Full wwPDB EM Validation Report

Nov 19, 2022 – 06:50 pm GMT

PDB ID	:	5OIK
EMDB ID	:	EMD-3817
Title	:	Structure of an RNA polymerase II-DSIF transcription elongation complex
Authors	:	Bernecky, C.; Plitzko, J.M.; Cramer, P.
Deposited on	:	2017-07-18
Resolution	:	3.70 Å(reported)

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

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

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

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

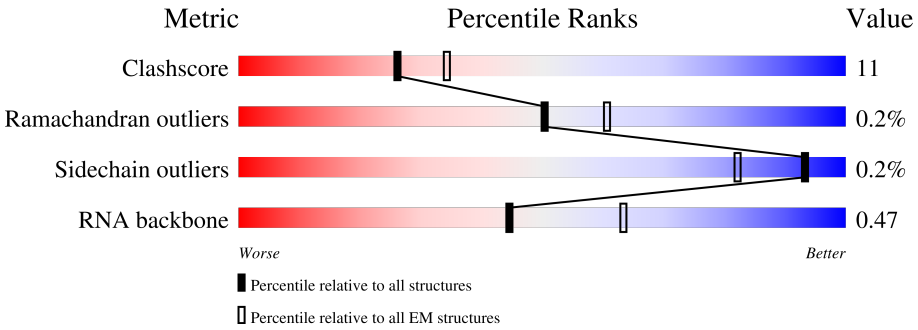
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1970	53% 19% 28%
2	B	1174	67% 31%
3	C	275	69% 25% 6%
4	D	142	23% 73% 18% 10%
5	E	210	74% 26%
6	F	127	54% 10% 35%
7	G	172	10% 68% 28%

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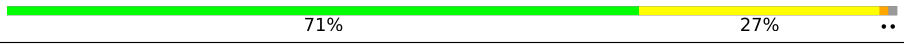
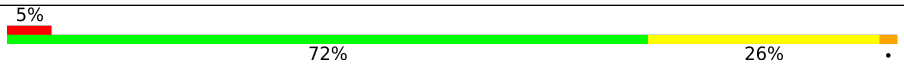
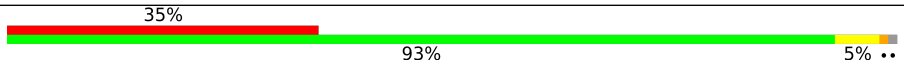
Mol	Chain	Length	Quality of chain
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	N	43	
14	P	50	
15	T	43	
16	Y	117	
17	Z	1087	

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 37988 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1421	11261	7084	2015	2090	72	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1147	9142	5780	1612	1686	64	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	259	2079	1305	357	411	6	0	0

- Molecule 4 is a protein called Polymerase (RNA) II (DNA directed) polypeptide D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	128	1008	635	170	199	4	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	209	1711	1084	300	319	8	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	82	658	419	113	121	5	0	0

- 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
			1341	871	218	244	8		

- Molecule 8 is a protein called Uncharacterized protein.

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	117	Total	C	N	O	S	0	0
			946	584	169	182	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	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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 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
			379	236	73	64	6		

- Molecule 13 is a DNA chain called DNA (43-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	43	Total	C	N	O	P	0	9
			709	335	130	202	42		

- Molecule 14 is a RNA chain called RNA (5'-R(P*UP*AP*UP*AP*UP*AP*CP*AP*UP*A

P*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	20	Total	C	N	O	P	0	0
			427	192	80	135	20		

- Molecule 15 is a DNA chain called DNA (43-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	43	Total	C	N	O	P	0	0
			874	419	157	256	42		

- Molecule 16 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	116	Total	C	N	O	S	0	0
			911	570	159	173	9		

- Molecule 17 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Z	488	Total	C	N	O	S	0	0
			3894	2475	686	716	17		

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
18	A	2	Total	Zn	0
			2	2	
18	B	1	Total	Zn	0
			1	1	
18	I	2	Total	Zn	0
			2	2	
18	J	1	Total	Zn	0
			1	1	
18	L	1	Total	Zn	0
			1	1	
18	Y	1	Total	Zn	0
			1	1	

- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

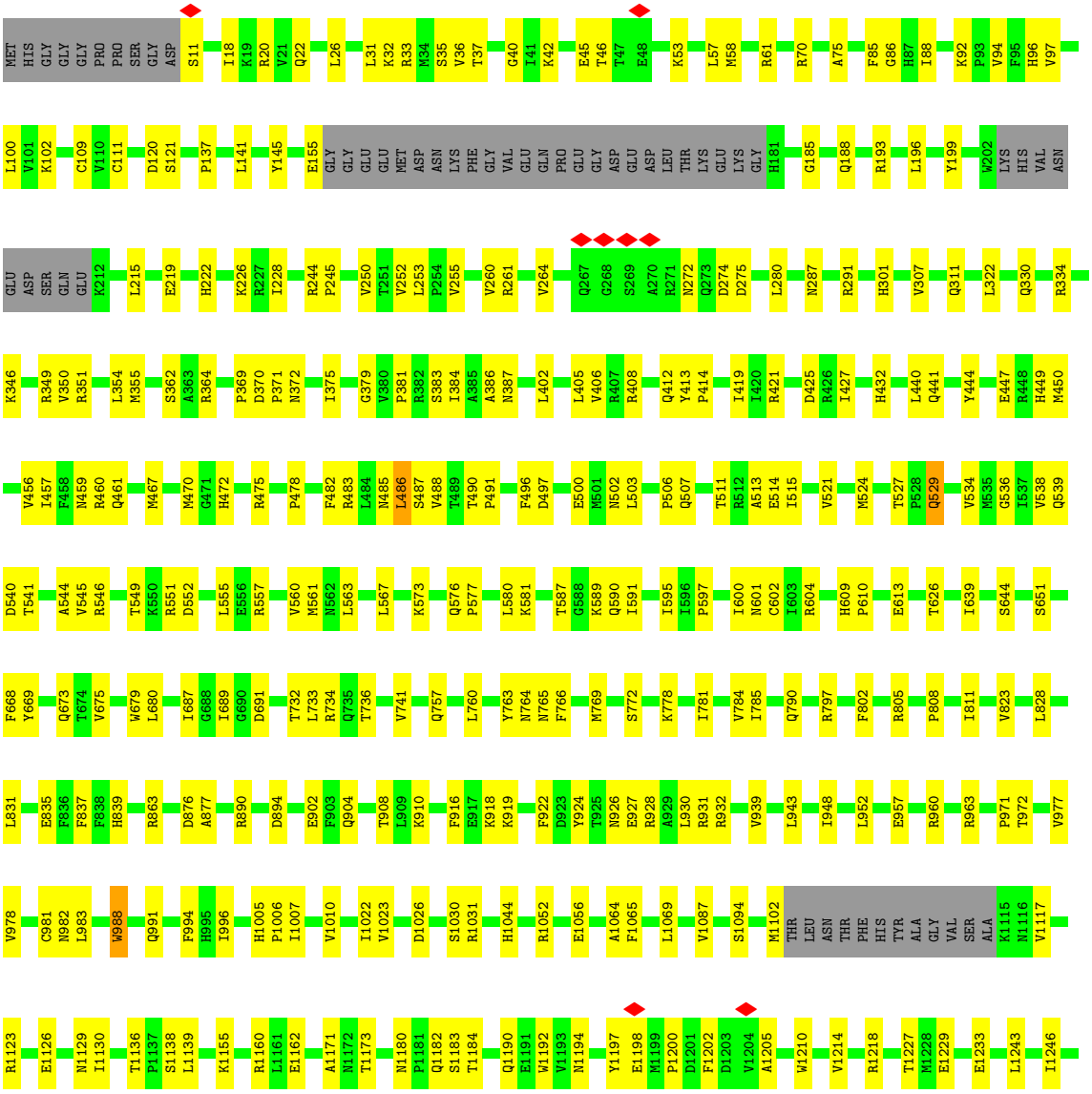
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
19	A	1	1	1	0

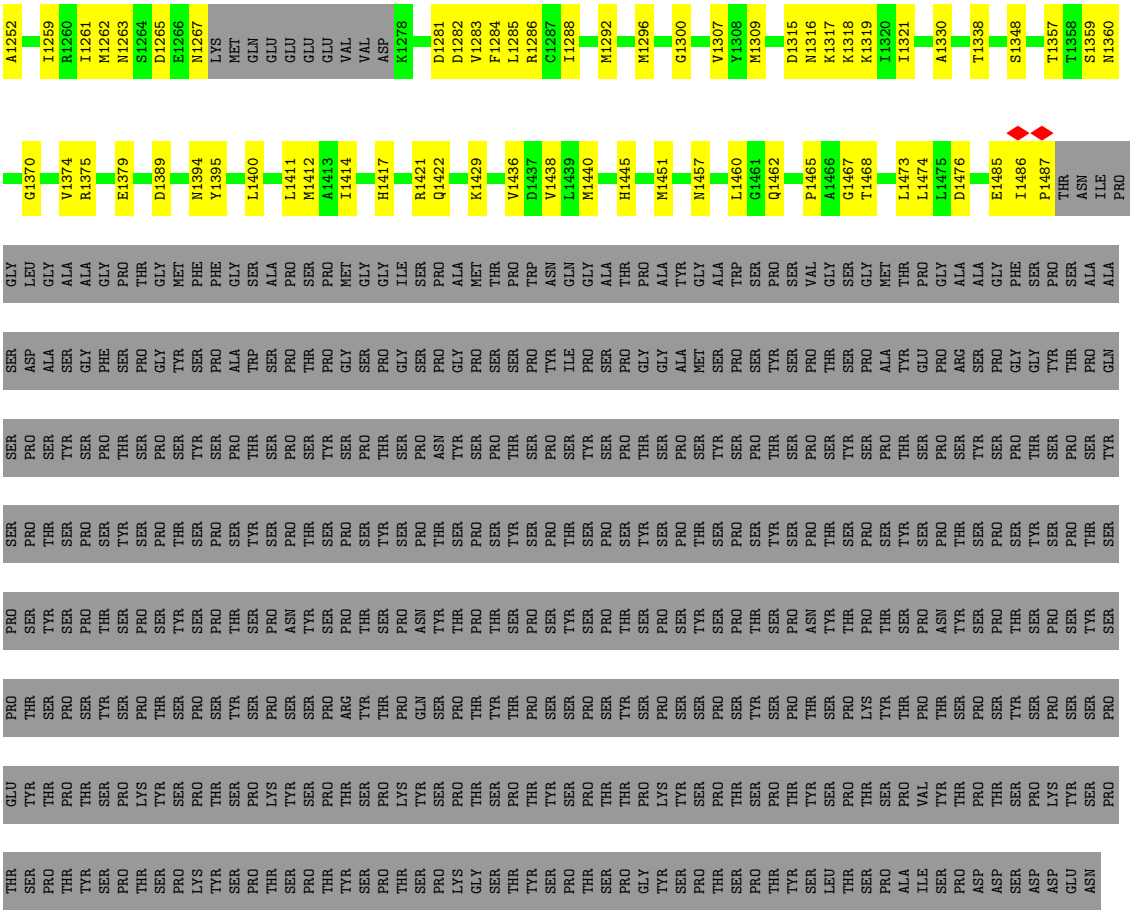
3 Residue-property plots (i)

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

• Molecule 1: DNA-directed RNA polymerase II subunit RPB1

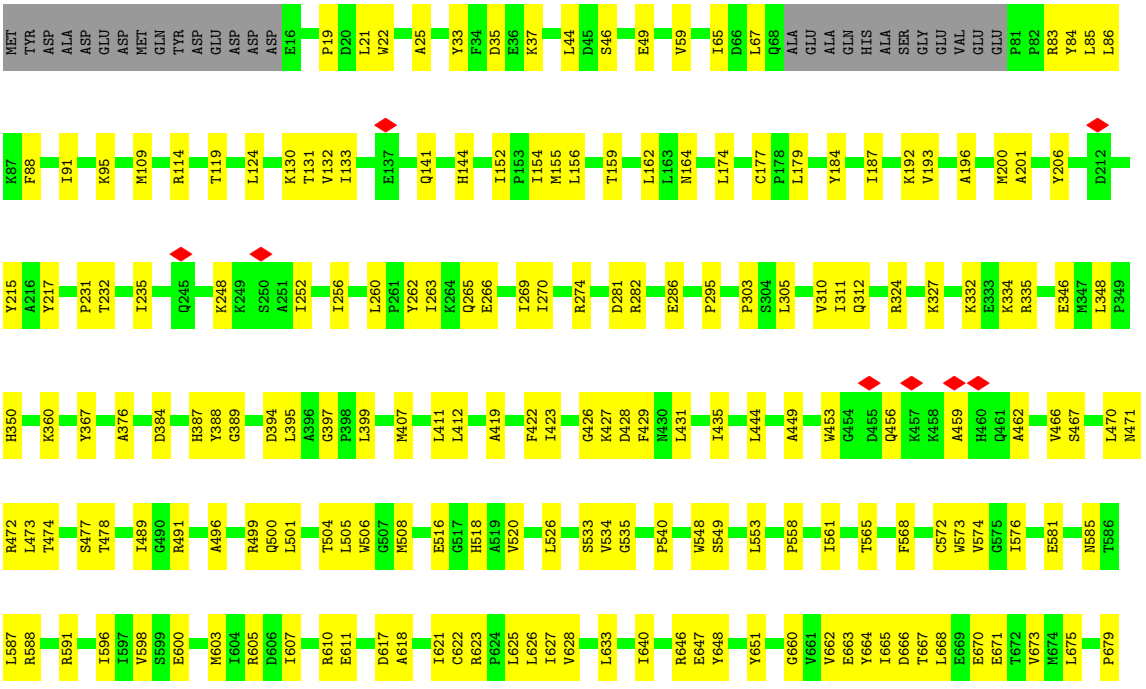
Chain A:

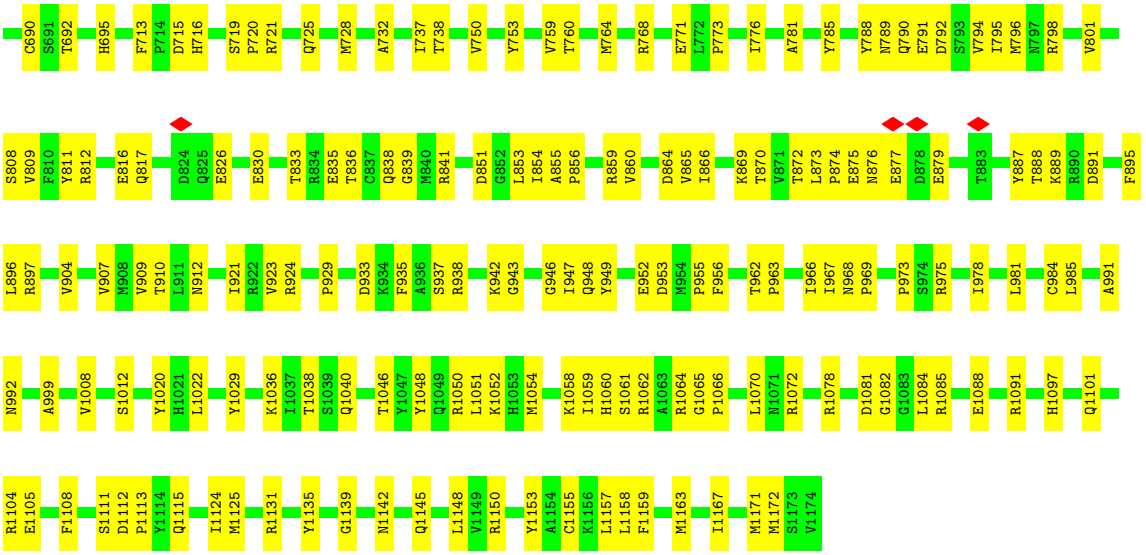




• Molecule 2: DNA-directed RNA polymerase subunit beta

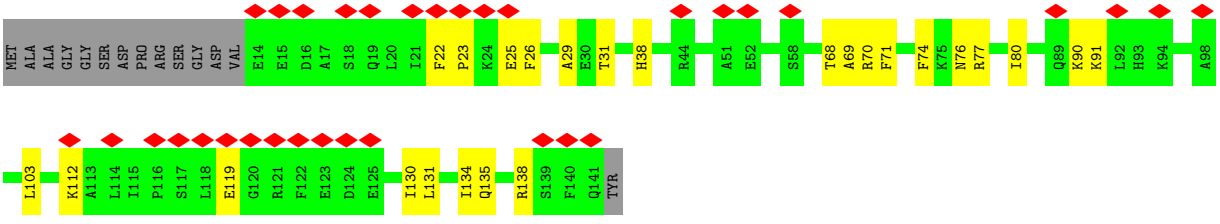
Chain B:



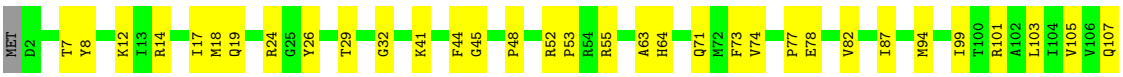


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

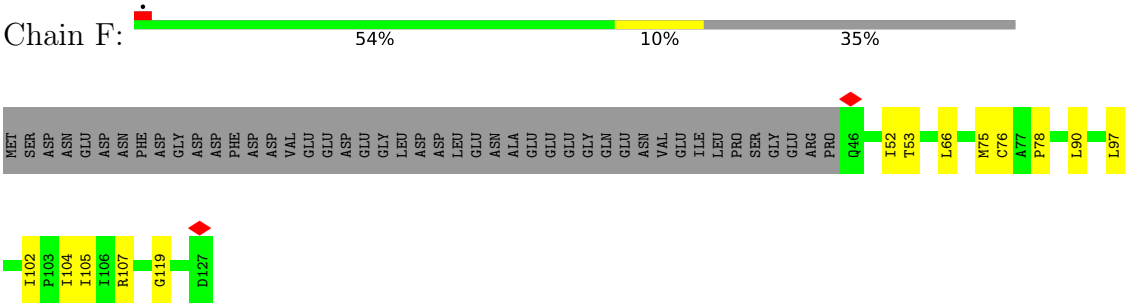
• Molecule 4: Polymerase (RNA) II (DNA directed) polypeptide D



