.40
22:Z:165:VAL:HA	22:Z:168:LEU:HD23	2.02	0.40
1:A:830:ARG:NH2	2:B:657:SER:O	2.55	0.40
2:B:1005:TYR:HH	3:C:293:ARG:NH2	2.16	0.40
16:P:199:GLU:HA	16:P:202:PRO:HG3	2.03	0.40
18:R:15:DG:H2"	18:R:16:DG:C8	2.56	0.40
19:S:51:DG:H2"	19:S:52:DT:C5	2.55	0.40
4:D:110:LEU:HB3	4:D:120:LYS:NZ	2.36	0.40
7:G:91:LYS:HZ3	7:G:98:LYS:NZ	2.16	0.40
1:A:848:VAL:HG23	1:A:860:GLU:HB3	2.04	0.40
1:A:881:GLU:OE2	1:A:1127:LYS:HD3	2.21	0.40
15:O:488:LYS:HZ2	15:O:651:PHE:HA	1.85	0.40
16:P:103:GLU:HA	16:P:155:PRO:HG3	2.03	0.40
18:R:23:DT:H6	18:R:23:DT:H2'	1.67	0.40
1:A:153:ARG:HG3	15:O:338:ASP:H	1.85	0.40
1:A:834:HIS:ND1	2:B:659:ILE:O	2.55	0.40
1:A:998:TYR:O	1:A:1002:ARG:NE	2.45	0.40
16:P:299:MET:HB2	16:P:302:ALA:H	1.86	0.40
20:V:421:THR:HG22	20:V:423:GLU:H	1.85	0.40
22:Z:124:ASN:HD21	22:Z:157:ILE:HA	1.86	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	1413/1460 (97%)	1199 (85%)	211 (15%)	3 (0%)	47 79
2	B	1110/1149 (97%)	918 (83%)	191 (17%)	1 (0%)	51 84
3	C	333/335 (99%)	282 (85%)	51 (15%)	0	100 100
4	D	136/161 (84%)	105 (77%)	26 (19%)	5 (4%)	3 28
5	E	213/215 (99%)	195 (92%)	17 (8%)	1 (0%)	29 67
6	F	81/155 (52%)	74 (91%)	7 (9%)	0	100 100
7	G	210/212 (99%)	164 (78%)	45 (21%)	1 (0%)	29 67
8	H	144/146 (99%)	128 (89%)	16 (11%)	0	100 100
9	I	39/110 (36%)	32 (82%)	7 (18%)	0	100 100
10	J	65/70 (93%)	56 (86%)	9 (14%)	0	100 100
11	K	100/142 (70%)	90 (90%)	10 (10%)	0	100 100
12	L	43/70 (61%)	32 (74%)	11 (26%)	0	100 100
13	M	195/282 (69%)	148 (76%)	45 (23%)	2 (1%)	15 53
14	N	101/422 (24%)	81 (80%)	20 (20%)	0	100 100
15	O	546/654 (84%)	481 (88%)	65 (12%)	0	100 100
16	P	294/317 (93%)	213 (72%)	74 (25%)	7 (2%)	6 36
17	Q	86/251 (34%)	69 (80%)	17 (20%)	0	100 100
20	V	265/594 (45%)	230 (87%)	35 (13%)	0	100 100
21	Y	178/240 (74%)	163 (92%)	15 (8%)	0	100 100
22	Z	333/596 (56%)	300 (90%)	33 (10%)	0	100 100
All	All	5885/7581 (78%)	4960 (84%)	905 (15%)	20 (0%)	44 75

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	14	TYR

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Mol	Chain	Res	Type
1	A	35	SER
1	A	496	ARG
2	B	586	GLU
4	D	13	ASP
16	P	210	PRO
16	P	313	ASP
1	A	566	HIS
7	G	123	PRO
13	M	131	TYR
16	P	211	ASN
5	E	38	PRO
13	M	222	PRO
16	P	214	ASN
16	P	300	PHE
4	D	50	TYR
4	D	53	PRO
16	P	212	VAL
16	P	209	ALA
4	D	49	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1228/1257 (98%)	1204 (98%)	24 (2%)	55 73
2	B	973/1006 (97%)	948 (97%)	25 (3%)	46 67
3	C	296/296 (100%)	292 (99%)	4 (1%)	67 81
4	D	126/145 (87%)	120 (95%)	6 (5%)	25 53
5	E	197/197 (100%)	194 (98%)	3 (2%)	65 80
6	F	73/137 (53%)	71 (97%)	2 (3%)	44 66
7	G	185/190 (97%)	184 (100%)	1 (0%)	88 93
8	H	128/128 (100%)	123 (96%)	5 (4%)	32 58
9	I	37/98 (38%)	37 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	J	62/65 (95%)	62 (100%)	0	100 100
11	K	92/130 (71%)	90 (98%)	2 (2%)	52 71
12	L	40/57 (70%)	40 (100%)	0	100 100
13	M	172/249 (69%)	167 (97%)	5 (3%)	42 65
14	N	88/360 (24%)	85 (97%)	3 (3%)	37 61
15	O	505/593 (85%)	498 (99%)	7 (1%)	67 81
16	P	257/285 (90%)	255 (99%)	2 (1%)	81 89
17	Q	56/212 (26%)	55 (98%)	1 (2%)	59 77
20	V	151/534 (28%)	145 (96%)	6 (4%)	31 57
21	Y	152/205 (74%)	151 (99%)	1 (1%)	84 90
22	Z	297/513 (58%)	288 (97%)	9 (3%)	41 64
All	All	5115/6657 (77%)	5009 (98%)	106 (2%)	56 72