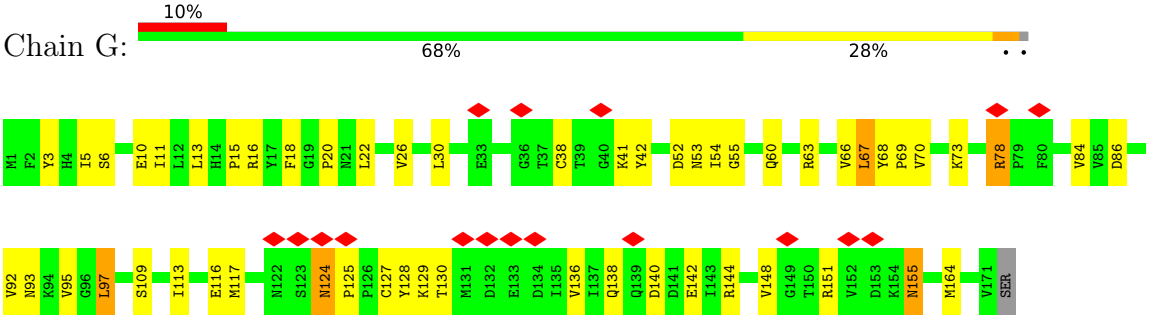
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



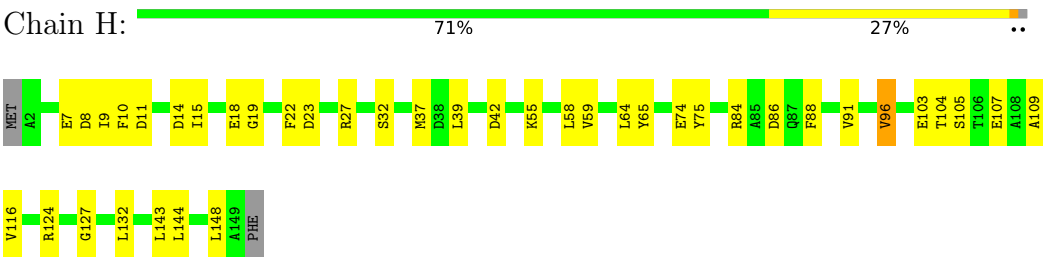
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



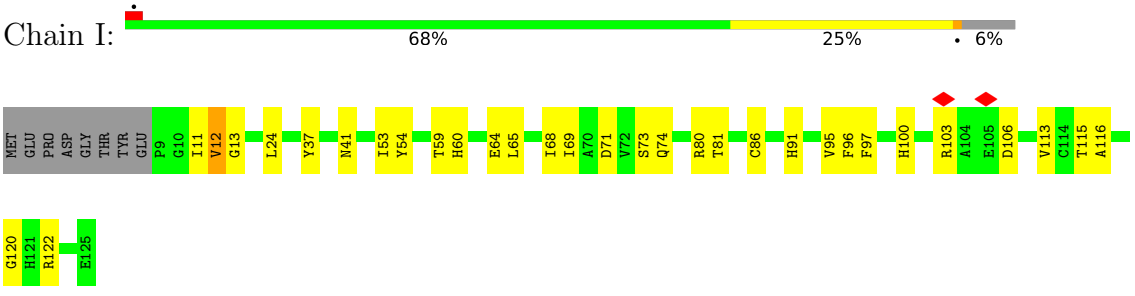
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7



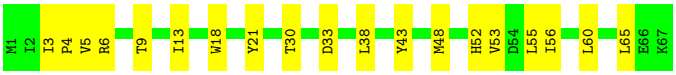
• Molecule 8: Uncharacterized protein



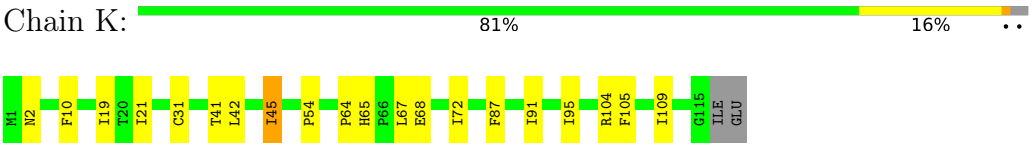
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9



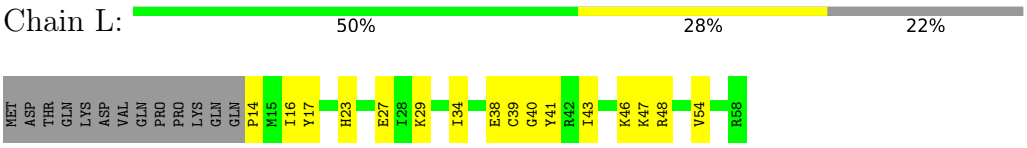
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



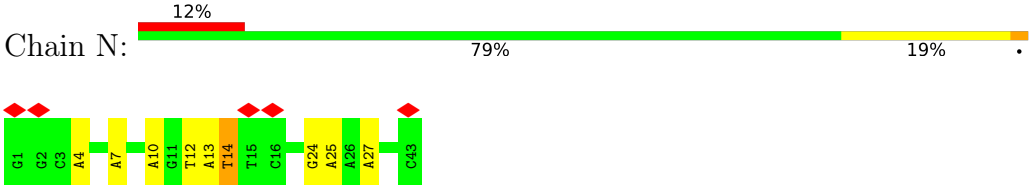
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11



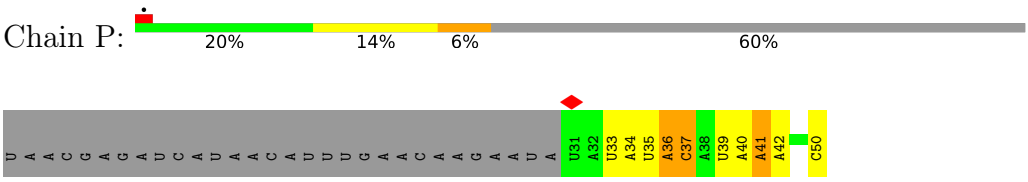
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



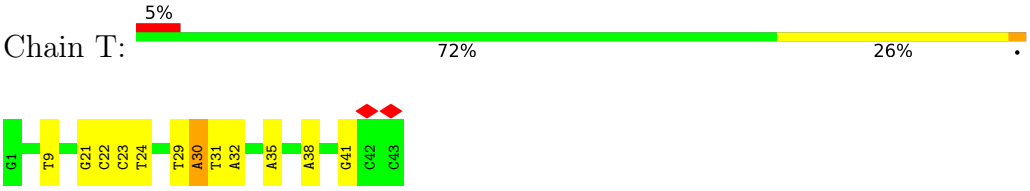
• Molecule 13: DNA (43-MER)



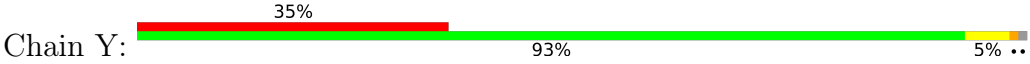
• Molecule 14: RNA (5'-R(P*UP*AP*UP*AP*UP*AP*CP*AP*UP*AP*AP*AP*GP*AP*CP* CP*AP*GP*GP*C)-3')



• Molecule 15: DNA (43-MER)



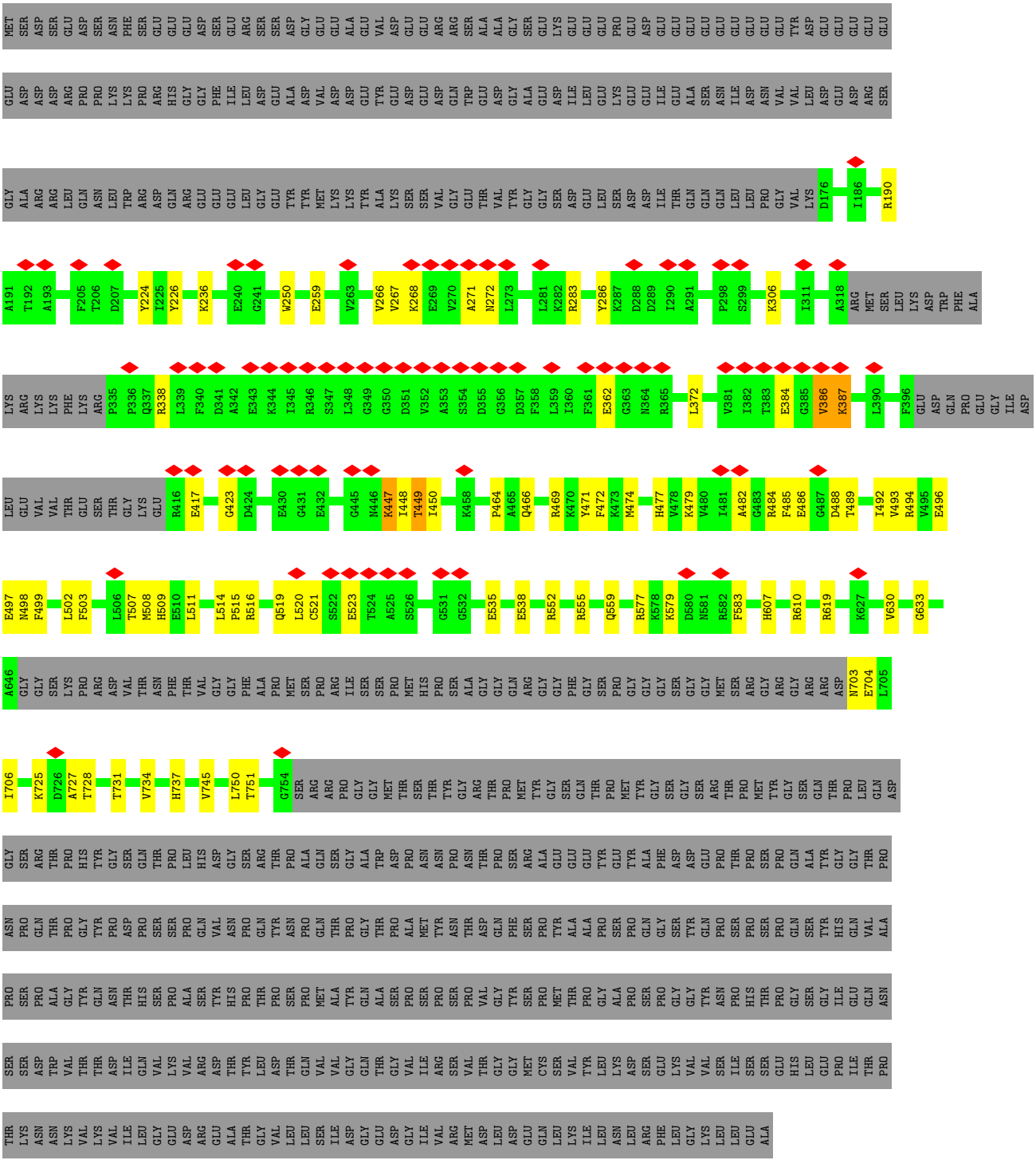
• Molecule 16: Transcription elongation factor SPT4



• Molecule 17: Transcription elongation factor SPT5

Chain Z:


8%
37%
7%
55%


MET SER ASP SER GLU ASP SER ASN PHE SER GLU GLU GLU ASP SER GLU ARG SER SER ASP GLY GLU GLU ALA GLU VAL ASP GLU GLU ARG ARG SER ALA ALA GLY SER GLU LYS GLU GLU GLU PRO GLU ASP GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU TYR ASP GLU GLU GLU GLU GLU
GLU ASP ASP ASP ARG PRO PRO LYS LYS PRO ARG HIS GLY GLY PHE ILE LEU ASP GLU ALA ASP VAL ASP ASP GLU TYR GLU ASP GLU ASP GLN TRP GLU ASP GLY ALA GLU ASP ILE LEU GLU LYS GLU GLU ILE GLU ALA SER ASN ILE ASP ASN VAL VAL LEU ASP GLU ASP ARG SER
GLY ALA ARG ARG LEU GLN ASN LEU TRP ARG ASP GLN ARG GLU GLU GLU LEU GLY GLU TYR TYR MET LYS LYS TYR ALA LYS SER SER VAL GLY GLU THR VAL TYR GLY GLY SER ASP GLU LEU SER ASP ASP ILE THR GLN GLN GLN LEU LEU PRO GLY VAL LYS D176 I186 R190
A191 T192 A193 F205 T206 D207 Y224 I225 Y226 K236 E240 G241 W250 E259 V263 V266 V267 K268 E269 V270 A271 N272 L273 L281 K282 R283 Y286 K287 D288 D289 I290 A291 P298 S299 K306 I311 A318 ARG MET SER LEU LYS ASP TRP PHE ALA
LYS ARG LYS LYS PHE LYS ARG P335 P336 Q337 R338 L339 F340 D341 A342 E343 K344 I345 R346 S347 L348 G349 G350 D351 V352 A353 S354 D355 G356 D357 F358 L359 I360 F361 E362 G363 N364 R365 L372 V381 I382 T383 E384 G385 V386 K387 L390 F396 GLU ASP GLN PRO GLU GLY ILE ASP
LEU GLU VAL VAL THR GLU SER THR GLY LYS GLU R416 E417 G423 D424 E430 G431 E432 G445 N446 K447 I448 T449 I450 K458 P464 A465 Q466 R469 K470 Y471 F472 K473 M474 H477 V478 K479 V480 I481 A482 G483 R484 F485 E486 G487 D488 T489 I492 V493 R494 V495 E496
E497 N498 F499 L502 F503 L506 T507 M508 H509 E510 L511 L514 P515 R516 Q519 L520 C521 S522 E523 T524 A525 S526 G531 G532 E535 E538 R552 R555 Q559 R577 K578 K579 D580 N581 R582 F583 H607 R610 R619 K627 V630 G633
A646 GLY GLY SER LYS PRO ARG ASP VAL THR ASN PHE THR VAL GLY GLY PHE ALA PRO MET SER PRO ARG ILE SER SER PRO MET HIS PRO SER ALA GLY GLY GLN ARG GLY GLY PHE GLY SER PRO GLY GLY GLY SER GLY GLY MET SER ARG GLY ARG GLY ARG ARG ASP N703 E704 L705
I706 K725 D726 A727 T728 T731 V734 H737 V745 L750 T751 G754 SER ARG ARG PRO GLY GLY MET THR SER THR TYR GLY ARG THR PRO MET TYR GLY GLY SER GLN THR PRO MET TYR GLY SER GLY SER ARG THR PRO MET TYR GLY SER GLN THR PRO LEU GLN ASP
GLY SER ARG THR PRO HIS TYR GLY SER GLN THR PRO LEU HIS ASP GLY SER ARG THR PRO ALA GLN SER GLY ALA TRP ASP PRO ASN ASN PRO ASN THR PRO SER ARG ALA GLU GLU GLU TYR GLU TYR ALA PHE ASP ASP GLU PRO THR PRO SER PRO GLN ALA TYR GLY GLY THR PRO
ASN PRO GLN THR PRO GLY TYR PRO ASP PRO SER SER PRO GLN VAL ASN PRO GLN TYR ASN PRO GLN THR PRO ALA MET TYR ASN THR ASP GLN PHE SER PRO TYR ALA ALA PRO SER PRO GLN GLY SER TYR GLN PRO SER PRO SER PRO GLN SER TYR HIS GLN VAL ALA
PRO SER PRO ALA GLY TYR GLN ASN THR HIS SER PRO ALA SER TYR HIS PRO THR PRO SER PRO MET THR PRO SER PRO ALA TYR GLN ALA SER PRO SER PRO VAL GLY TYR SER PRO MET THR PRO GLY ALA PRO SER PRO GLY GLY TYR ASN PRO HIS THR PRO GLY SER GLY ILE GLU GLN ASN
SER SER ASP TRP VAL THR THR ASP ILE GLN VAL LYS VAL ARG ASP THR TYR LEU ASP THR GLN VAL VAL GLY GLN THR GLY VAL ILE ARG SER VAL THR GLY GLY GLY MET CYS SER VAL TYR LEU LYS ASP SER GLU LYS VAL VAL SER ILE GLU GLY GLN GLN HIS LEU GLU PRO ILE THR PRO
THR LYS ASN LYS VAL LYS VAL ILE LEU LEU GLY GLU ASP ARG GLU ALA THR GLY VAL LEU LEU SER ILE ASP GLY GLU ASP GLY ILE VAL ARG MET ASP LEU ASP GLU GLN LEU LYS ILE LEU ASN LEU ARG PHE LEU GLY LYS LEU LEU GLU ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	101140	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 ($e^-/Å^2$)	33	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	37037	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.153	Depositor
Minimum map value	-0.053	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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: 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	0.52	1/11467 (0.0%)	0.57	1/15479 (0.0%)
2	B	0.59	0/9325	0.60	1/12589 (0.0%)
3	C	0.64	0/2122	0.59	0/2883
4	D	0.29	0/1022	0.53	0/1377
5	E	0.50	0/1742	0.54	0/2353
6	F	0.55	0/668	0.56	0/903
7	G	0.34	0/1372	0.71	3/1861 (0.2%)
8	H	0.60	0/1207	0.57	0/1628
9	I	0.45	0/968	0.52	0/1311
10	J	0.68	0/542	0.64	0/730
11	K	0.54	0/939	0.56	1/1271 (0.1%)
12	L	0.61	0/385	0.54	0/511
13	N	0.78	0/785	1.28	4/1209 (0.3%)
14	P	0.66	0/478	0.74	0/742
15	T	0.92	1/979 (0.1%)	1.20	0/1508
16	Y	0.60	1/927 (0.1%)	0.67	1/1250 (0.1%)
17	Z	0.66	0/3963	0.67	5/5339 (0.1%)
All	All	0.58	3/38891 (0.0%)	0.65	16/52944 (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	1
16	Y	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	105	GLY	CA-C	10.69	1.69	1.51
15	T	30	DA	O3'-P	-6.03	1.53	1.61
1	A	988	TRP	CB-CG	-5.13	1.41	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	486	LEU	CA-CB-CG	-7.26	98.60	115.30
16	Y	104	ARG	N-CA-C	6.43	128.35	111.00
7	G	78	ARG	NE-CZ-NH1	-6.38	117.11	120.30
2	B	526	LEU	CA-CB-CG	6.23	129.63	115.30
17	Z	450	ILE	N-CA-C	-6.23	94.18	111.00
7	G	78	ARG	NE-CZ-NH2	6.19	123.40	120.30
17	Z	449	THR	N-CA-C	-6.11	94.49	111.00
13	N	14	DT	O4'-C1'-N1	6.08	112.26	108.00
13	N	14	DT	C3'-C2'-C1'	-6.07	95.21	102.50
7	G	67	LEU	CA-CB-CG	5.74	128.51	115.30
13	N	14	DT	O4'-C4'-C3'	-5.60	102.26	104.50
17	Z	423	GLY	N-CA-C	5.56	127.01	113.10
17	Z	447	LYS	N-CA-C	-5.38	96.48	111.00
17	Z	286	TYR	CA-CB-CG	-5.28	103.36	113.40
11	K	45	ILE	CG1-CB-CG2	-5.17	100.03	111.40
13	N	27	DA	O4'-C1'-N9	5.08	111.56	108.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	910	LYS	Peptide
16	Y	105	GLY	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	11261	0	11390	302	0
2	B	9142	0	9157	288	0
3	C	2079	0	2032	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1008	0	970	18	0
5	E	1711	0	1733	41	0
6	F	658	0	686	15	0
7	G	1341	0	1348	43	0
8	H	1186	0	1147	37	0
9	I	946	0	881	24	0
10	J	533	0	553	15	0
11	K	920	0	942	18	0
12	L	379	0	386	16	0
13	N	709	0	387	11	0
14	P	427	0	216	10	0
15	T	874	0	487	14	0
16	Y	911	0	904	5	0
17	Z	3894	0	3957	86	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	I	2	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
18	Y	1	0	0	0	0
19	A	1	0	0	0	0
All	All	37988	0	37176	841	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 11.