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	46	ARG
1	A	108	LYS
1	A	109	ASN
1	A	153	ARG
1	A	184	ARG
1	A	281	ASN
1	A	328	ASN
1	A	333	ASN
1	A	351	ARG
1	A	464	ARG
1	A	482	ARG
1	A	637	LYS
1	A	664	MET
1	A	674	LYS
1	A	789	ASN
1	A	964	ASN
1	A	973	ARG
1	A	1002	ARG
1	A	1024	LYS
1	A	1037	LYS
1	A	1118	ASN

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Mol	Chain	Res	Type
1	A	1313	ARG
1	A	1453	ASN
2	B	99	ARG
2	B	286	ASN
2	B	343	ARG
2	B	354	ARG
2	B	362	ASN
2	B	365	MET
2	B	397	ASN
2	B	408	LYS
2	B	409	LYS
2	B	411	ASN
2	B	428	ASN
2	B	449	MET
2	B	512	LYS
2	B	607	ARG
2	B	610	ARG
2	B	664	LYS
2	B	774	ASN
2	B	797	ARG
2	B	859	ASN
2	B	861	ASN
2	B	901	ARG
2	B	970	ASN
2	B	1003	MET
2	B	1028	LYS
2	B	1061	ARG
3	C	11	ARG
3	C	68	ARG
3	C	174	ARG
3	C	240	LYS
4	D	1	MET
4	D	2	LYS
4	D	61	ASN
4	D	69	ASN
4	D	97	LYS
4	D	117	LYS
5	E	5	ASN
5	E	17	ARG
5	E	56	LYS
6	F	76	LYS
6	F	104	ASN

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Mol	Chain	Res	Type
7	G	98	LYS
8	H	55	LEU
8	H	87	ARG
8	H	124	ARG
8	H	133	ASN
8	H	146	ARG
11	K	44	ARG
11	K	140	LYS
13	M	92	ASN
13	M	155	ASN
13	M	175	ARG
13	M	184	LYS
13	M	214	MET
14	N	297	MET
14	N	364	ARG
14	N	384	LYS
15	O	50	LYS
15	O	194	LEU
15	O	268	LYS
15	O	294	LYS
15	O	469	ASN
15	O	528	MET
15	O	631	ASN
16	P	23	MET
16	P	298	LYS
17	Q	50	LYS
20	V	314	ARG
20	V	343	ARG
20	V	391	ASN
20	V	440	ASN
20	V	460	ASN
20	V	464	LYS
21	Y	159	ASN
22	Z	20	ASN
22	Z	82	ASN
22	Z	84	ARG
22	Z	124	ASN
22	Z	188	LYS
22	Z	260	ASN
22	Z	286	ARG
22	Z	294	ARG
22	Z	298	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	109	ASN
1	A	134	ASN
1	A	161	ASN
1	A	229	ASN
1	A	328	ASN
1	A	333	ASN
1	A	355	GLN
1	A	625	ASN
1	A	630	ASN
1	A	789	ASN
1	A	843	GLN
1	A	964	ASN
1	A	1118	ASN
1	A	1180	ASN
1	A	1185	GLN
1	A	1284	ASN
1	A	1317	ASN
1	A	1345	ASN
1	A	1346	HIS
1	A	1354	HIS
1	A	1453	ASN
2	B	80	ASN
2	B	144	HIS
2	B	199	GLN
2	B	270	GLN
2	B	286	ASN
2	B	362	ASN
2	B	382	GLN
2	B	397	ASN
2	B	411	ASN
2	B	428	ASN
2	B	519	HIS
2	B	574	GLN
2	B	655	ASN
2	B	672	HIS
2	B	694	ASN
2	B	708	GLN
2	B	717	GLN
2	B	774	ASN
2	B	840	GLN

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Mol	Chain	Res	Type
2	B	859	ASN
2	B	861	ASN
2	B	865	GLN
2	B	902	GLN
2	B	903	ASN
2	B	970	ASN
2	B	1036	HIS
3	C	3	ASN
3	C	130	ASN
3	C	216	HIS
4	D	8	ASN
4	D	61	ASN
4	D	69	ASN
4	D	71	ASN
4	D	122	GLN
4	D	126	GLN
5	E	5	ASN
5	E	153	HIS
6	F	104	ASN
7	G	17	GLN
7	G	28	HIS
7	G	32	ASN
7	G	173	GLN
8	H	11	GLN
8	H	35	GLN
8	H	133	ASN
11	K	95	HIS
11	K	106	GLN
13	M	92	ASN
13	M	132	ASN
13	M	155	ASN
13	M	167	GLN
13	M	210	GLN
15	O	128	HIS
15	O	152	HIS
15	O	257	ASN
15	O	295	GLN
15	O	469	ASN
15	O	544	ASN
15	O	631	ASN
16	P	19	HIS
16	P	117	HIS

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Mol	Chain	Res	Type
16	P	118	GLN
16	P	119	HIS
16	P	229	GLN
17	Q	93	ASN
20	V	391	ASN
20	V	400	ASN
20	V	440	ASN
20	V	444	GLN
20	V	460	ASN
21	Y	68	GLN
21	Y	159	ASN
22	Z	82	ASN
22	Z	118	GLN
22	Z	124	ASN
22	Z	183	GLN
22	Z	207	GLN
22	Z	241	HIS
22	Z	249	HIS
22	Z	293	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

Of 8 ligands modelled in this entry, 8 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.