All (841) 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)
2:B:327:LYS:NZ	17:Z:250:TRP:CE3	2.09	1.20
17:Z:417:GLU:OE2	17:Z:516:ARG:NH1	1.84	1.08
17:Z:471:TYR:O	17:Z:472:PHE:CG	2.23	0.90
2:B:888:THR:HG23	2:B:889:LYS:HG3	1.56	0.88
1:A:425:ASP:HB2	17:Z:583:PHE:CZ	2.08	0.87
8:H:58:LEU:HD11	8:H:143:LEU:HD11	1.56	0.86
4:D:26:PHE:CE2	7:G:78:ARG:HD3	2.10	0.85
7:G:60:GLN:OE1	7:G:63:ARG:NH2	2.09	0.85
17:Z:538:GLU:HG3	17:Z:577:ARG:HH22	1.44	0.83
5:E:45:GLY:HA3	5:E:52:ARG:HD2	1.60	0.83
15:T:29:DT:H2"	15:T:30:DA:OP1	1.77	0.83
14:P:37:C:OP2	17:Z:579:LYS:NZ	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Z:479:LYS:HD3	17:Z:521:CYS:HB2	1.62	0.82
1:A:948:ILE:HG23	1:A:1007:ILE:HD11	1.61	0.82
17:Z:496:GLU:HB2	17:Z:499:PHE:HB2	1.62	0.80
1:A:425:ASP:OD2	17:Z:583:PHE:CZ	2.35	0.80
7:G:55:GLY:HA3	7:G:69:PRO:HG2	1.64	0.79
1:A:733:LEU:HB3	9:I:106:ASP:HB2	1.67	0.77
3:C:259:LEU:HD11	11:K:42:LEU:HD21	1.65	0.77
2:B:265:GLN:HE21	2:B:324:ARG:HE	1.31	0.77
2:B:109:MET:HE1	2:B:174:LEU:HD13	1.64	0.77
1:A:372:ASN:ND2	2:B:788:TYR:OH	2.17	0.77
2:B:910:THR:HG22	12:L:43:ILE:HA	1.67	0.77
1:A:691:ASP:OD2	1:A:765:ASN:ND2	2.16	0.76
1:A:904:GLN:NE2	1:A:981:CYS:O	2.19	0.76
2:B:924:ARG:NH1	3:C:62:GLU:OE2	2.15	0.76
1:A:425:ASP:OD2	17:Z:583:PHE:CE1	2.39	0.76
2:B:591:ARG:NH2	2:B:663:GLU:OE2	2.18	0.76
2:B:841:ARG:HD2	2:B:895:PHE:HE2	1.51	0.76
17:Z:272:ASN:OD1	17:Z:384:GLU:HB2	1.85	0.76
1:A:447:GLU:OE1	2:B:1064:ARG:NH2	2.19	0.75
2:B:984:CYS:HG	2:B:1046:THR:HG1	1.25	0.75
1:A:425:ASP:CG	17:Z:583:PHE:CZ	2.60	0.75
1:A:538:VAL:HG12	1:A:539:GLN:HG2	1.68	0.75
17:Z:471:TYR:O	17:Z:472:PHE:CD2	2.40	0.74
9:I:65:LEU:O	9:I:122:ARG:NH1	2.15	0.74
9:I:86:CYS:HB3	9:I:91:HIS:H	1.53	0.74
1:A:425:ASP:CB	17:Z:583:PHE:CZ	2.71	0.74
2:B:568:PHE:HE1	2:B:573:TRP:HD1	1.35	0.74
2:B:367:TYR:OH	2:B:611:GLU:OE2	2.04	0.73
1:A:18:ILE:H	1:A:1462:GLN:HE22	1.36	0.73
2:B:851:ASP:OD2	12:L:17:TYR:OH	2.06	0.73
1:A:1374:VAL:HG11	1:A:1411:LEU:HD21	1.71	0.73
2:B:327:LYS:NZ	17:Z:250:TRP:CZ3	2.57	0.73
2:B:953:ASP:OD1	3:C:36:ARG:NH2	2.21	0.72
5:E:55:ARG:HB2	5:E:78:GLU:HG2	1.70	0.72
7:G:10:GLU:HB3	7:G:67:LEU:HG	1.71	0.72
5:E:185:ILE:HG21	5:E:209:VAL:HG21	1.72	0.72
2:B:193:VAL:HG21	2:B:470:LEU:HD13	1.72	0.72
5:E:19:GLN:OE1	5:E:138:ASN:ND2	2.22	0.72
4:D:26:PHE:HE2	7:G:78:ARG:HD3	1.53	0.72
2:B:984:CYS:SG	2:B:1046:THR:OG1	2.42	0.71
2:B:581:GLU:OE2	9:I:74:GLN:NE2	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:70:ARG:NH2	7:G:140:ASP:OD1	2.23	0.71
2:B:37:LYS:NZ	2:B:664:TYR:OH	2.22	0.71
1:A:1192:TRP:HZ3	1:A:1246:ILE:HG22	1.56	0.71
1:A:863:ARG:NH2	1:A:1129:ASN:OD1	2.24	0.70
6:F:75:MET:O	7:G:15:PRO:HB2	1.91	0.70
3:C:2:PRO:HB3	11:K:54:PRO:HD2	1.73	0.70
1:A:413:TYR:OH	1:A:450:MET:O	2.10	0.70
1:A:1138:SER:OG	1:A:1360:ASN:ND2	2.25	0.70
2:B:759:VAL:HG12	2:B:999:ALA:HB2	1.74	0.70
3:C:42:VAL:HB	3:C:178:PRO:HG3	1.74	0.69
10:J:65:LEU:O	12:L:23:HIS:ND1	2.25	0.69
1:A:244:ARG:HD2	1:A:245:PRO:HD2	1.74	0.69
2:B:471:ASN:ND2	2:B:477:SER:OG	2.24	0.69
5:E:29:THR:HG23	5:E:32:GLY:H	1.56	0.69
1:A:577:PRO:HG2	1:A:580:LEU:HD23	1.75	0.69
2:B:565:THR:HA	2:B:610:ARG:HG2	1.75	0.68
2:B:1062:ARG:NH1	2:B:1081:ASP:O	2.26	0.68
2:B:360:LYS:HG2	2:B:553:LEU:HD13	1.75	0.68
1:A:877:ALA:HB3	1:A:890:ARG:NH1	2.09	0.68
7:G:97:LEU:HD13	7:G:113:ILE:HD11	1.76	0.68
1:A:597:PRO:HD3	1:A:668:PHE:CD1	2.28	0.68
2:B:781:ALA:HB3	2:B:966:ILE:HG12	1.76	0.68
1:A:760:LEU:HD22	1:A:764:ASN:HD22	1.59	0.68
1:A:540:ASP:HB2	2:B:790:GLN:HE21	1.59	0.67
1:A:877:ALA:HB3	1:A:890:ARG:HH11	1.59	0.67
1:A:757:GLN:HE22	1:A:778:LYS:HB3	1.59	0.67
1:A:1184:THR:HG21	1:A:1190:GLN:HA	1.77	0.67
2:B:327:LYS:NZ	17:Z:250:TRP:CD2	2.63	0.67
2:B:1029:TYR:CE1	2:B:1036:LYS:HG2	2.30	0.67
2:B:833:THR:HB	2:B:836:THR:HG22	1.76	0.67
9:I:115:THR:HG22	9:I:116:ALA:H	1.60	0.67
1:A:70:ARG:NH1	17:Z:535:GLU:OE2	2.28	0.67
1:A:560:VAL:HG22	1:A:591:ILE:HD11	1.77	0.67
2:B:270:ILE:HG13	2:B:305:LEU:HD23	1.76	0.66
1:A:760:LEU:HD22	1:A:764:ASN:ND2	2.11	0.66
1:A:111:CYS:SG	1:A:188:GLN:NE2	2.68	0.66
1:A:459:ASN:OD1	1:A:460:ARG:N	2.29	0.66
9:I:69:ILE:HG22	9:I:71:ASP:H	1.59	0.66
2:B:860:VAL:HG23	2:B:896:LEU:HD11	1.77	0.65
2:B:310:VAL:HG23	2:B:311:ILE:HD12	1.77	0.65
5:E:17:ILE:HD13	5:E:74:VAL:HG11	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:7:PRO:O	11:K:104:ARG:NH1	2.28	0.65
2:B:992:ASN:HD21	2:B:1020:TYR:HE2	1.44	0.65
1:A:425:ASP:HB2	17:Z:583:PHE:HZ	1.60	0.65
17:Z:479:LYS:NZ	17:Z:521:CYS:O	2.30	0.65
4:D:31:THR:HG22	7:G:3:TYR:HE1	1.62	0.64
5:E:73:PHE:HE2	5:E:99:ILE:HG12	1.61	0.64
1:A:425:ASP:OD2	17:Z:583:PHE:CE2	2.49	0.64
2:B:937:SER:HB3	2:B:1048:TYR:HE1	1.61	0.64
8:H:14:ASP:OD1	8:H:15:ILE:N	2.30	0.64
2:B:1085:ARG:HD3	15:T:22:DC:H5”	1.80	0.64
1:A:971:PRO:O	1:A:972:THR:OG1	2.15	0.64
2:B:489:ILE:HD11	13:N:25:DA:C6	2.32	0.64
3:C:205:LYS:NZ	3:C:212:ASP:O	2.31	0.64
17:Z:703:ASN:OD1	17:Z:704:GLU:N	2.31	0.64
1:A:904:GLN:HE21	1:A:982:ASN:HA	1.63	0.64
1:A:1030:SER:HG	5:E:162:ARG:HE	1.42	0.64
1:A:402:LEU:HD23	1:A:405:LEU:HD12	1.80	0.64
1:A:1218:ARG:NH2	1:A:1252:ALA:O	2.31	0.64
3:C:31:ALA:O	3:C:231:TYR:OH	2.16	0.64
2:B:937:SER:HB3	2:B:1048:TYR:CE1	2.34	0.63
2:B:1062:ARG:NH2	2:B:1066:PRO:O	2.30	0.63
2:B:65:ILE:HB	2:B:86:LEU:HB2	1.80	0.63
2:B:952:GLU:OE2	3:C:40:ALA:HB2	1.98	0.63
5:E:55:ARG:NH1	5:E:107:GLN:HE21	1.97	0.63
15:T:30:DA:H2’	15:T:31:DT:C6	2.33	0.63
2:B:690:CYS:SG	2:B:692:THR:OG1	2.56	0.63
2:B:956:PHE:CE2	3:C:184:PHE:HB3	2.34	0.63
1:A:1348:SER:O	5:E:12:LYS:NZ	2.32	0.62
2:B:907:VAL:HG22	2:B:921:ILE:HG12	1.81	0.62
3:C:105:VAL:HG11	3:C:115:VAL:HG22	1.79	0.62
1:A:1457:ASN:HD22	1:A:1465:PRO:HD3	1.64	0.62
8:H:64:LEU:HB3	8:H:84:ARG:HB2	1.79	0.62
17:Z:479:LYS:HG3	17:Z:489:THR:HG22	1.81	0.62
2:B:274:ARG:NH2	2:B:281:ASP:OD1	2.29	0.62
1:A:486:LEU:HD13	2:B:790:GLN:OE1	2.00	0.62
1:A:364:ARG:NH1	1:A:502:ASN:OD1	2.33	0.62
1:A:507:GLN:HB2	2:B:1105:GLU:OE2	2.00	0.62
1:A:802:PHE:HE2	1:A:808:PRO:HD3	1.64	0.62
13:N:13:DA:C2	15:T:32:DA:C2	2.88	0.62
1:A:1202:PHE:O	1:A:1263:ASN:ND2	2.33	0.62
1:A:478:PRO:O	1:A:483:ARG:NH2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Z:469:ARG:HD2	17:Z:515:PRO:CG	2.30	0.61
1:A:957:GLU:HG2	1:A:960:ARG:HH21	1.64	0.61
5:E:52:ARG:HG3	5:E:53:PRO:HD3	1.80	0.61
3:C:99:VAL:HG21	3:C:127:VAL:HG21	1.81	0.61
3:C:41:GLU:OE2	3:C:255:LYS:NZ	2.27	0.61
1:A:45:GLU:OE2	1:A:53:LYS:NZ	2.34	0.61
1:A:1474:LEU:HB2	6:F:105:ILE:HG13	1.82	0.61
2:B:1060:HIS:NE2	2:B:1082:GLY:O	2.24	0.61
1:A:595:ILE:HD11	1:A:675:VAL:HG21	1.83	0.61
17:Z:267:VAL:O	17:Z:268:LYS:HD3	2.01	0.61
2:B:785:TYR:CZ	2:B:955:PRO:HD3	2.36	0.60
2:B:826:GLU:H	2:B:872:THR:HG22	1.67	0.60
2:B:839:GLY:O	2:B:891:ASP:HB3	2.02	0.60
1:A:540:ASP:HB2	2:B:790:GLN:NE2	2.17	0.60
1:A:1417:HIS:O	1:A:1421:ARG:HG2	2.02	0.59
3:C:70:LEU:HD22	10:J:6:ARG:HG3	1.84	0.59
11:K:65:HIS:HE1	11:K:67:LEU:HD12	1.66	0.59
17:Z:745:VAL:HG21	17:Z:750:LEU:HD21	1.85	0.59
1:A:369:PRO:HB3	1:A:486:LEU:HD21	1.84	0.59
1:A:811:ILE:HD11	2:B:690:CYS:HB2	1.82	0.59
2:B:841:ARG:HD2	2:B:895:PHE:CE2	2.34	0.59
2:B:628:VAL:HG22	2:B:633:LEU:HD23	1.84	0.59
7:G:117:MET:SD	7:G:130:THR:HG23	2.42	0.59
1:A:20:ARG:NH2	2:B:1172:MET:SD	2.75	0.59
1:A:687:ILE:HD13	1:A:766:PHE:HE1	1.67	0.59
2:B:1112:ASP:OD1	2:B:1112:ASP:N	2.34	0.59
3:C:72:PRO:HG3	10:J:13:ILE:HD11	1.84	0.59
17:Z:472:PHE:HE1	17:Z:520:LEU:HB2	1.67	0.59
1:A:541:THR:O	1:A:545:VAL:HG23	2.03	0.59
1:A:576:GLN:HG3	1:A:577:PRO:HD2	1.85	0.59
1:A:919:LYS:O	1:A:1052:ARG:HD3	2.03	0.59
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.84	0.59
1:A:467:MET:SD	1:A:524:MET:HE2	2.42	0.58
1:A:475:ARG:NH2	11:K:68:GLU:OE2	2.36	0.58
1:A:551:ARG:HH12	8:H:27:ARG:HH21	1.51	0.58
2:B:130:LYS:NZ	2:B:429:PHE:O	2.35	0.58
2:B:933:ASP:OD2	2:B:1050:ARG:NH2	2.36	0.58
7:G:53:ASN:OD1	7:G:54:ILE:N	2.35	0.58
1:A:425:ASP:OD2	17:Z:583:PHE:CD1	2.55	0.58
1:A:908:THR:HG23	1:A:916:PHE:HE1	1.67	0.58
1:A:1123:ARG:NH1	1:A:1126:GLU:OE1	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:75:SER:HB3	3:C:79:VAL:HG21	1.84	0.58
5:E:101:ARG:HG2	5:E:126:ILE:HD11	1.84	0.58
3:C:133:ARG:NH2	3:C:237:GLY:O	2.36	0.58
1:A:904:GLN:NE2	1:A:982:ASN:HA	2.18	0.58
8:H:32:SER:HB3	8:H:37:MET:H	1.67	0.58
1:A:274:ASP:OD1	1:A:275:ASP:N	2.35	0.58
5:E:26:TYR:HD1	5:E:64:HIS:HA	1.67	0.58
6:F:52:ILE:O	6:F:53:THR:HG23	2.03	0.58
2:B:67:LEU:HD21	2:B:423:ILE:HG13	1.86	0.58
5:E:112:PRO:HB3	15:T:9:DT:H5"	1.85	0.58
1:A:461:GLN:HE22	1:A:502:ASN:ND2	2.01	0.57
2:B:508:MET:SD	2:B:667:THR:HG23	2.43	0.57
2:B:864:ASP:OD1	17:Z:725:LYS:NZ	2.36	0.57
2:B:663:GLU:OE1	2:B:695:HIS:NE2	2.27	0.57
2:B:956:PHE:HE2	3:C:184:PHE:HB3	1.66	0.57
3:C:5:ASN:HD21	3:C:26:THR:HA	1.70	0.57
5:E:48:PRO:HA	5:E:53:PRO:HG2	1.87	0.57
5:E:118:LEU:HD22	5:E:127:LEU:HB2	1.86	0.57
1:A:387:ASN:ND2	2:B:1061:SER:OG	2.30	0.57
2:B:84:TYR:CE2	2:B:423:ILE:HD12	2.39	0.57
1:A:1451:MET:HE1	1:A:1460:LEU:HD12	1.85	0.57
1:A:370:ASP:CG	11:K:65:HIS:HE2	2.07	0.57
1:A:576:GLN:HE21	1:A:580:LEU:HD21	1.68	0.57
2:B:841:ARG:NH2	14:P:39:U:O2	2.38	0.57
1:A:381:PRO:HG2	1:A:384:ILE:HB	1.85	0.57
1:A:1473:LEU:HD22	6:F:104:ILE:HG21	1.86	0.57
2:B:760:THR:OG1	2:B:764:MET:SD	2.62	0.57
1:A:11:SER:N	2:B:1135:TYR:OH	2.38	0.57
1:A:876:ASP:O	1:A:890:ARG:NH1	2.37	0.57
1:A:1281:ASP:O	1:A:1285:LEU:N	2.36	0.57
1:A:802:PHE:HE2	1:A:808:PRO:CD	2.18	0.57
2:B:875:GLU:O	2:B:879:GLU:N	2.34	0.57
2:B:1115:GLN:HB3	2:B:1148:LEU:HD11	1.86	0.57
3:C:74:THR:O	3:C:127:VAL:HG12	2.05	0.57
2:B:179:LEU:HD22	2:B:768:ARG:HD3	1.87	0.56
2:B:667:THR:O	2:B:670:GLU:N	2.35	0.56
17:Z:507:THR:HG22	17:Z:633:GLY:HA3	1.87	0.56
1:A:576:GLN:O	1:A:590:GLN:NE2	2.38	0.56
2:B:177:CYS:HG	2:B:738:THR:HG1	1.53	0.56
5:E:74:VAL:HG22	5:E:103:LEU:HD12	1.86	0.56
1:A:346:LYS:NZ	15:T:21:DG:OP2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:ILE:HD11	3:C:101:PHE:HD2	1.70	0.56
1:A:994:PHE:CE2	1:A:1064:ALA:HA	2.41	0.56
4:D:112:LYS:HB3	4:D:119:GLU:OE2	2.06	0.56
7:G:6:SER:HG	7:G:73:LYS:HZ3	1.53	0.56
1:A:555:LEU:HD12	1:A:591:ILE:HD12	1.86	0.56
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.38	0.56
1:A:1262:MET:HG2	1:A:1265:ASP:H	1.71	0.56
5:E:73:PHE:CE2	5:E:99:ILE:HG12	2.40	0.56
2:B:193:VAL:O	2:B:467:SER:HA	2.05	0.56
2:B:968:ASN:OD1	2:B:969:PRO:HD2	2.06	0.56
2:B:585:ASN:OD1	2:B:588:ARG:NH2	2.39	0.55
1:A:137:PRO:HB2	1:A:1445:HIS:HB3	1.88	0.55
1:A:457:ILE:HD11	1:A:515:ILE:HG12	1.87	0.55
1:A:1087:VAL:HG12	1:A:1400:LEU:HD22	1.88	0.55
1:A:1476:ASP:HB2	6:F:105:ILE:HG23	1.88	0.55
7:G:116:GLU:O	7:G:130:THR:HA	2.04	0.55
1:A:805:ARG:NH2	2:B:673:VAL:O	2.25	0.55
1:A:92:LYS:HD3	1:A:307:VAL:HG21	1.89	0.55
2:B:217:TYR:OH	9:I:103:ARG:NH2	2.39	0.55
3:C:18:ASN:OD1	3:C:19:VAL:N	2.39	0.55
16:Y:25:ILE:HD11	16:Y:50:TYR:CZ	2.42	0.55
17:Z:448:ILE:O	17:Z:449:THR:OG1	2.23	0.55
2:B:131:THR:HG22	2:B:141:GLN:HB3	1.88	0.55
2:B:876:ASN:OD1	2:B:877:GLU:N	2.40	0.55
7:G:30:LEU:HD22	7:G:70:VAL:HG11	1.88	0.55
1:A:92:LYS:NZ	1:A:219:GLU:OE2	2.30	0.55
1:A:644:SER:O	1:A:651:SER:HB2	2.07	0.55
1:A:1130:ILE:HD13	1:A:1411:LEU:HD22	1.89	0.55
2:B:95:LYS:HB3	2:B:162:LEU:HD21	1.88	0.55
2:B:419:ALA:O	2:B:423:ILE:HG12	2.07	0.55
2:B:427:LYS:HG3	2:B:428:ASP:H	1.71	0.55
8:H:88:PHE:CD2	8:H:144:LEU:HB3	2.41	0.55
1:A:355:MET:O	2:B:1091:ARG:HD2	2.07	0.55
7:G:92:VAL:HG13	7:G:128:TYR:CE2	2.41	0.55
17:Z:552:ARG:HB3	17:Z:559:GLN:HB2	1.88	0.55
1:A:514:GLU:OE2	2:B:1101:GLN:HB2	2.07	0.55
1:A:890:ARG:HE	1:A:1023:VAL:HG22	1.72	0.55
8:H:91:VAL:HG22	8:H:144:LEU:HD23	1.89	0.55
2:B:114:ARG:NH2	2:B:184:TYR:OH	2.39	0.54
2:B:773:PRO:HG2	10:J:53:VAL:HG21	1.88	0.54
7:G:124:ASN:CB	7:G:125:PRO:HD3	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1117:VAL:HA	1:A:1136:THR:HG21	1.89	0.54
8:H:112:LEU:HB2	8:H:132:LEU:HD23	1.90	0.54
5:E:63:ALA:HA	5:E:71:GLN:HA	1.89	0.54
17:Z:498:ASN:O	17:Z:515:PRO:HD3	2.08	0.54
3:C:5:ASN:ND2	3:C:26:THR:HA	2.22	0.54
5:E:171:PRO:HB2	5:E:207:ARG:HD3	1.90	0.54
15:T:29:DT:C2'	15:T:30:DA:OP1	2.51	0.54
2:B:407:MET:HE1	2:B:444:LEU:N	2.23	0.54
2:B:617:ASP:OD1	2:B:618:ALA:N	2.40	0.54
1:A:386:ALA:O	1:A:449:HIS:ND1	2.41	0.54
2:B:422:PHE:HE2	2:B:429:PHE:HA	1.73	0.54
3:C:190:ASN:ND2	3:C:195:THR:O	2.40	0.54
1:A:26:LEU:HD13	1:A:31:LEU:HD21	1.90	0.54
1:A:228:ILE:O	1:A:244:ARG:NH2	2.26	0.54
1:A:573:LYS:NZ	8:H:74:GLU:OE2	2.33	0.54
2:B:692:THR:HG21	9:I:80:ARG:HH12	1.73	0.54
1:A:155:GLU:HA	1:A:185:GLY:HA2	1.90	0.54
2:B:833:THR:HG22	2:B:835:GLU:H	1.73	0.54
17:Z:466:GLN:OE1	17:Z:466:GLN:N	2.38	0.54
17:Z:607:HIS:HB3	17:Z:610:ARG:HD2	1.90	0.54
1:A:1005:HIS:ND1	1:A:1006:PRO:HD2	2.23	0.53
2:B:811:TYR:CD1	2:B:924:ARG:HB3	2.43	0.53
8:H:96:VAL:HA	8:H:116:VAL:HA	1.89	0.53
1:A:97:VAL:HG21	1:A:322:LEU:HD11	1.90	0.53
1:A:375:ILE:HD11	1:A:669:TYR:CD1	2.43	0.53
1:A:1184:THR:OG1	1:A:1190:GLN:NE2	2.41	0.53
2:B:119:THR:HG23	2:B:187:ILE:HA	1.90	0.53
2:B:587:LEU:HB3	2:B:603:MET:SD	2.49	0.53
4:D:31:THR:HG22	7:G:3:TYR:CE1	2.43	0.53
2:B:192:LYS:NZ	2:B:449:ALA:O	2.41	0.53
2:B:924:ARG:HH12	3:C:62:GLU:CD	2.09	0.53
2:B:516:GLU:HA	2:B:520:VAL:HG22	1.91	0.53
17:Z:519:GLN:NE2	17:Z:521:CYS:SG	2.81	0.53
1:A:384:ILE:HD11	2:B:1059:ILE:HG13	1.91	0.53
1:A:18:ILE:HD12	2:B:1171:MET:HB3	1.90	0.53
1:A:511:THR:HG21	2:B:1105:GLU:OE1	2.08	0.53
1:A:601:ASN:CG	1:A:988:TRP:HZ3	2.12	0.53
1:A:1205:ALA:HB1	1:A:1267:ASN:HB2	1.90	0.53
2:B:533:SER:HB2	2:B:600:GLU:HG3	1.91	0.53
2:B:865:VAL:HG22	2:B:895:PHE:CE1	2.44	0.53
3:C:59:LEU:HD13	3:C:63:PHE:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:863:ARG:NH2	1:A:1414:ILE:O	2.41	0.53
1:A:1370:GLY:HA2	5:E:177:ASP:OD1	2.09	0.53
2:B:625:LEU:HD13	2:B:675:LEU:HD21	1.91	0.53
10:J:21:TYR:HB2	10:J:38:LEU:HD11	1.91	0.53
2:B:789:ASN:HB3	2:B:795:ILE:HG13	1.92	0.52
3:C:44:ILE:HD12	3:C:178:PRO:HA	1.91	0.52
2:B:334:LYS:NZ	17:Z:236:LYS:NZ	2.57	0.52
2:B:728:MET:SD	2:B:942:LYS:HD3	2.50	0.52
1:A:1030:SER:OG	5:E:162:ARG:NE	2.28	0.52
1:A:1171:ALA:HA	9:I:59:THR:HB	1.92	0.52
9:I:113:VAL:HG22	9:I:122:ARG:HG2	1.90	0.52
1:A:287:ASN:O	1:A:291:ARG:HG2	2.09	0.52
2:B:1115:GLN:HG2	2:B:1150:ARG:HD2	1.91	0.52
8:H:58:LEU:HD11	8:H:143:LEU:CD1	2.35	0.52
1:A:20:ARG:NH1	1:A:22:GLN:OE1	2.43	0.52
3:C:35:ARG:HB3	3:C:231:TYR:HE2	1.74	0.52
2:B:796:MET:SD	2:B:935:PHE:HE2	2.33	0.52
7:G:109:SER:HB3	17:Z:493:VAL:HG11	1.90	0.52
3:C:40:ALA:O	3:C:170:GLY:N	2.38	0.52
5:E:14:ARG:O	5:E:18:MET:HG2	2.10	0.52
17:Z:488:ASP:OD1	17:Z:489:THR:N	2.42	0.52
1:A:413:TYR:HB3	1:A:414:PRO:HD3	1.92	0.52
1:A:1026:ASP:OD1	1:A:1031:ARG:NH2	2.42	0.52
2:B:873:LEU:HD12	2:B:874:PRO:HD2	1.92	0.52
4:D:71:PHE:CZ	7:G:142:GLU:HG2	2.45	0.52
11:K:64:PRO:HG3	11:K:72:ILE:HD12	1.92	0.52
14:P:33:U:H2'	14:P:34:A:H8	1.75	0.52
1:A:364:ARG:HB2	2:B:1084:LEU:HD11	1.92	0.51
7:G:148:VAL:HG21	17:Z:474:MET:HE2	1.92	0.51
9:I:81:THR:HG23	9:I:96:PHE:HE2	1.74	0.51
2:B:59:VAL:HG21	2:B:91:ILE:HD12	1.90	0.51
1:A:199:TYR:HE1	1:A:215:LEU:HD23	1.74	0.51
1:A:1485:GLU:HB3	6:F:78:PRO:HB3	1.92	0.51
2:B:1142:ASN:HD21	2:B:1145:GLN:HG3	1.75	0.51
1:A:994:PHE:HE2	1:A:1064:ALA:HA	1.76	0.51
2:B:295:PRO:HG3	9:I:11:ILE:HG23	1.92	0.51
2:B:798:ARG:HB2	2:B:948:GLN:HB3	1.92	0.51
2:B:1072:ARG:O	2:B:1112:ASP:HB3	2.11	0.51
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.91	0.51
13:N:4:DA:C2	15:T:41:DG:N2	2.78	0.51
2:B:217:TYR:CE2	2:B:376:ALA:HA	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:423:ILE:O	2:B:426:GLY:N	2.38	0.51
7:G:22:LEU:O	7:G:26:VAL:HG23	2.11	0.51
9:I:64:GLU:O	9:I:68:ILE:HG12	2.10	0.51
1:A:46:THR:HG23	1:A:58:MET:HB3	1.93	0.51
1:A:222:HIS:CD2	1:A:226:LYS:HE3	2.46	0.51
1:A:828:LEU:HD11	2:B:1008:VAL:HG21	1.92	0.51
2:B:470:LEU:HD11	2:B:478:THR:HG23	1.92	0.51
2:B:534:VAL:N	2:B:600:GLU:OE2	2.44	0.51
1:A:383:SER:OG	11:K:2:ASN:ND2	2.35	0.51
2:B:19:PRO:C	2:B:21:LEU:H	2.15	0.51
8:H:18:GLU:HG3	8:H:19:GLY:H	1.75	0.51
1:A:1102:MET:HG2	1:A:1389:ASP:OD2	2.10	0.51
2:B:22:TRP:O	2:B:25:ALA:N	2.43	0.51
2:B:474:THR:OG1	2:B:732:ALA:O	2.29	0.51
5:E:45:GLY:HA3	5:E:52:ARG:HH11	1.75	0.51
16:Y:25:ILE:CD1	16:Y:50:TYR:CZ	2.93	0.50
17:Z:471:TYR:C	17:Z:472:PHE:CG	2.85	0.50
2:B:231:PRO:O	2:B:232:THR:HG23	2.10	0.50
2:B:411:LEU:HD11	2:B:435:ILE:HG23	1.94	0.50
5:E:148:HIS:CE1	5:E:179:VAL:HG11	2.46	0.50
3:C:40:ALA:HB1	3:C:171:LYS:HG3	1.94	0.50
8:H:64:LEU:HD13	8:H:84:ARG:HD2	1.94	0.50
1:A:784:VAL:HG22	2:B:978:ILE:HD11	1.93	0.50
2:B:792:ASP:O	2:B:943:GLY:HA3	2.12	0.50
14:P:36:A:H4'	14:P:37:C:OP1	2.11	0.50
1:A:552:ASP:OD1	8:H:22:PHE:HB3	2.11	0.50
2:B:692:THR:CG2	9:I:80:ARG:HH12	2.25	0.50
8:H:7:GLU:HG2	8:H:59:VAL:HG22	1.93	0.50
1:A:421:ARG:HA	1:A:444:TYR:CD1	2.46	0.50
7:G:92:VAL:HG21	7:G:127:CYS:HA	1.94	0.50
1:A:918:LYS:O	1:A:1052:ARG:NH2	2.45	0.50
2:B:459:ALA:HA	2:B:462:ALA:HB3	1.93	0.50
2:B:473:LEU:HD21	2:B:1052:LYS:HD3	1.93	0.50
3:C:193:ARG:HH12	3:C:217:GLN:CD	2.15	0.50
4:D:103:LEU:HD11	7:G:84:VAL:HB	1.94	0.50
1:A:425:ASP:OD2	17:Z:583:PHE:CD2	2.66	0.49
1:A:733:LEU:HA	1:A:736:THR:HG22	1.94	0.49
2:B:548:TRP:O	2:B:549:SER:OG	2.24	0.49
5:E:87:ILE:HD11	5:E:110:MET:HE1	1.94	0.49
17:Z:471:TYR:O	17:Z:472:PHE:CD1	2.63	0.49
1:A:506:PRO:HG3	1:A:515:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:ILE:HD11	1:A:769:MET:SD	2.53	0.49
3:C:159:LEU:HD11	3:C:161:LEU:HD23	1.94	0.49
16:Y:60:ILE:CD1	17:Z:190:ARG:HG3	2.42	0.49
2:B:193:VAL:HG23	2:B:470:LEU:HB2	1.94	0.49
5:E:7:THR:HG21	5:E:41:LYS:HZ3	1.76	0.49
10:J:56:ILE:O	10:J:60:LEU:HG	2.13	0.49
1:A:908:THR:HG23	1:A:916:PHE:CE1	2.46	0.49
1:A:1292:MET:O	1:A:1296:MET:HG2	2.11	0.49
2:B:35:ASP:OD2	2:B:646:ARG:NH2	2.44	0.49
7:G:11:ILE:N	7:G:11:ILE:HD13	2.28	0.49
1:A:1139:LEU:HB3	1:A:1338:THR:OG1	2.12	0.49
2:B:144:HIS:ND1	2:B:431:LEU:HD12	2.27	0.49
2:B:713:PHE:HB3	2:B:716:HIS:HD2	1.77	0.49
1:A:1182:GLN:O	1:A:1190:GLN:NE2	2.29	0.49
1:A:1286:ARG:HH21	9:I:54:TYR:HB2	1.78	0.49
6:F:97:LEU:HD13	6:F:102:ILE:HD12	1.95	0.49
1:A:11:SER:N	2:B:1135:TYR:HH	2.11	0.49
1:A:1227:THR:HG22	1:A:1229:GLU:H	1.76	0.49
2:B:85:LEU:HB2	2:B:131:THR:OG1	2.12	0.49
3:C:56:SER:HB2	3:C:158:GLU:H	1.78	0.49
3:C:169:PHE:HE1	3:C:171:LYS:HD2	1.77	0.49
14:P:33:U:H2'	14:P:34:A:C8	2.47	0.49
17:Z:474:MET:HA	17:Z:492:ILE:HG13	1.94	0.49
4:D:135:GLN:HA	4:D:138:ARG:HD3	1.95	0.49
5:E:122:ALA:HB3	5:E:123:PRO:HD3	1.94	0.49
9:I:73:SER:HA	9:I:95:VAL:HG11	1.95	0.49
10:J:3:ILE:HG13	10:J:4:PRO:HD2	1.95	0.49
17:Z:266:VAL:CG1	17:Z:268:LYS:HE2	2.43	0.49
1:A:255:VAL:HG13	1:A:280:LEU:HD13	1.95	0.49
1:A:421:ARG:NE	1:A:427:ILE:HD11	2.27	0.49
1:A:769:MET:SD	2:B:973:PRO:HG3	2.53	0.49
1:A:1319:LYS:HE2	1:A:1321:ILE:HD11	1.93	0.49
2:B:256:ILE:HG22	2:B:269:ILE:HG13	1.95	0.49
2:B:491:ARG:HB3	2:B:518:HIS:HD2	1.77	0.49
3:C:9:VAL:HG11	11:K:105:PHE:HD1	1.78	0.49
1:A:601:ASN:CG	1:A:988:TRP:CZ3	2.86	0.48
1:A:1155:LYS:HA	1:A:1309:MET:HE1	1.94	0.48
1:A:1210:TRP:HZ3	9:I:53:ILE:HD12	1.77	0.48
2:B:159:THR:HA	2:B:164:ASN:ND2	2.28	0.48
2:B:196:ALA:HB2	2:B:395:LEU:HD23	1.94	0.48
3:C:45:ILE:HG13	3:C:79:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:173:ILE:HG23	5:E:209:VAL:HG22	1.94	0.48
8:H:11:ASP:OD1	8:H:55:LYS:HG2	2.13	0.48
13:N:12:DT:H5"	17:Z:283:ARG:NH2	2.27	0.48
1:A:40:GLY:O	1:A:42:LYS:HG3	2.13	0.48
1:A:425:ASP:CG	17:Z:583:PHE:CE2	2.86	0.48
2:B:334:LYS:NZ	17:Z:236:LYS:HZ3	2.11	0.48
2:B:910:THR:HG21	12:L:43:ILE:HG12	1.95	0.48
2:B:1101:GLN:HA	2:B:1104:ARG:HG2	1.96	0.48
7:G:93:ASN:O	7:G:128:TYR:OH	2.24	0.48
1:A:757:GLN:NE2	1:A:778:LYS:HB3	2.27	0.48
8:H:115:TYR:HE1	8:H:124:ARG:HD3	1.77	0.48
9:I:97:PHE:HB2	9:I:100:HIS:HE2	1.78	0.48
11:K:87:PHE:CE2	11:K:91:ILE:HD11	2.48	0.48
1:A:497:ASP:OD1	1:A:497:ASP:N	2.46	0.48
1:A:514:GLU:OE2	1:A:1468:THR:HG21	2.12	0.48
1:A:732:THR:HG22	1:A:734:ARG:H	1.79	0.48
2:B:84:TYR:HE2	2:B:423:ILE:HG23	1.79	0.48
2:B:795:ILE:HG12	2:B:947:ILE:HG22	1.95	0.48
2:B:835:GLU:O	2:B:887:TYR:HE1	1.96	0.48
17:Z:471:TYR:CG	17:Z:472:PHE:N	2.81	0.48
17:Z:521:CYS:HB3	17:Z:523:GLU:OE1	2.14	0.48
1:A:349:ARG:NH2	2:B:1070:LEU:HD21	2.29	0.48
2:B:384:ASP:HB3	2:B:387:HIS:HB2	1.95	0.48
2:B:598:VAL:HG12	2:B:600:GLU:H	1.79	0.48
10:J:5:VAL:HG12	10:J:6:ARG:HG2	1.96	0.48
1:A:470:MET:HG2	1:A:524:MET:SD	2.54	0.48
1:A:485:ASN:ND2	1:A:673:GLN:OE1	2.37	0.48
8:H:104:THR:OG1	8:H:107:GLU:OE2	2.31	0.48
17:Z:728:THR:OG1	17:Z:731:THR:N	2.47	0.48
1:A:1052:ARG:HE	1:A:1056:GLU:CD	2.17	0.48
3:C:47:ILE:HD11	3:C:101:PHE:CD2	2.49	0.48
1:A:100:LEU:HD21	1:A:193:ARG:HD2	1.95	0.48
1:A:472:HIS:CE1	1:A:521:VAL:HG21	2.49	0.48
1:A:602:CYS:SG	1:A:604:ARG:HG2	2.54	0.48
1:A:823:VAL:HG11	1:A:831:LEU:HD22	1.95	0.48
2:B:866:ILE:HD11	2:B:896:LEU:HG	1.95	0.48
2:B:907:VAL:HG13	2:B:921:ILE:HG12	1.96	0.48
5:E:44:PHE:O	5:E:53:PRO:HD3	2.14	0.47
8:H:88:PHE:HD2	8:H:144:LEU:HD22	1.79	0.47
1:A:456:VAL:HG21	1:A:503:LEU:HD11	1.96	0.47
2:B:1104:ARG:O	2:B:1108:PHE:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:926:ASN:C	1:A:928:ARG:H	2.17	0.47
2:B:19:PRO:O	2:B:21:LEU:N	2.44	0.47
2:B:812:ARG:HH12	2:B:897:ARG:HE	1.62	0.47
2:B:835:GLU:O	2:B:887:TYR:CE1	2.66	0.47
7:G:95:VAL:HG11	17:Z:630:VAL:HG21	1.96	0.47
1:A:96:HIS:HB2	1:A:250:VAL:HG23	1.96	0.47
17:Z:706:ILE:HD11	17:Z:727:ALA:H	1.79	0.47
1:A:351:ARG:HG3	2:B:1088:GLU:OE2	2.15	0.47
2:B:109:MET:CE	2:B:174:LEU:HD13	2.39	0.47
2:B:854:ILE:HG22	2:B:855:ALA:O	2.15	0.47
7:G:127:CYS:HB2	7:G:138:GLN:HB3	1.97	0.47
17:Z:503:PHE:HD1	17:Z:508:MET:O	1.98	0.47
2:B:427:LYS:HG3	2:B:428:ASP:N	2.30	0.47
2:B:456:GLN:H	2:B:456:GLN:CD	2.16	0.47
3:C:77:ASP:HB2	3:C:126:ARG:HH21	1.79	0.47
1:A:350:VAL:O	1:A:355:MET:HG2	2.14	0.47
1:A:496:PHE:HD2	2:B:791:GLU:HB2	1.79	0.47
1:A:924:TYR:HA	1:A:930:LEU:HD11	1.96	0.47
1:A:1318:LYS:HE2	1:A:1330:ALA:HB1	1.96	0.47
2:B:399:LEU:HB3	2:B:453:TRP:CZ2	2.49	0.47
2:B:535:GLY:N	2:B:600:GLU:OE2	2.27	0.47
4:D:135:GLN:OE1	4:D:138:ARG:NH1	2.47	0.47
15:T:23:DC:H2"	15:T:24:DT:H5'	1.96	0.47
2:B:44:LEU:HD23	2:B:155:MET:SD	2.55	0.47
3:C:59:LEU:HD13	3:C:63:PHE:HE2	1.80	0.47
3:C:72:PRO:HG3	10:J:13:ILE:CD1	2.45	0.47
5:E:171:PRO:HD2	5:E:206:TYR:O	2.15	0.47
1:A:610:PRO:HG2	1:A:613:GLU:HB2	1.96	0.47
2:B:389:GLY:O	2:B:668:LEU:HD23	2.15	0.47
13:N:4:DA:C2	15:T:41:DG:C2	3.03	0.47
17:Z:535:GLU:O	17:Z:538:GLU:HG2	2.14	0.47
1:A:406:VAL:HG11	1:A:419:ILE:HD11	1.97	0.47
1:A:457:ILE:HG13	1:A:515:ILE:HD13	1.97	0.47
1:A:460:ARG:NH2	14:P:50:C:O2'	2.42	0.46
1:A:524:MET:CE	2:B:1097:HIS:HE1	2.28	0.46
1:A:902:GLU:OE1	1:A:982:ASN:HB2	2.15	0.46
1:A:379:GLY:O	1:A:482:PHE:HA	2.16	0.46
1:A:425:ASP:OD2	17:Z:583:PHE:CG	2.68	0.46
5:E:77:PRO:HD2	5:E:105:VAL:O	2.15	0.46
7:G:86:ASP:OD1	7:G:144:ARG:NE	2.48	0.46
1:A:1026:ASP:O	1:A:1031:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ARG:HH21	1:A:412:GLN:HB3	1.79	0.46
1:A:587:THR:HG22	1:A:589:LYS:H	1.80	0.46
1:A:760:LEU:HD11	1:A:781:ILE:HG21	1.97	0.46
1:A:839:HIS:CD2	2:B:719:SER:HB3	2.50	0.46
2:B:572:CYS:O	2:B:574:VAL:HG23	2.15	0.46
5:E:24:ARG:NH2	5:E:181:ARG:O	2.48	0.46
17:Z:447:LYS:HA	17:Z:464:PRO:HA	1.97	0.46
2:B:750:VAL:O	2:B:808:SER:HB2	2.16	0.46
8:H:103:GLU:HB3	8:H:109:ALA:HB2	1.96	0.46
1:A:301:HIS:HD2	17:Z:259:GLU:OE1	1.98	0.46
14:P:33:U:H4'	17:Z:619:ARG:HG2	1.97	0.46
17:Z:502:LEU:HD11	17:Z:511:LEU:HD12	1.98	0.46
1:A:527:THR:HB	1:A:534:VAL:CG2	2.45	0.46
1:A:557:ARG:O	1:A:561:MET:HG2	2.16	0.46
2:B:201:ALA:HB3	2:B:206:TYR:OH	2.16	0.46
2:B:812:ARG:HH12	2:B:897:ARG:NE	2.13	0.46
2:B:904:VAL:HG22	2:B:923:VAL:HG22	1.98	0.46
5:E:94:MET:HG2	5:E:99:ILE:HD11	1.98	0.46
1:A:362:SER:HA	1:A:503:LEU:O	2.16	0.46
2:B:633:LEU:HD11	2:B:679:PRO:HG3	1.98	0.46
2:B:812:ARG:NH1	2:B:897:ARG:HE	2.13	0.46
2:B:854:ILE:CD1	2:B:866:ILE:HA	2.46	0.46
2:B:540:PRO:HB2	2:B:596:ILE:HG23	1.97	0.46
2:B:753:TYR:O	2:B:776:ILE:HG12	2.16	0.46
1:A:33:ARG:HB3	2:B:1139:GLY:HA2	1.98	0.46
1:A:597:PRO:HD3	1:A:668:PHE:HD1	1.78	0.46
1:A:802:PHE:HE1	2:B:504:THR:HG22	1.81	0.46
1:A:1394:ASN:OD1	1:A:1395:TYR:N	2.48	0.46
2:B:949:TYR:HB3	2:B:953:ASP:HB2	1.98	0.46
6:F:52:ILE:O	6:F:52:ILE:HG13	2.15	0.46
7:G:10:GLU:HB3	7:G:67:LEU:CG	2.43	0.46
1:A:37:THR:HG22	1:A:61:ARG:HD2	1.98	0.45
1:A:432:HIS:NE2	17:Z:728:THR:HG22	2.31	0.45
1:A:790:GLN:NE2	1:A:797:ARG:HG3	2.31	0.45
2:B:605:ARG:NH1	2:B:607:ILE:HG12	2.31	0.45
2:B:622:CYS:HB3	2:B:666:ASP:HB3	1.98	0.45
2:B:1062:ARG:NH1	2:B:1065:GLY:HA3	2.31	0.45
3:C:103:LEU:O	3:C:160:ARG:HA	2.17	0.45
6:F:105:ILE:HA	6:F:119:GLY:HA2	1.97	0.45
12:L:16:ILE:HG12	12:L:27:GLU:HG2	1.99	0.45
1:A:1451:MET:CE	1:A:1460:LEU:HD12	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1467:GLY:O	1:A:1468:THR:HB	2.17	0.45
2:B:955:PRO:O	2:B:963:PRO:HD2	2.16	0.45
2:B:1029:TYR:CD1	2:B:1036:LYS:HG2	2.50	0.45
8:H:18:GLU:HG3	8:H:19:GLY:N	2.31	0.45
1:A:488:VAL:O	1:A:491:PRO:HD2	2.16	0.45
1:A:741:VAL:HG11	1:A:797:ARG:NH1	2.31	0.45
3:C:7:PRO:HB3	3:C:26:THR:OG1	2.17	0.45
3:C:259:LEU:HD22	11:K:19:ILE:HD11	1.98	0.45
1:A:922:PHE:CD2	1:A:952:LEU:HD23	2.52	0.45
2:B:856:PRO:HG2	12:L:48:ARG:HA	1.97	0.45
1:A:350:VAL:HA	1:A:354:LEU:HD12	1.98	0.45
1:A:487:SER:OG	1:A:673:GLN:NE2	2.49	0.45
2:B:388:TYR:CE2	2:B:621:ILE:HG21	2.52	0.45
2:B:627:ILE:HD12	2:B:660:GLY:O	2.16	0.45
2:B:715:ASP:N	2:B:715:ASP:OD1	2.47	0.45
3:C:77:ASP:OD2	3:C:126:ARG:NH2	2.50	0.45
5:E:82:VAL:HB	5:E:110:MET:SD	2.56	0.45
8:H:10:PHE:CE2	8:H:39:LEU:HD22	2.50	0.45
12:L:17:TYR:HE1	12:L:46:LYS:HD2	1.82	0.45
1:A:375:ILE:HD11	1:A:669:TYR:CG	2.51	0.45
3:C:172:GLU:HG2	11:K:10:PHE:CE1	2.52	0.45
7:G:97:LEU:HD12	7:G:128:TYR:CE2	2.52	0.45
3:C:49:TRP:NE1	12:L:54:VAL:HG11	2.32	0.45
8:H:55:LYS:O	8:H:148:LEU:N	2.46	0.45
1:A:932:ARG:NH2	8:H:103:GLU:OE1	2.45	0.45
1:A:1262:MET:HB3	1:A:1265:ASP:HB2	1.99	0.45
2:B:419:ALA:HA	2:B:429:PHE:CE1	2.52	0.45