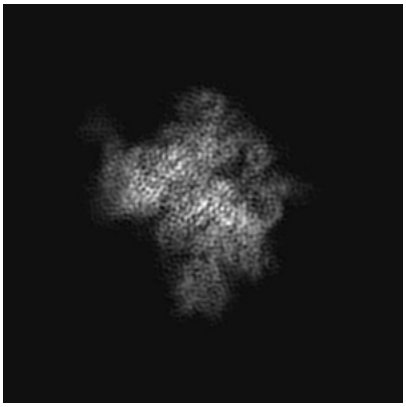
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3955. These allow visual inspection of the internal detail of the map and identification of artifacts.

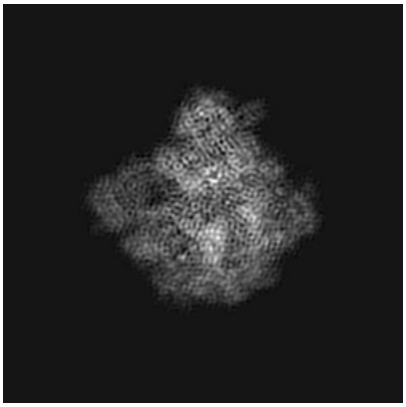
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

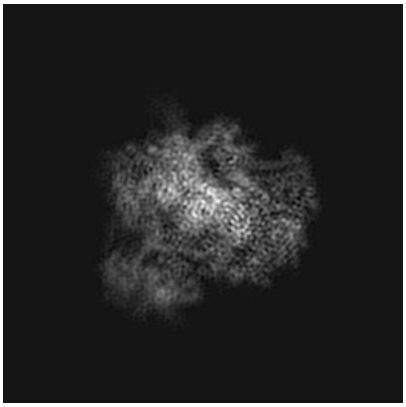
6.1.1 Primary map



X



Y

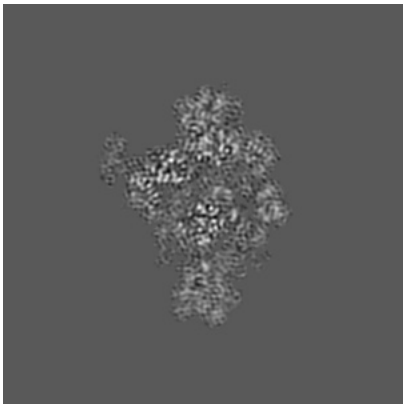


Z

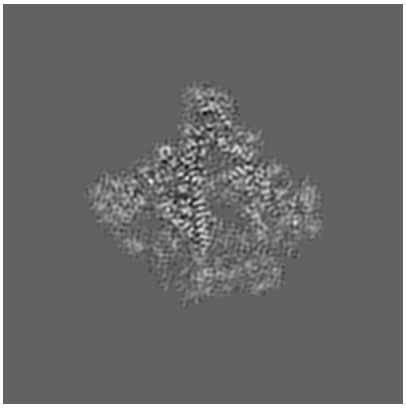
The images above show the map projected in three orthogonal directions.

6.2 Central slices

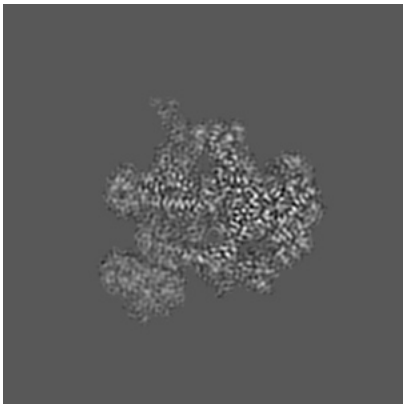
6.2.1 Primary map



X Index: 155



Y Index: 155

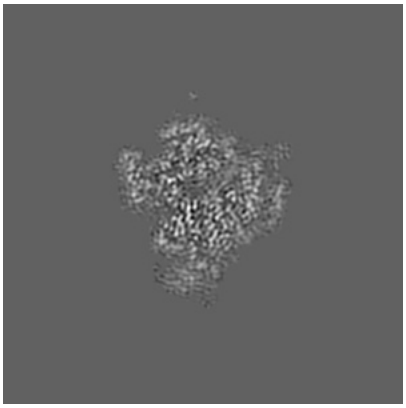


Z Index: 155

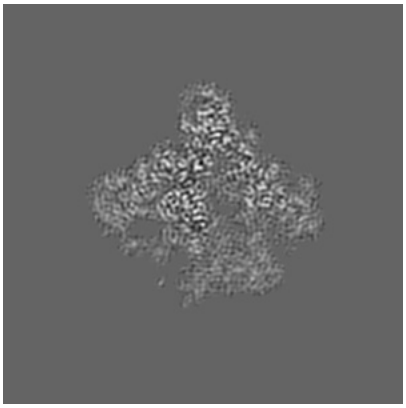
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