3:C:197:TYR:HD2	3:C:217:GLN:HE21	1.64	0.45
7:G:129:LYS:CB	7:G:136:VAL:HG22	2.47	0.45
1:A:1065:PHE:CE2	1:A:1069:LEU:HD11	2.52	0.45
2:B:496:ALA:O	2:B:500:GLN:HG3	2.16	0.45
2:B:794:VAL:O	2:B:946:GLY:N	2.30	0.45
2:B:859:ARG:HD2	17:Z:737:HIS:HA	1.99	0.45
1:A:109:CYS:SG	1:A:145:TYR:HA	2.57	0.45
1:A:529:GLN:O	1:A:1394:ASN:HB2	2.17	0.45
1:A:922:PHE:H	1:A:1052:ARG:HD2	1.82	0.45
3:C:19:VAL:HG12	3:C:21:PHE:HD1	1.81	0.45
6:F:76:CYS:O	7:G:16:ARG:HA	2.18	0.45
7:G:92:VAL:HG13	7:G:128:TYR:CD2	2.52	0.45
11:K:21:ILE:HG23	11:K:31:CYS:SG	2.57	0.45
17:Z:509:HIS:HD2	17:Z:552:ARG:NH1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:837:PHE:HB2	2:B:506:TRP:HZ3	1.81	0.44
2:B:350:HIS:HD2	2:B:572:CYS:SG	2.41	0.44
2:B:489:ILE:HD11	13:N:25:DA:C5	2.51	0.44
2:B:801:VAL:HG13	2:B:929:PRO:HG2	1.98	0.44
2:B:962:THR:O	10:J:9:THR:HG23	2.18	0.44
2:B:978:ILE:O	2:B:981:LEU:N	2.44	0.44
6:F:75:MET:HB2	7:G:15:PRO:HG2	2.00	0.44
17:Z:224:TYR:HE2	17:Z:226:TYR:CZ	2.35	0.44
1:A:35:SER:OG	1:A:86:GLY:HA2	2.17	0.44
1:A:1197:TYR:HD1	1:A:1200:PRO:HB3	1.81	0.44
2:B:1012:SER:HB3	2:B:1022:LEU:HB2	2.00	0.44
2:B:1124:ILE:HG22	2:B:1125:MET:N	2.31	0.44
8:H:8:ASP:OD2	8:H:32:SER:OG	2.24	0.44
1:A:983:LEU:HD23	1:A:983:LEU:HA	1.80	0.44
2:B:466:VAL:O	2:B:467:SER:OG	2.32	0.44
2:B:838:GLN:HB2	2:B:887:TYR:HB3	1.99	0.44
3:C:19:VAL:HG23	3:C:241:PRO:HB2	1.99	0.44
17:Z:482:ALA:HA	17:Z:486:GLU:OE1	2.17	0.44
17:Z:514:LEU:HB3	17:Z:515:PRO:HD2	1.99	0.44
1:A:461:GLN:HE22	1:A:502:ASN:HD21	1.66	0.44
1:A:549:THR:O	1:A:589:LYS:HE3	2.18	0.44
1:A:1173:THR:HG23	1:A:1214:VAL:HG12	1.99	0.44
2:B:568:PHE:HE1	2:B:573:TRP:CD1	2.25	0.44
2:B:991:ALA:HB1	10:J:43:TYR:HB2	1.99	0.44
8:H:37:MET:HG2	8:H:127:GLY:HA3	2.00	0.44
9:I:106:ASP:OD1	9:I:106:ASP:N	2.50	0.44
17:Z:484:ARG:HH11	17:Z:485:PHE:HE1	1.64	0.44
1:A:576:GLN:HA	8:H:75:TYR:HB2	1.98	0.44
2:B:1078:ARG:N	15:T:24:DT:OP1	2.51	0.44
17:Z:734:VAL:HG21	17:Z:750:LEU:HD21	1.99	0.44
1:A:441:GLN:HG2	1:A:444:TYR:CE2	2.52	0.44
2:B:809:VAL:HG21	3:C:60:HIS:CE1	2.52	0.44
10:J:3:ILE:HD13	10:J:18:TRP:HB2	1.99	0.44
14:P:39:U:H2'	14:P:40:A:C8	2.52	0.44
1:A:581:LYS:NZ	8:H:86:ASP:O	2.50	0.44
1:A:1486:ILE:HG13	1:A:1487:PRO:HD3	1.99	0.44
2:B:533:SER:HB2	2:B:600:GLU:CG	2.47	0.44
9:I:24:LEU:HB3	9:I:37:TYR:HB3	1.98	0.44
1:A:551:ARG:NH1	8:H:42:ASP:OD2	2.51	0.44
1:A:802:PHE:CE1	2:B:504:THR:HG22	2.53	0.44
1:A:1243:LEU:HD11	1:A:1259:ILE:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:TYR:OH	2:B:266:GLU:OE2	2.27	0.44
2:B:262:TYR:CD2	2:B:346:GLU:HG3	2.53	0.44
5:E:177:ASP:OD1	5:E:178:PRO:HD2	2.18	0.44
12:L:46:LYS:O	12:L:46:LYS:HG3	2.18	0.44
1:A:544:ALA:HB2	1:A:680:LEU:HD13	2.00	0.43
2:B:1163:MET:HA	2:B:1167:ILE:O	2.18	0.43
17:Z:479:LYS:NZ	17:Z:523:GLU:O	2.31	0.43
1:A:371:PRO:HD2	2:B:788:TYR:CE2	2.52	0.43
1:A:1139:LEU:HD13	1:A:1359:SER:HB3	1.99	0.43
2:B:49:GLU:OE1	2:B:534:VAL:HG22	2.18	0.43
2:B:472:ARG:HD3	2:B:472:ARG:HA	1.82	0.43
10:J:48:MET:O	10:J:52:HIS:HB2	2.18	0.43
17:Z:469:ARG:HD2	17:Z:515:PRO:HG3	1.99	0.43
1:A:1436:VAL:O	1:A:1440:MET:HG2	2.19	0.43
2:B:794:VAL:HG22	2:B:967:ILE:HG22	2.01	0.43
2:B:1155:CYS:O	2:B:1158:LEU:HB3	2.18	0.43
1:A:57:LEU:O	1:A:261:ARG:NH2	2.49	0.43
2:B:1111:SER:O	2:B:1113:PRO:HD3	2.18	0.43
3:C:212:ASP:OD1	3:C:215:GLU:HG2	2.19	0.43
7:G:38:CYS:HB3	7:G:155:ASN:O	2.19	0.43
10:J:30:THR:O	10:J:33:ASP:N	2.51	0.43
11:K:105:PHE:CE2	11:K:109:ILE:HD11	2.53	0.43
17:Z:492:ILE:HG13	17:Z:492:ILE:O	2.19	0.43
1:A:196:LEU:HD13	1:A:311:GLN:HG3	2.01	0.43
1:A:927:GLU:HG3	1:A:943:LEU:HD11	2.00	0.43
1:A:1229:GLU:O	1:A:1233:GLU:HG2	2.19	0.43
1:A:1284:PHE:CE2	1:A:1288:ILE:HD11	2.54	0.43
2:B:187:ILE:HG21	2:B:449:ALA:HB2	2.00	0.43
2:B:235:ILE:HG21	2:B:348:LEU:HD11	2.00	0.43
4:D:25:GLU:OE2	7:G:41:LYS:HE3	2.19	0.43
17:Z:386:VAL:O	17:Z:387:LYS:HB2	2.18	0.43
1:A:760:LEU:HD21	1:A:785:ILE:CD1	2.48	0.43
1:A:1429:LYS:HB2	1:A:1438:VAL:HG11	2.01	0.43
2:B:1050:ARG:HH21	2:B:1054:MET:HG2	1.83	0.43
4:D:90:LYS:HE2	4:D:130:ILE:HD11	1.99	0.43
17:Z:469:ARG:HD2	17:Z:515:PRO:CB	2.49	0.43
1:A:354:LEU:HD21	2:B:1155:CYS:HA	2.00	0.43
1:A:540:ASP:CB	2:B:790:GLN:HE21	2.30	0.43
1:A:1162:GLU:O	1:A:1300:GLY:HA3	2.18	0.43
1:A:1316:ASN:OD1	1:A:1317:LYS:HG2	2.19	0.43
12:L:14:PRO:HG3	12:L:29:LYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Z:471:TYR:C	17:Z:472:PHE:CD2	2.91	0.43
1:A:260:VAL:HG22	2:B:1157:LEU:HD12	2.01	0.43
2:B:558:PRO:O	2:B:561:ILE:HG22	2.19	0.43
9:I:60:HIS:O	9:I:60:HIS:ND1	2.52	0.43
1:A:609:HIS:ND1	1:A:626:THR:OG1	2.31	0.43
2:B:192:LYS:HZ2	2:B:449:ALA:HA	1.84	0.43
2:B:561:ILE:HG13	2:B:576:ILE:HG21	2.00	0.43
2:B:647:GLU:O	2:B:648:TYR:CG	2.72	0.43
4:D:22:PHE:HB3	4:D:23:PRO:HD2	2.01	0.43
8:H:10:PHE:CE1	8:H:32:SER:HB2	2.53	0.43
17:Z:486:GLU:OE2	17:Z:555:ARG:NH2	2.52	0.43
1:A:597:PRO:HG2	1:A:600:ILE:HD12	2.00	0.42
2:B:332:LYS:O	2:B:335:ARG:N	2.49	0.42
1:A:36:VAL:HG22	1:A:85:PHE:O	2.19	0.42
1:A:500:GLU:OE2	2:B:1058:LYS:HB3	2.18	0.42
2:B:719:SER:OG	2:B:720:PRO:HD3	2.20	0.42
2:B:1159:PHE:CD2	2:B:1171:MET:HE3	2.53	0.42
3:C:40:ALA:O	3:C:169:PHE:HB2	2.19	0.42
16:Y:14:ARG:HD2	16:Y:25:ILE:HD12	2.01	0.42
1:A:764:ASN:OD1	1:A:765:ASN:N	2.52	0.42
1:A:823:VAL:HG13	1:A:835:GLU:HB3	2.01	0.42
1:A:1007:ILE:O	1:A:1010:VAL:N	2.51	0.42
1:A:1316:ASN:OD1	1:A:1317:LYS:N	2.52	0.42
1:A:1357:THR:O	5:E:142:HIS:NE2	2.50	0.42
1:A:1412:MET:SD	1:A:1422:GLN:NE2	2.92	0.42
2:B:428:ASP:OD1	2:B:429:PHE:N	2.47	0.42
2:B:1038:THR:HA	3:C:195:THR:HA	2.01	0.42
7:G:13:LEU:HD22	7:G:68:TYR:CE1	2.55	0.42
13:N:7:DA:C2	15:T:38:DA:C2	3.07	0.42
17:Z:271:ALA:O	17:Z:272:ASN:HB3	2.18	0.42
1:A:94:VAL:HG13	1:A:311:GLN:OE1	2.19	0.42
1:A:527:THR:HB	1:A:534:VAL:HG22	2.01	0.42
1:A:1474:LEU:HB2	6:F:105:ILE:CG1	2.48	0.42
12:L:39:CYS:SG	12:L:40:GLY:N	2.92	0.42
12:L:41:TYR:CE2	12:L:43:ILE:HB	2.55	0.42
2:B:84:TYR:CD1	2:B:132:VAL:HG12	2.55	0.42
2:B:499:ARG:NH1	2:B:520:VAL:O	2.50	0.42
2:B:1159:PHE:CE2	2:B:1171:MET:HE3	2.54	0.42
3:C:253:LYS:HE3	11:K:95:ILE:HG23	2.02	0.42
5:E:8:TYR:CZ	5:E:12:LYS:HE3	2.54	0.42
15:T:30:DA:H2"	15:T:31:DT:H5'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:991:GLN:HA	1:A:996:ILE:HD12	2.01	0.42
2:B:33:TYR:CE1	2:B:37:LYS:HD2	2.54	0.42
2:B:1072:ARG:NH1	2:B:1153:TYR:CZ	2.88	0.42
1:A:1282:ASP:OD1	1:A:1283:VAL:N	2.52	0.42
2:B:665:ILE:HD11	2:B:695:HIS:NE2	2.35	0.42
2:B:737:ILE:HD12	2:B:737:ILE:HG23	1.85	0.42
2:B:909:VAL:HG12	12:L:34:ILE:HD11	2.00	0.42
3:C:37:VAL:HG13	3:C:41:GLU:HB2	2.02	0.42
12:L:47:LYS:HG2	12:L:48:ARG:H	1.83	0.42
1:A:264:VAL:HB	1:A:272:ASN:HB2	2.00	0.42
1:A:490:THR:HB	1:A:491:PRO:HD3	2.02	0.42
1:A:977:VAL:HG12	1:A:978:VAL:N	2.35	0.42
2:B:548:TRP:O	2:B:548:TRP:CG	2.73	0.42
2:B:1040:GLN:HG2	3:C:203:TRP:CH2	2.55	0.42
3:C:49:TRP:CH2	3:C:51:GLN:HB2	2.54	0.42
8:H:10:PHE:HE1	8:H:32:SER:HB2	1.84	0.42
1:A:1194:ASN:O	1:A:1198:GLU:HG3	2.20	0.42
1:A:1315:ASP:HA	1:A:1318:LYS:HD3	2.00	0.42
3:C:91:GLU:OE2	17:Z:751:THR:HG21	2.19	0.42
3:C:106:ARG:NH1	3:C:158:GLU:OE1	2.53	0.42
3:C:172:GLU:OE1	3:C:176:TRP:CZ3	2.73	0.42
4:D:29:ALA:HB2	7:G:5:ILE:HG22	2.00	0.42
1:A:1005:HIS:CD2	1:A:1007:ILE:HB	2.55	0.42
1:A:1307:VAL:HG22	1:A:1338:THR:HG22	2.02	0.42
2:B:312:GLN:HE21	9:I:41:ASN:HD21	1.68	0.42
2:B:666:ASP:OD1	2:B:666:ASP:N	2.53	0.42
6:F:66:LEU:HD23	6:F:66:LEU:HA	1.87	0.42
1:A:513:ALA:HB2	6:F:90:LEU:HD21	2.02	0.41
4:D:76:ASN:OD1	4:D:77:ARG:N	2.53	0.41
9:I:12:VAL:HG13	9:I:13:GLY:N	2.34	0.41
17:Z:472:PHE:CE1	17:Z:520:LEU:HB2	2.53	0.41
1:A:551:ARG:HH12	8:H:27:ARG:NH2	2.16	0.41
1:A:757:GLN:NE2	1:A:778:LYS:O	2.54	0.41
2:B:422:PHE:CE2	2:B:429:PHE:HA	2.54	0.41
2:B:792:ASP:OD1	2:B:975:ARG:NH2	2.53	0.41
7:G:52:ASP:OD2	7:G:73:LYS:HE2	2.20	0.41
11:K:41:THR:O	11:K:45:ILE:HG13	2.20	0.41
11:K:45:ILE:HG21	11:K:45:ILE:HD13	1.83	0.41
1:A:916:PHE:CE1	1:A:963:ARG:HD2	2.55	0.41
2:B:83:ARG:HB2	2:B:133:ILE:HB	2.01	0.41
2:B:200:MET:HB2	13:N:24:DG:N1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:ILE:O	2:B:303:PRO:HB3	2.20	0.41
7:G:41:LYS:HE2	7:G:42:TYR:CZ	2.55	0.41
7:G:54:ILE:HD13	7:G:54:ILE:HA	1.88	0.41
1:A:120:ASP:OD1	1:A:121:SER:N	2.53	0.41
1:A:524:MET:HE3	2:B:1097:HIS:HE1	1.84	0.41
1:A:902:GLU:O	1:A:978:VAL:HA	2.20	0.41
2:B:156:LEU:HD22	2:B:184:TYR:CZ	2.56	0.41
2:B:535:GLY:HA3	2:B:618:ALA:HB2	2.02	0.41
1:A:563:LEU:HD23	1:A:563:LEU:HA	1.82	0.41
2:B:235:ILE:HG21	2:B:348:LEU:CD1	2.50	0.41
2:B:623:ARG:NH1	2:B:625:LEU:HD21	2.36	0.41
2:B:626:LEU:HD23	2:B:662:VAL:HG12	2.02	0.41
2:B:1062:ARG:HH12	2:B:1066:PRO:HD2	1.85	0.41
5:E:8:TYR:CE2	5:E:12:LYS:HE3	2.56	0.41
16:Y:60:ILE:HD11	17:Z:190:ARG:HG3	2.02	0.41
1:A:330:GLN:HG2	1:A:334:ARG:O	2.20	0.41
1:A:931:ARG:HD3	1:A:939:VAL:HG11	2.03	0.41
1:A:1474:LEU:HD11	6:F:107:ARG:NE	2.35	0.41
4:D:74:PHE:HB2	4:D:80:ILE:HG12	2.02	0.41
13:N:13:DA:C8	13:N:14:DT:H72	2.56	0.41
1:A:546:ARG:HG3	1:A:639:ILE:HG21	2.03	0.41
1:A:567:LEU:HD21	1:A:595:ILE:HG12	2.03	0.41
1:A:932:ARG:HG2	8:H:105:SER:O	2.21	0.41
1:A:1261:ILE:HG22	1:A:1262:MET:N	2.35	0.41
2:B:196:ALA:HA	2:B:394:ASP:O	2.21	0.41
2:B:817:GLN:HE21	2:B:912:ASN:ND2	2.18	0.41
3:C:75:SER:HB3	3:C:79:VAL:CG2	2.50	0.41
3:C:197:TYR:HD2	3:C:217:GLN:NE2	2.18	0.41
14:P:41:A:H2'	14:P:42:A:O4'	2.21	0.41
1:A:102:LYS:HZ1	1:A:141:LEU:HD13	1.86	0.41
1:A:529:GLN:HG3	1:A:1094:SER:HB3	2.01	0.41
1:A:689:ILE:HD12	2:B:985:LEU:HD22	2.03	0.41
2:B:130:LYS:O	2:B:141:GLN:HA	2.20	0.41
2:B:154:ILE:HG22	2:B:155:MET:O	2.20	0.41
2:B:1124:ILE:HG22	2:B:1125:MET:H	1.86	0.41
1:A:88:ILE:HD12	1:A:253:LEU:HD23	2.03	0.41
1:A:375:ILE:HD11	1:A:669:TYR:HB2	2.02	0.41
1:A:406:VAL:HG21	1:A:440:LEU:HD11	2.02	0.41
1:A:1160:ARG:O	1:A:1300:GLY:HA2	2.21	0.41
2:B:25:ALA:HB1	2:B:640:ILE:HD13	2.02	0.41
2:B:46:SER:OG	2:B:397:GLY:N	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:721:ARG:HD3	2:B:721:ARG:HA	1.79	0.41
2:B:725:GLN:HG2	2:B:938:ARG:O	2.20	0.41
2:B:1104:ARG:HG3	2:B:1105:GLU:N	2.36	0.41
13:N:10:DA:C2	15:T:35:DA:C2	3.08	0.41
14:P:37:C:P	17:Z:579:LYS:HZ2	2.36	0.41
1:A:1130:ILE:HG21	1:A:1411:LEU:HD13	2.02	0.41
2:B:816:GLU:OE2	2:B:869:LYS:NZ	2.34	0.41
8:H:65:TYR:CE1	8:H:84:ARG:HB3	2.56	0.41
12:L:38:GLU:O	12:L:38:GLU:HG2	2.21	0.41
1:A:601:ASN:CB	1:A:988:TRP:CZ3	3.03	0.40
1:A:894:ASP:O	1:A:1022:ILE:HD13	2.21	0.40
1:A:1180:ASN:OD1	1:A:1183:SER:HB3	2.21	0.40
1:A:1197:TYR:O	1:A:1200:PRO:HD3	2.21	0.40
1:A:1375:ARG:HH12	1:A:1379:GLU:CD	2.25	0.40
8:H:8:ASP:OD1	8:H:9:ILE:N	2.48	0.40
13:N:12:DT:H5"	17:Z:283:ARG:HH21	1.85	0.40
1:A:32:LYS:HE3	1:A:252:VAL:HG21	2.02	0.40
1:A:75:ALA:CB	2:B:1131:ARG:HD2	2.52	0.40
1:A:546:ARG:HD2	1:A:772:SER:HB3	2.04	0.40
1:A:601:ASN:HB3	1:A:988:TRP:CZ3	2.57	0.40
1:A:983:LEU:HD12	1:A:1044:HIS:CD2	2.57	0.40
2:B:67:LEU:O	2:B:84:TYR:N	2.39	0.40
2:B:88:PHE:CE2	2:B:412:LEU:HD21	2.56	0.40
2:B:771:GLU:O	10:J:55:LEU:HD21	2.20	0.40
2:B:830:GLU:OE2	2:B:870:THR:OG1	2.31	0.40
2:B:1051:LEU:HD23	2:B:1051:LEU:HA	1.77	0.40
3:C:26:THR:HG22	3:C:27:ASP:N	2.37	0.40
4:D:130:ILE:O	4:D:134:ILE:HG13	2.21	0.40
5:E:87:ILE:HD11	5:E:110:MET:CE	2.51	0.40
8:H:96:VAL:HB	8:H:116:VAL:HG22	2.03	0.40
9:I:120:GLY:O	9:I:122:ARG:HG3	2.22	0.40
2:B:124:LEU:HD22	2:B:152:ILE:HD11	2.03	0.40
2:B:646:ARG:HG3	2:B:651:TYR:O	2.22	0.40
7:G:151:ARG:HH22	17:Z:477:HIS:HD2	1.68	0.40
7:G:164:MET:CE	17:Z:494:ARG:HH12	2.34	0.40
1:A:425:ASP:CB	17:Z:583:PHE:CE1	3.05	0.40
1:A:536:GLY:O	1:A:538:VAL:HG23	2.22	0.40
2:B:248:LYS:O	2:B:252:ILE:HG12	2.21	0.40
2:B:260:LEU:HB2	2:B:263:ILE:HD12	2.03	0.40
2:B:853:LEU:O	12:L:46:LYS:NZ	2.55	0.40
4:D:38:HIS:CE1	4:D:69:ALA:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:185:ILE:CG2	5:E:209:VAL:HG21	2.47	0.40
17:Z:306:LYS:HA	17:Z:372:LEU:O	2.22	0.40
1:A:86:GLY:O	1:A:255:VAL:N	2.48	0.40
1:A:370:ASP:OD2	11:K:65:HIS:NE2	2.55	0.40
1:A:555:LEU:HD21	1:A:679:TRP:HE1	1.87	0.40
1:A:763:TYR:OH	8:H:23:ASP:OD2	2.18	0.40
1:A:1210:TRP:CZ3	1:A:1282:ASP:HB3	2.57	0.40
2:B:282:ARG:O	2:B:286:GLU:HB2	2.22	0.40
17:Z:417:GLU:CD	17:Z:516:ARG:NH1	2.68	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	1411/1970 (72%)	1353 (96%)	57 (4%)	1 (0%)	51 83
2	B	1143/1174 (97%)	1088 (95%)	55 (5%)	0	100 100
3	C	255/275 (93%)	238 (93%)	17 (7%)	0	100 100
4	D	126/142 (89%)	113 (90%)	12 (10%)	1 (1%)	19 56
5	E	207/210 (99%)	197 (95%)	10 (5%)	0	100 100
6	F	80/127 (63%)	78 (98%)	2 (2%)	0	100 100
7	G	169/172 (98%)	162 (96%)	3 (2%)	4 (2%)	6 35
8	H	146/150 (97%)	140 (96%)	6 (4%)	0	100 100
9	I	115/125 (92%)	105 (91%)	9 (8%)	1 (1%)	17 54
10	J	65/67 (97%)	62 (95%)	3 (5%)	0	100 100
11	K	113/117 (97%)	113 (100%)	0	0	100 100
12	L	43/58 (74%)	40 (93%)	3 (7%)	0	100 100
16	Y	114/117 (97%)	113 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	Z	480/1087 (44%)	463 (96%)	13 (3%)	4 (1%)	19 56
All	All	4467/5791 (77%)	4265 (96%)	191 (4%)	11 (0%)	50 78