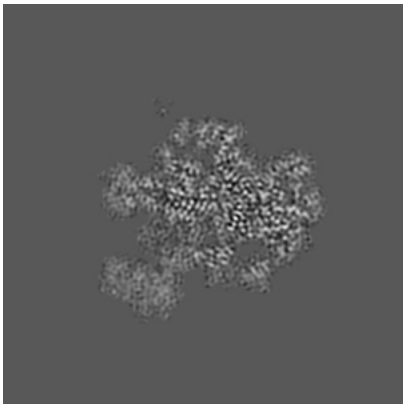
6.3.1 Primary map



X Index: 180



Y Index: 152

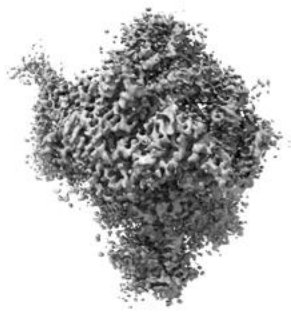


Z Index: 151

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

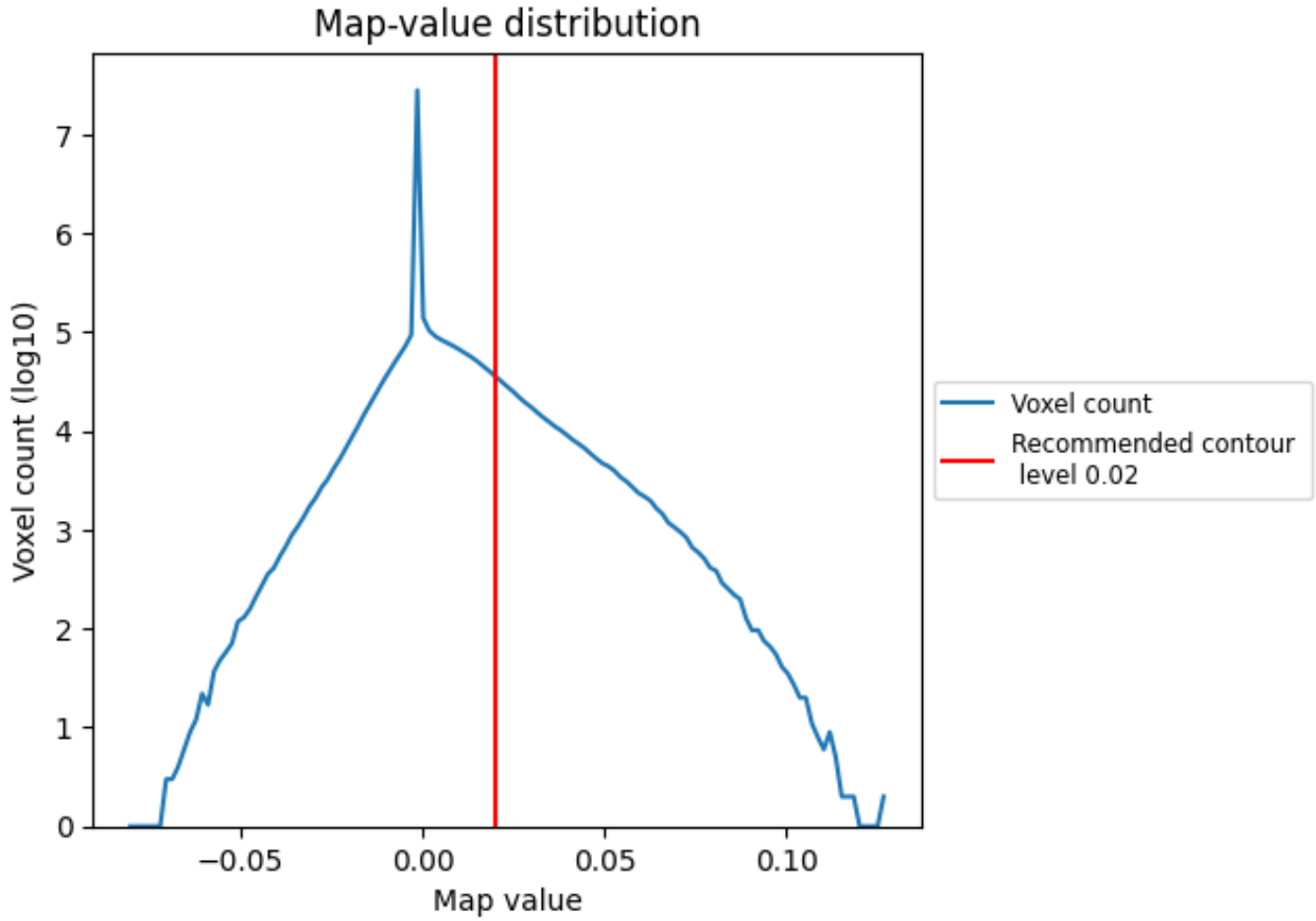
6.5 Mask visualisation (i)

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

7 Map analysis

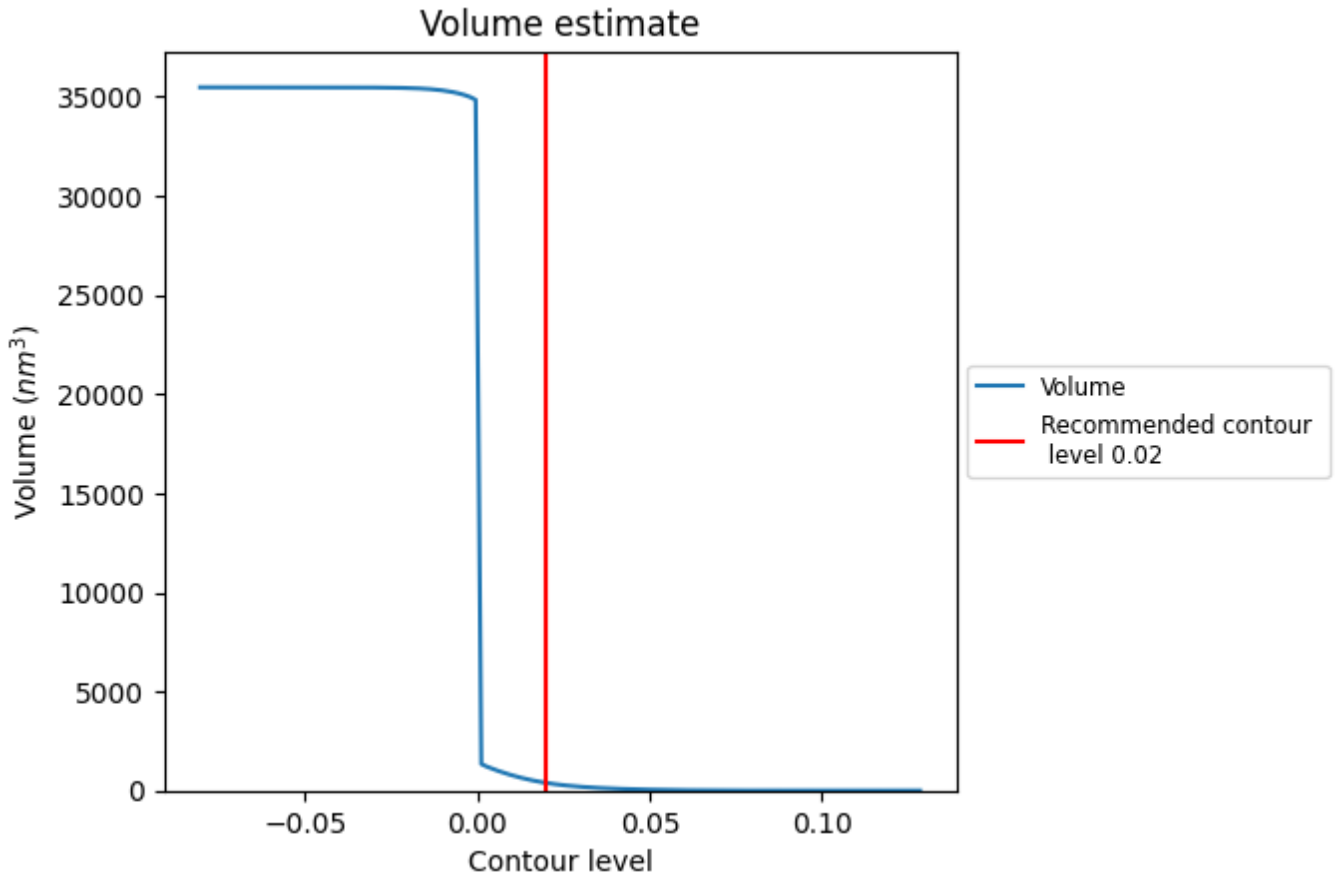
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