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	18	PHE
7	G	124	ASN
4	D	91	LYS
9	I	12	VAL
17	Z	362	GLU
7	G	155	ASN
17	Z	387	LYS
17	Z	497	GLU
1	A	529	GLN
7	G	20	PRO
17	Z	386	VAL

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	1252/1749 (72%)	1252 (100%)	0	100 100
2	B	996/1027 (97%)	996 (100%)	0	100 100
3	C	236/252 (94%)	236 (100%)	0	100 100
4	D	107/127 (84%)	105 (98%)	2 (2%)	57 76
5	E	189/190 (100%)	189 (100%)	0	100 100
6	F	71/111 (64%)	71 (100%)	0	100 100
7	G	149/153 (97%)	147 (99%)	2 (1%)	69 83
8	H	129/131 (98%)	128 (99%)	1 (1%)	81 89
9	I	105/112 (94%)	105 (100%)	0	100 100
10	J	56/56 (100%)	56 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	K	104/106 (98%)	104 (100%)	0	100 100
12	L	42/55 (76%)	42 (100%)	0	100 100
16	Y	102/103 (99%)	101 (99%)	1 (1%)	76 86
17	Z	429/940 (46%)	428 (100%)	1 (0%)	93 97
All	All	3967/5112 (78%)	3960 (100%)	7 (0%)	93 97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	68	THR
4	D	131	LEU
7	G	66	VAL
7	G	97	LEU
8	H	96	VAL
16	Y	37	ASP
17	Z	338	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	A	301	HIS
1	A	372	ASN
1	A	461	GLN
1	A	576	GLN
1	A	757	GLN
1	A	780	ASN
1	A	790	GLN
1	A	791	GLN
1	A	839	HIS
1	A	913	ASN
1	A	1163	HIS
1	A	1360	ASN
1	A	1462	GLN
2	B	111	ASN
2	B	265	GLN
2	B	312	GLN
2	B	350	HIS
2	B	370	HIS
2	B	471	ASN

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Mol	Chain	Res	Type
2	B	518	HIS
2	B	731	GLN
2	B	817	GLN
2	B	1021	HIS
2	B	1097	HIS
2	B	1142	ASN
4	D	38	HIS
4	D	48	ASN
7	G	4	HIS
9	I	22	ASN
9	I	45	GLN
11	K	69	HIS
16	Y	41	GLN
17	Z	477	HIS
17	Z	509	HIS
17	Z	519	GLN
17	Z	534	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	19/50 (38%)	4 (21%)	1 (5%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	35	U
14	P	36	A
14	P	37	C
14	P	41	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	P	36	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	14:DT	O3'	15:DT	P	3.16

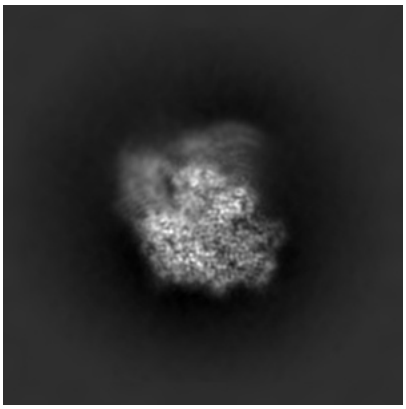
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3817. These allow visual inspection of the internal detail of the map and identification of artifacts.

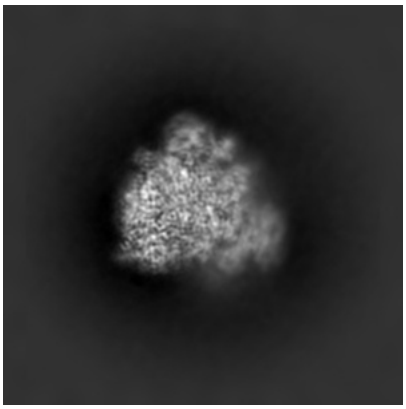
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

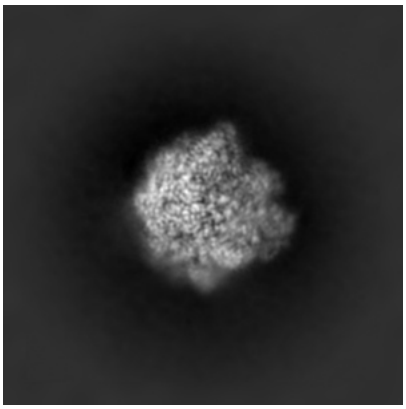
6.1.1 Primary map



X

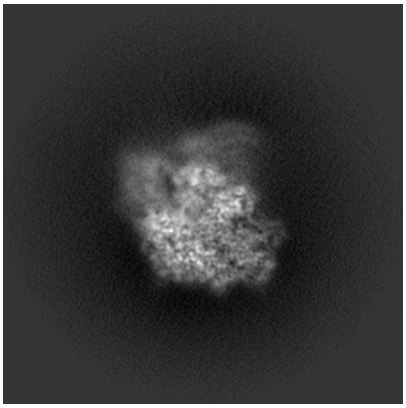


Y

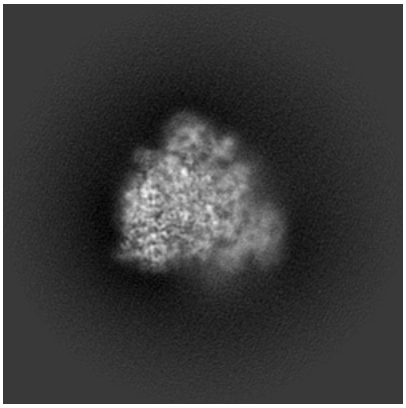


Z

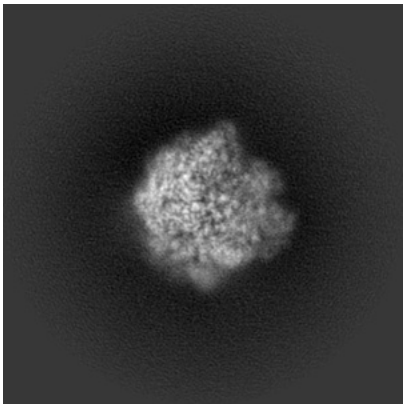
6.1.2 Raw map



X



Y

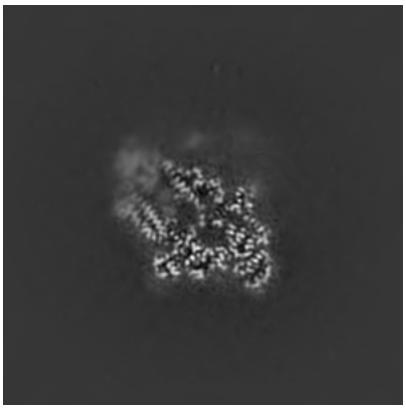


Z

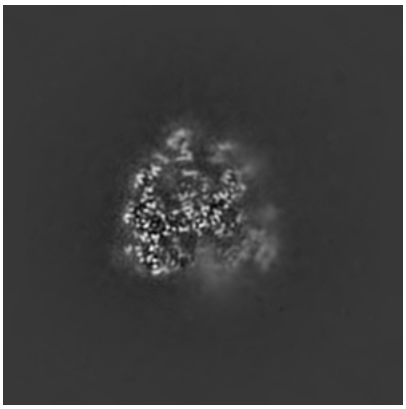
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

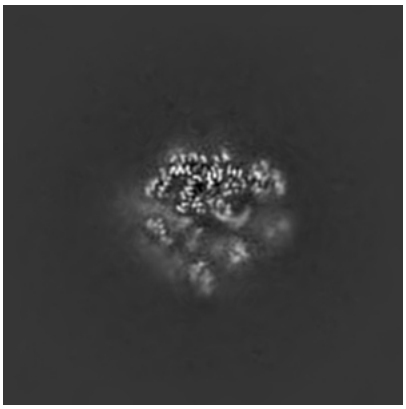
6.2.1 Primary map



X Index: 128

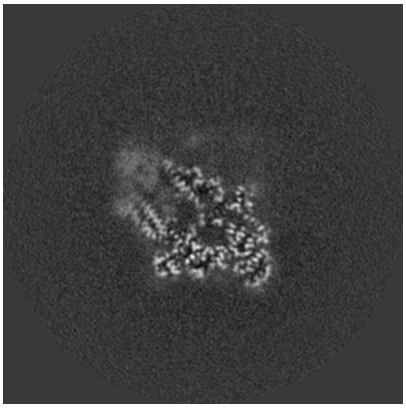


Y Index: 128

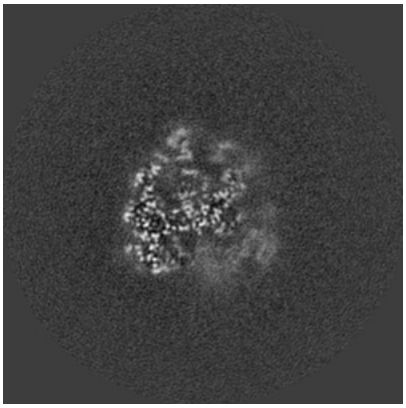


Z Index: 128

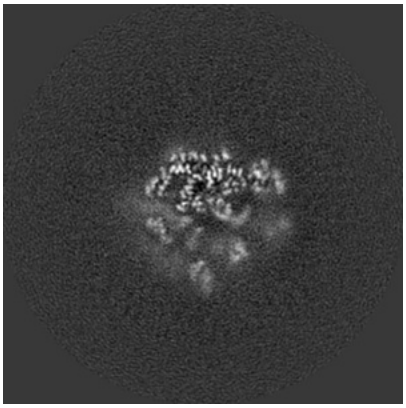
6.2.2 Raw map



X Index: 128



Y Index: 128

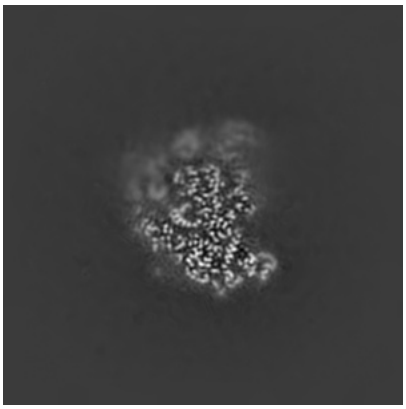


Z Index: 128

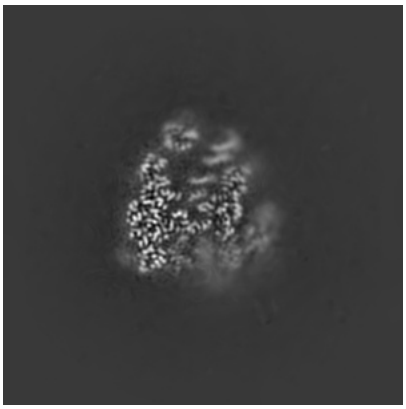
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

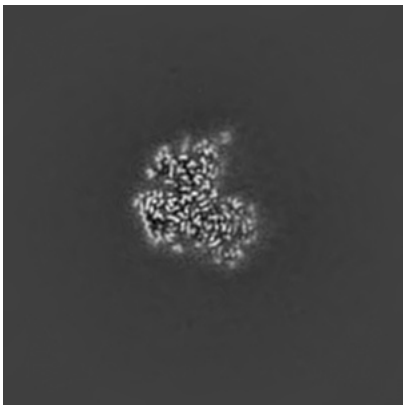
6.3.1 Primary map



X Index: 117

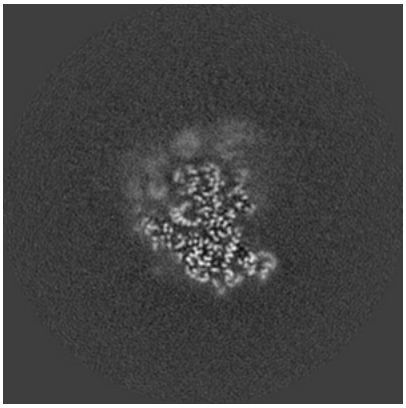


Y Index: 124

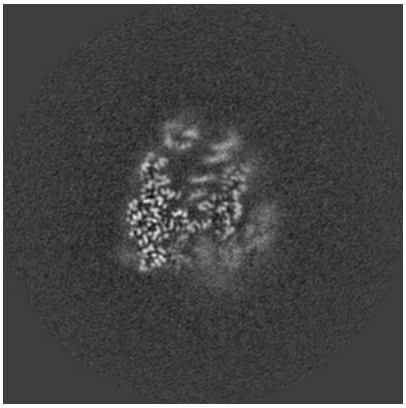


Z Index: 96

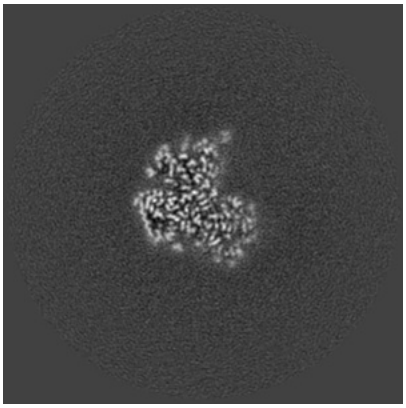
6.3.2 Raw map



X Index: 117



Y Index: 124

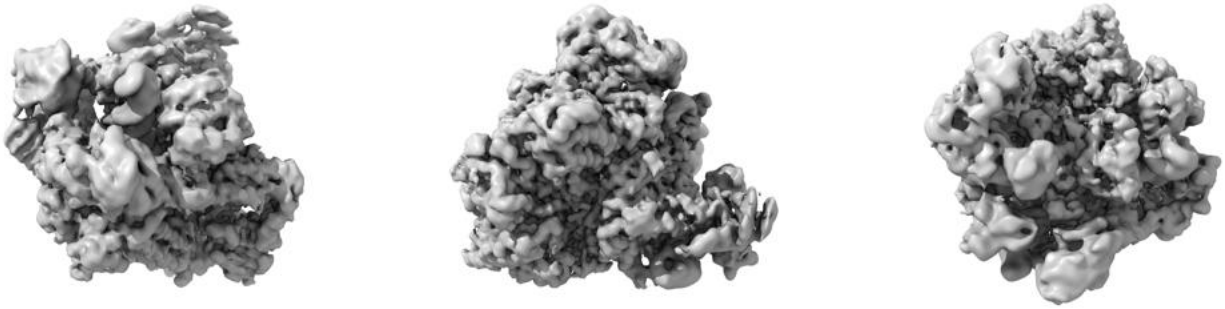


Z Index: 96

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

6.4 Orthogonal surface views (i)

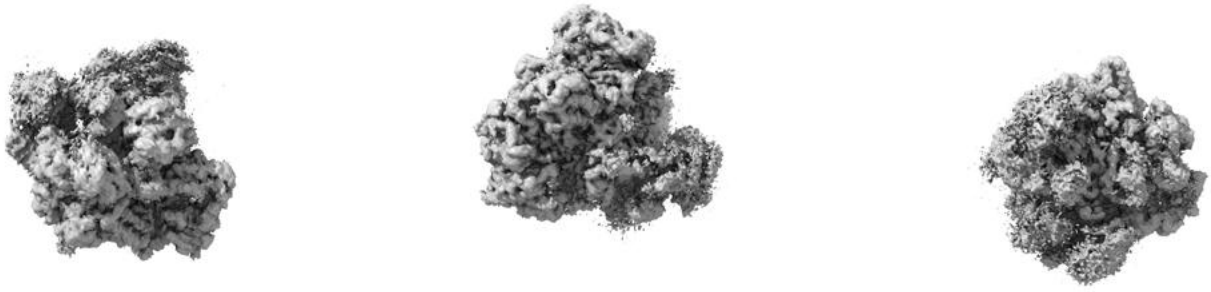
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