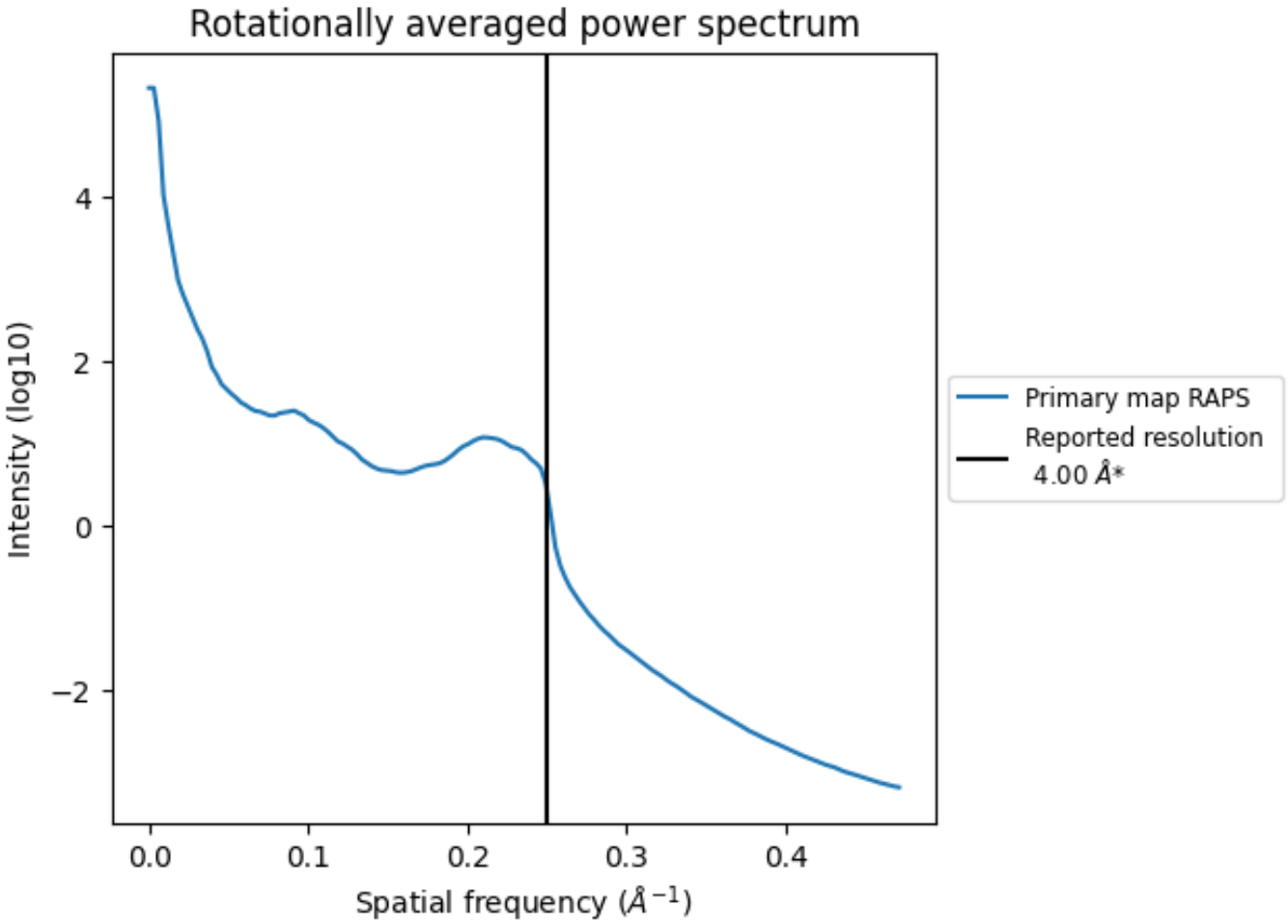
7.2 Volume estimate (i)



The volume at the recommended contour level is 387 nm^3; this corresponds to an approximate mass of 350 kDa.

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

7.3 Rotationally averaged power spectrum (i)

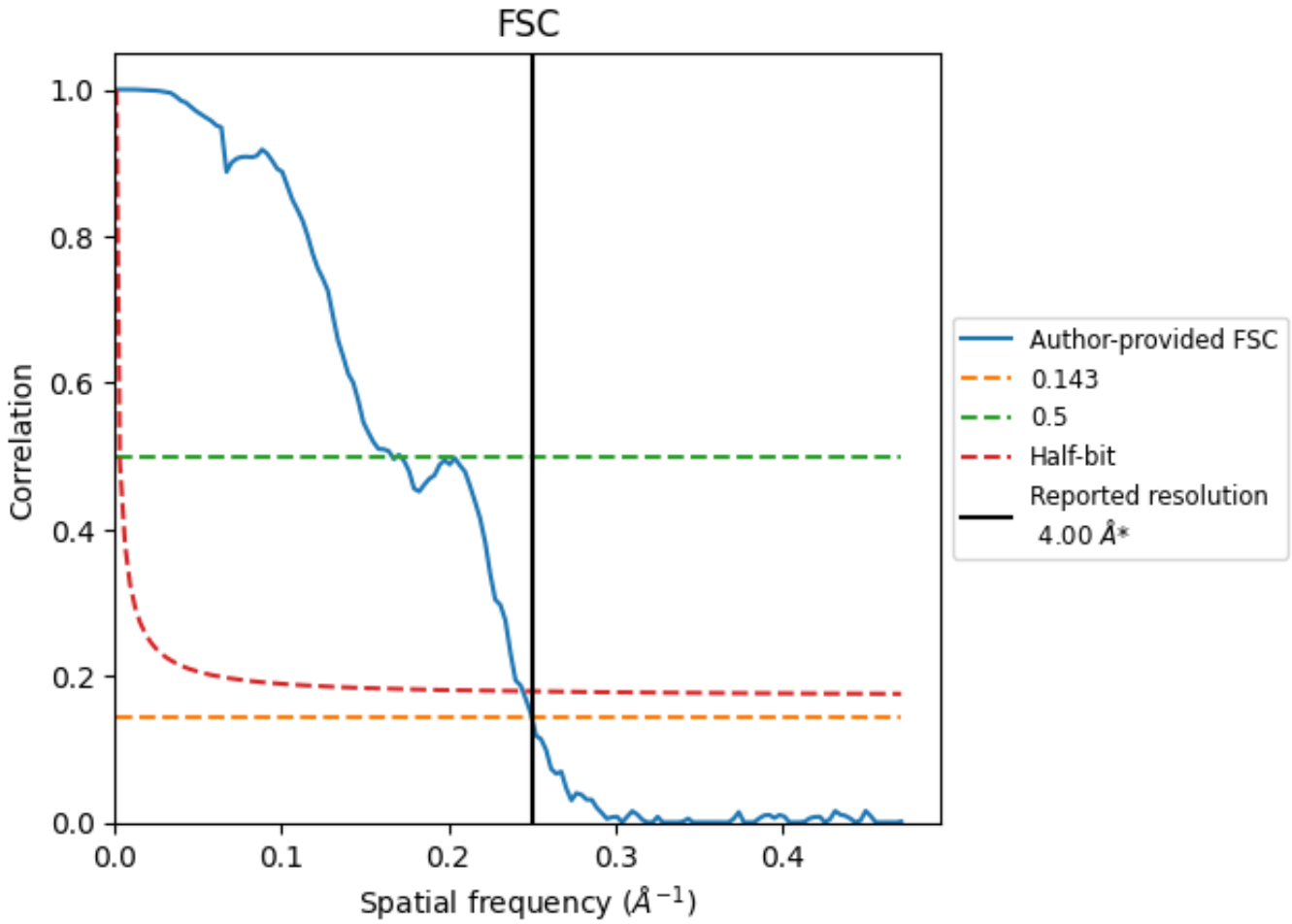


*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8.2 Resolution estimates (i)

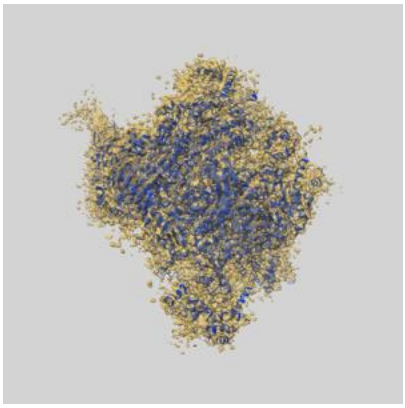
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.00	6.02	4.08
Unmasked-calculated*	-	-	-

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

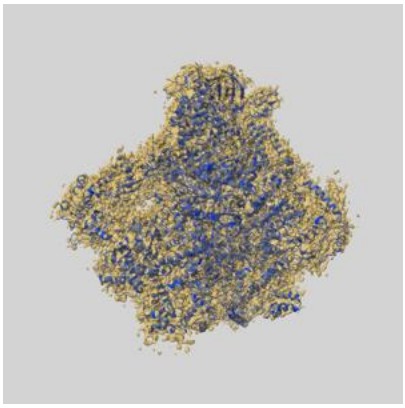
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3955 and PDB model 6EU0. Per-residue inclusion information can be found in section 3 on page 8.

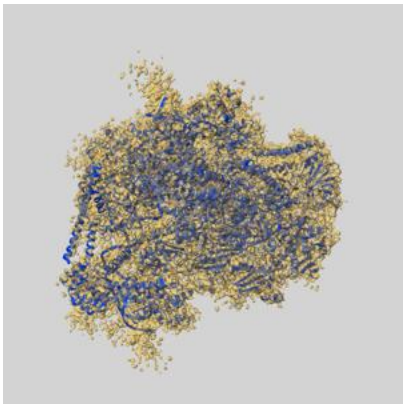
9.1 Map-model overlay



X



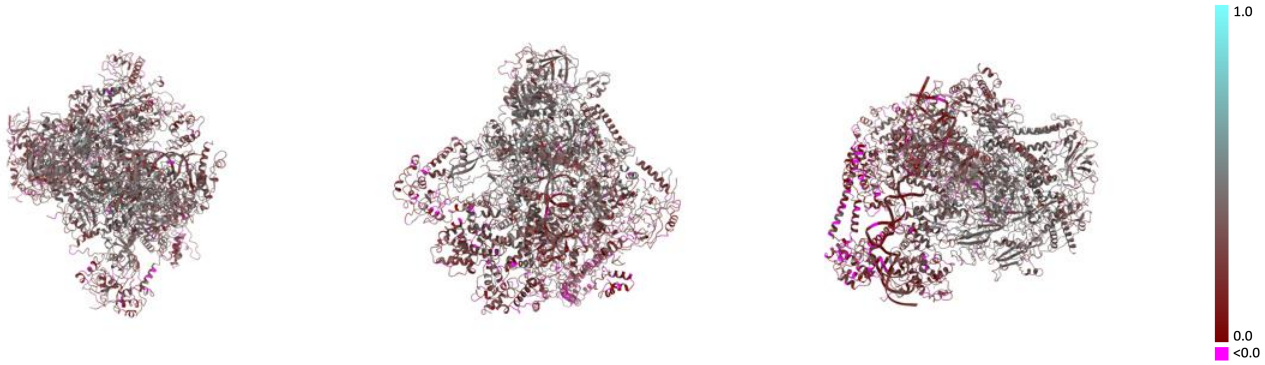
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

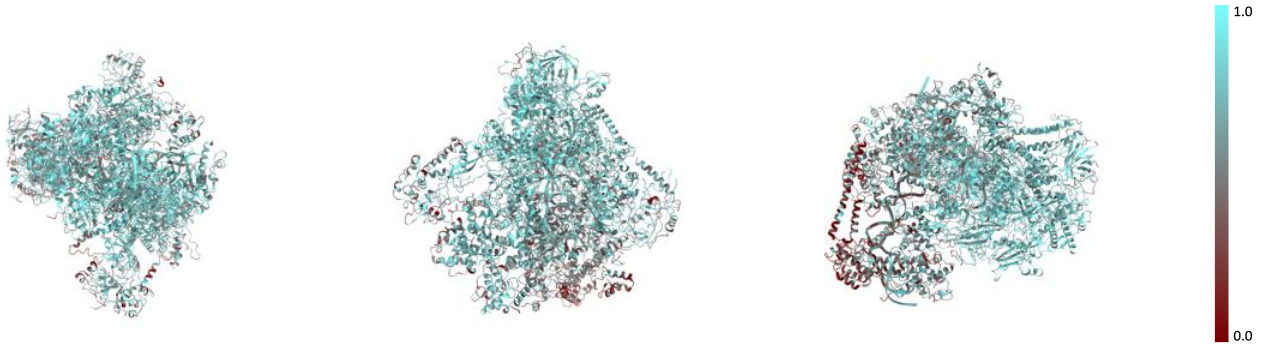
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

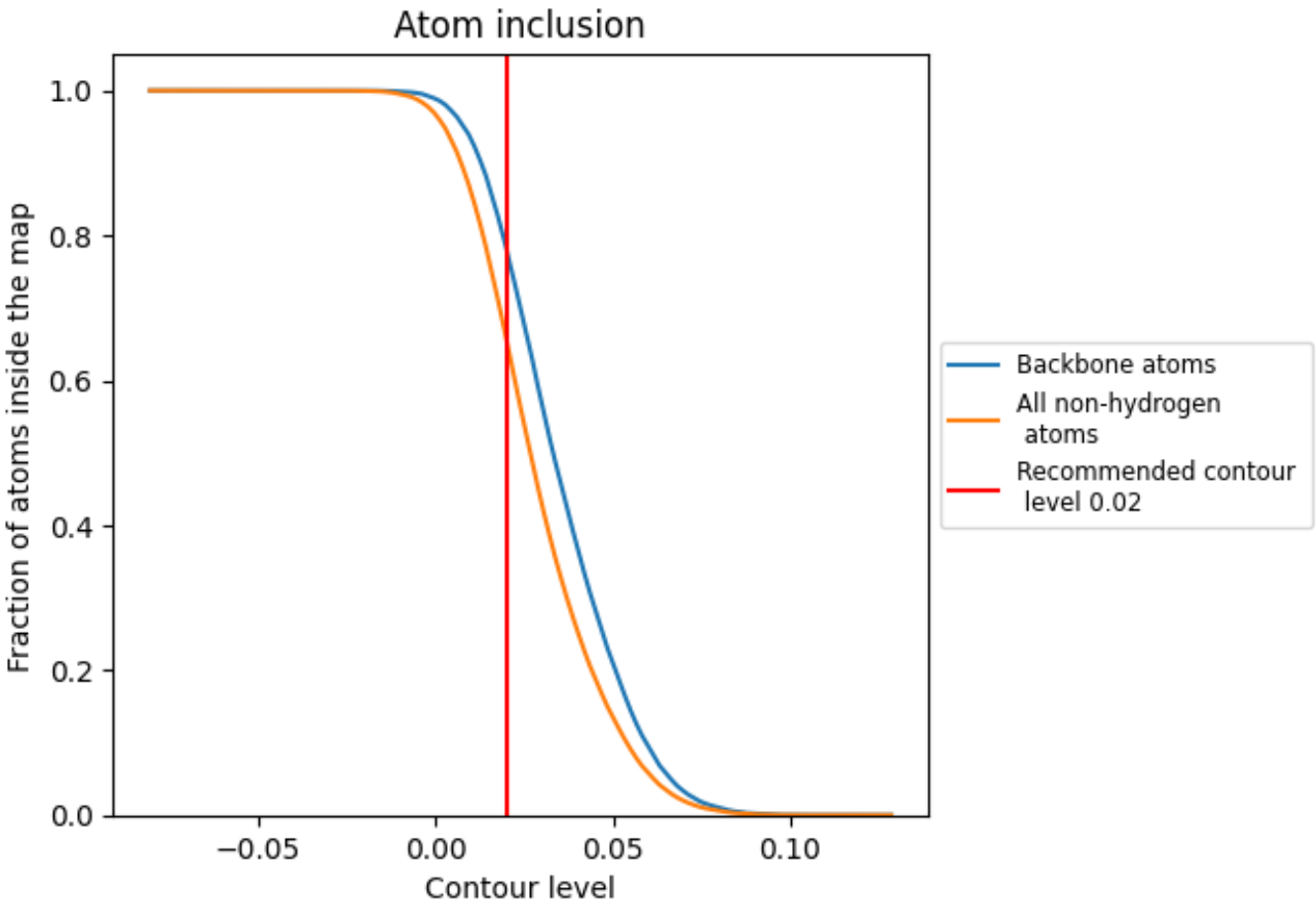
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6579	0.3130
A	0.7315	0.3730
B	0.7371	0.3720
C	0.7500	0.3720
D	0.5593	0.2220
E	0.7063	0.3440
F	0.7871	0.3900
G	0.6038	0.2650
H	0.6946	0.3500
I	0.5728	0.2240
J	0.7884	0.4060
K	0.7412	0.3880
L	0.7428	0.3810
M	0.5776	0.2480
N	0.6199	0.2610
O	0.6646	0.2990
P	0.4951	0.1880
Q	0.5969	0.2230
R	0.5925	0.2040
S	0.6210	0.2080
V	0.4102	0.1800
Y	0.4171	0.1880
Z	0.4908	0.2350