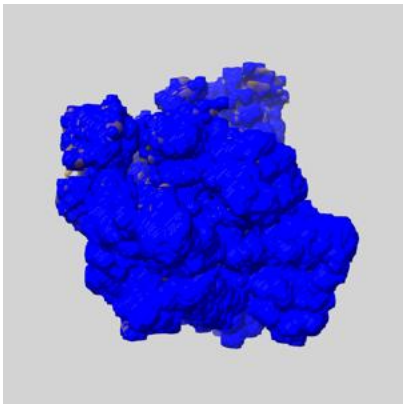
6.5 Mask visualisation

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

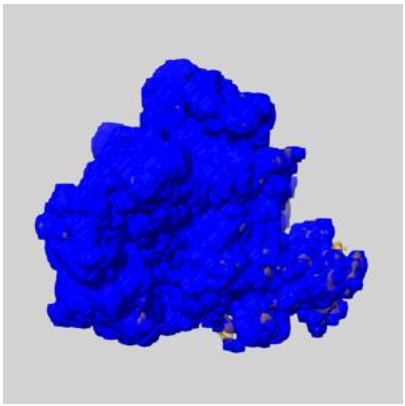
A mask typically either:

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

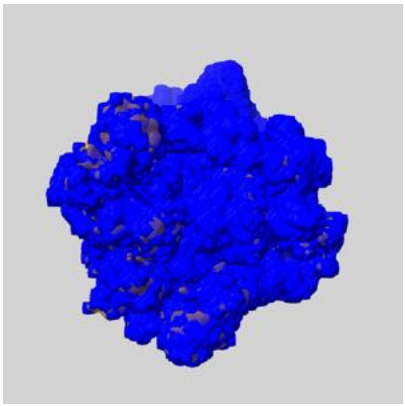
6.5.1 emd_3817_msk_1.map



X



Y

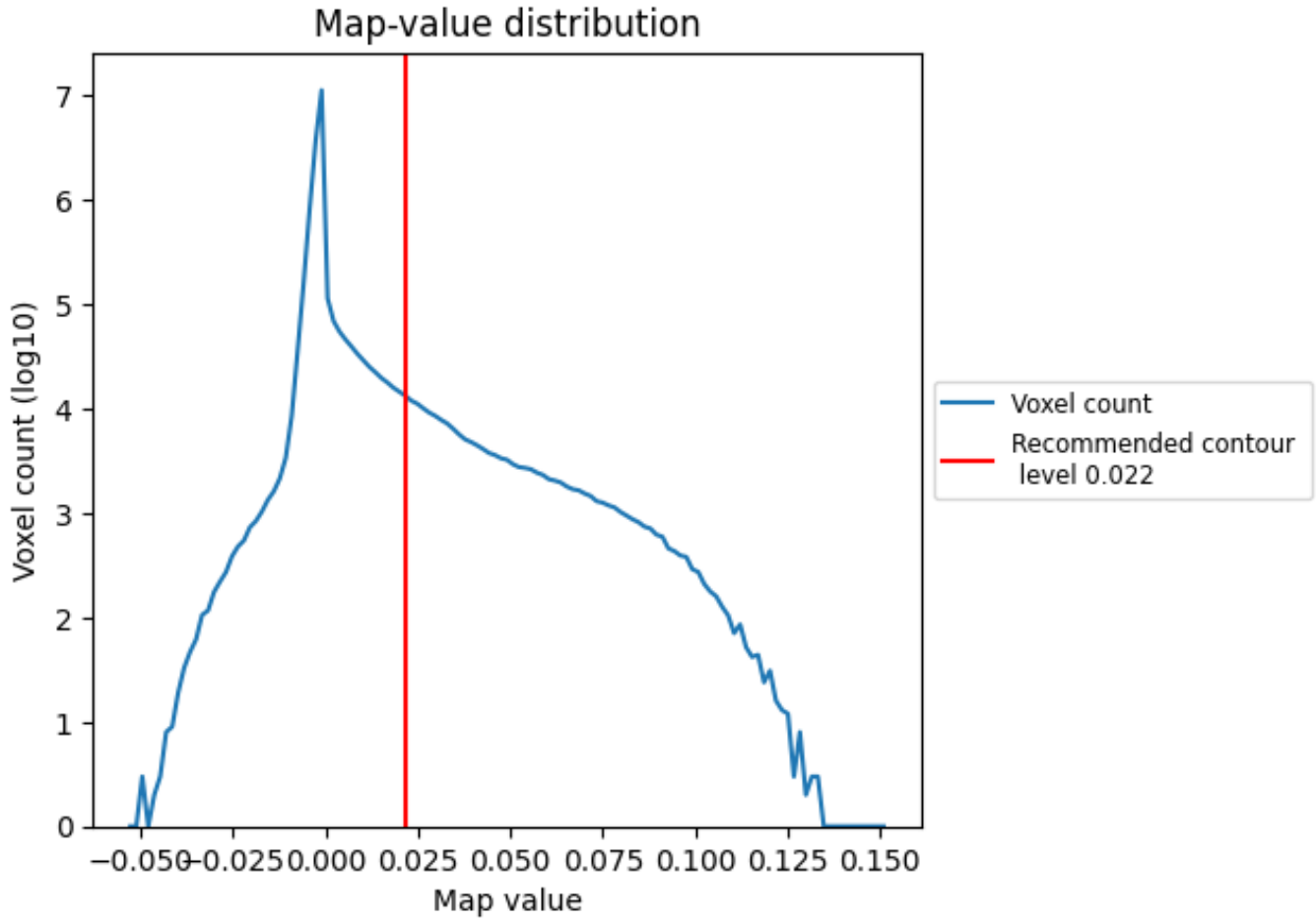


Z

7 Map analysis

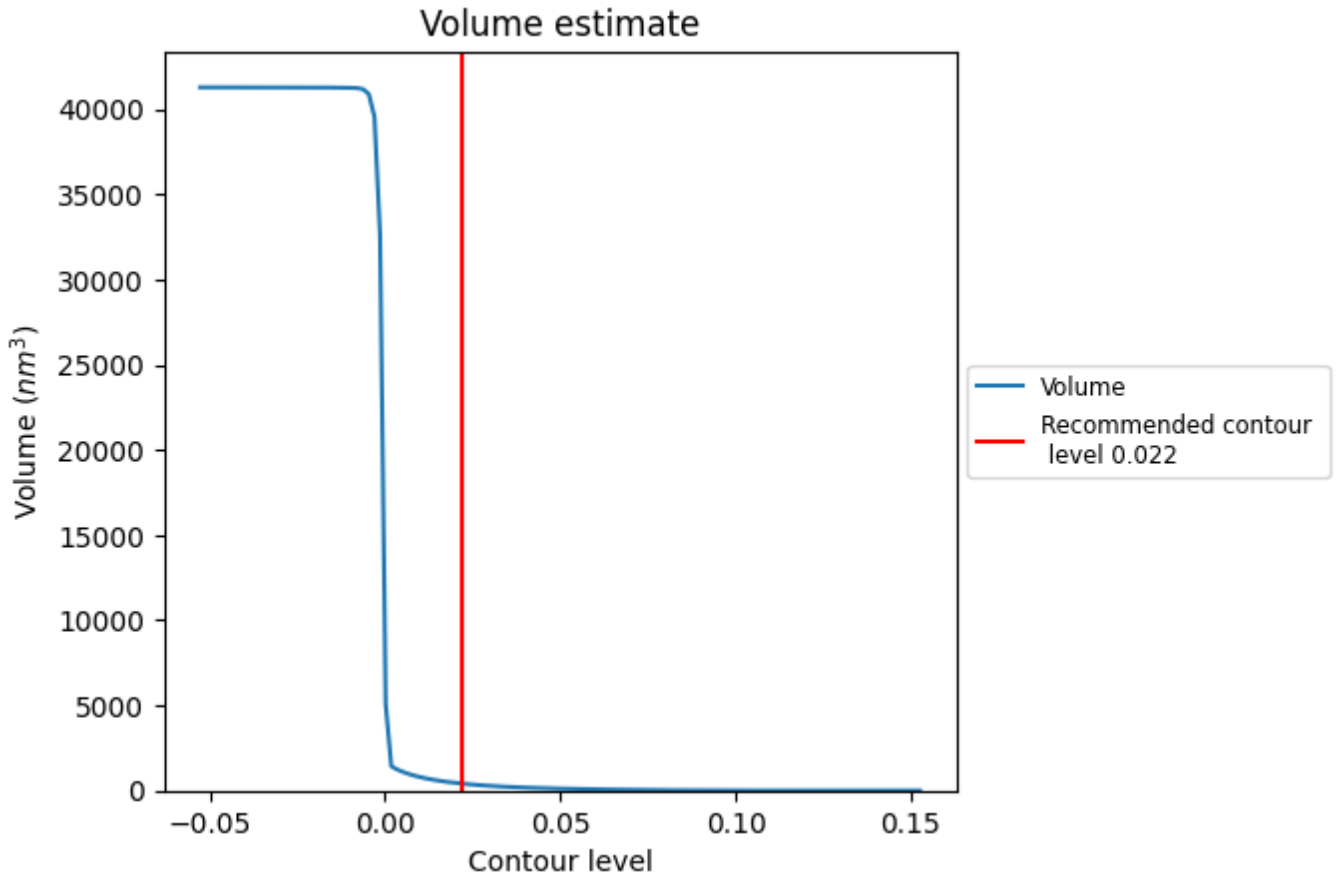
This section contains the results of statistical analysis of the map.

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.

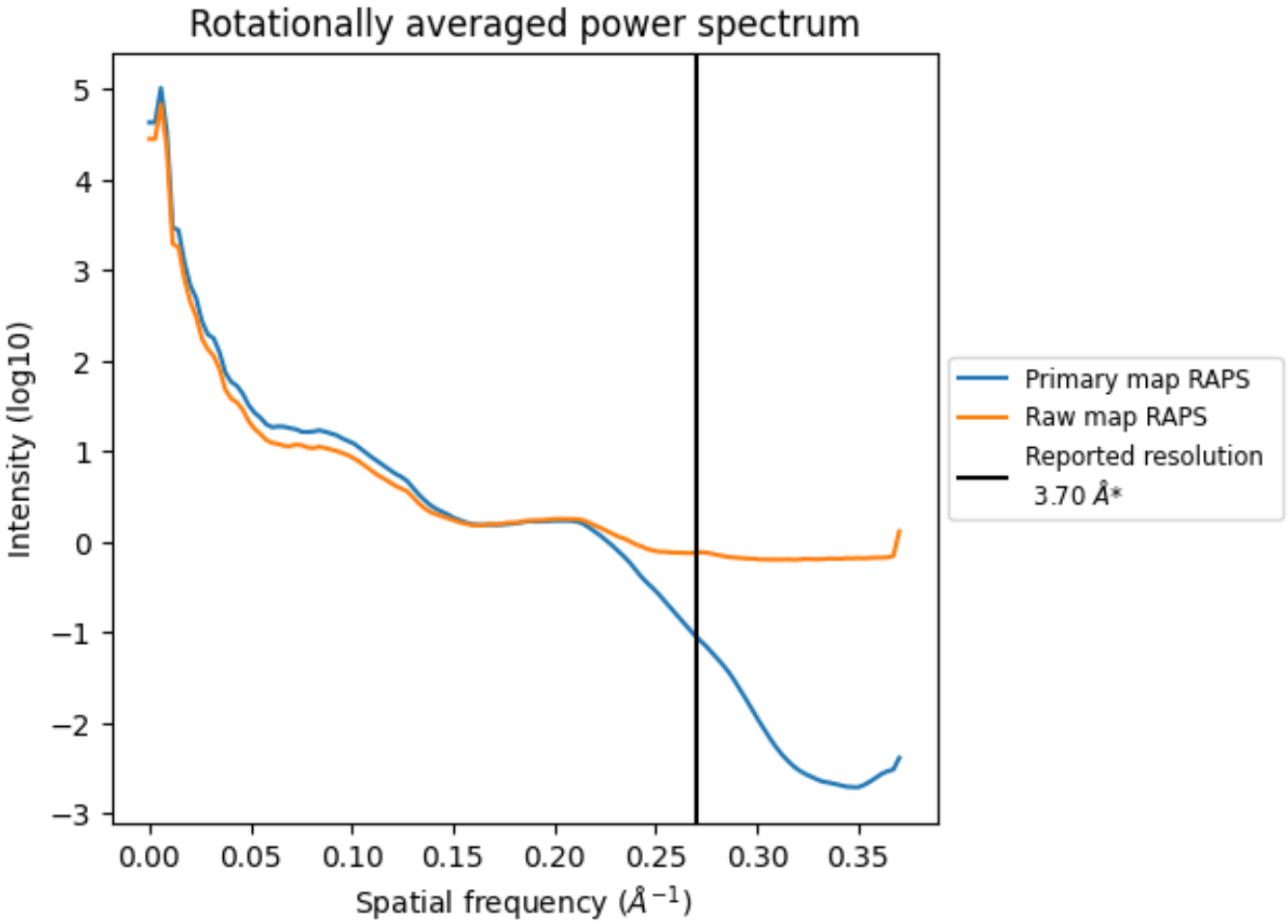
7.2 Volume estimate (i)



The volume at the recommended contour level is 409 nm^3; this corresponds to an approximate mass of 370 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)

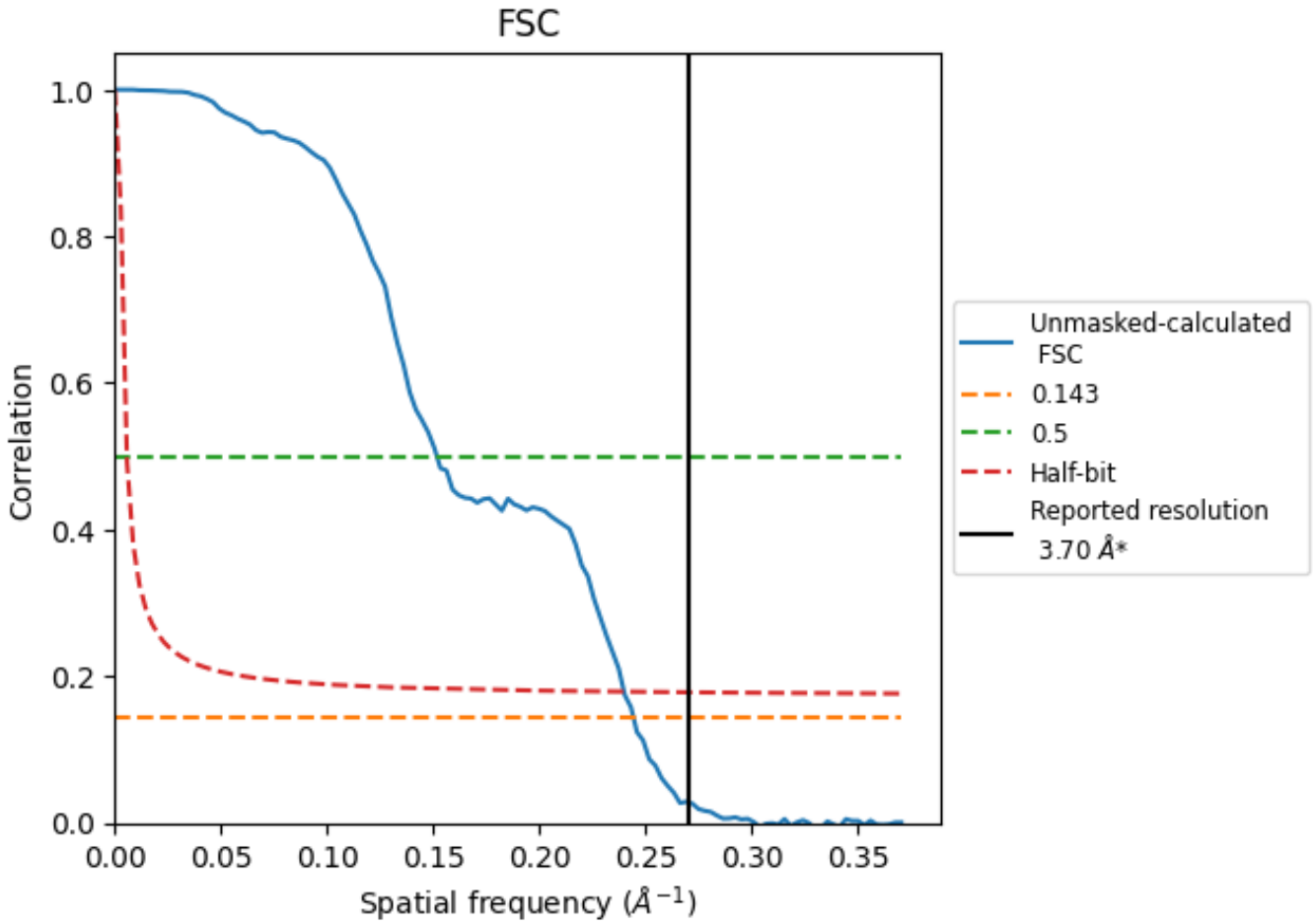


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

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 0.270 Å^{-1}

8.2 Resolution estimates (i)

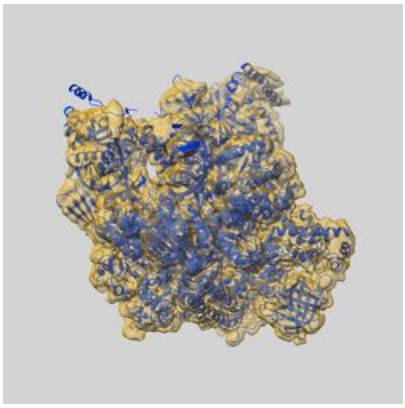
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.09	6.60	4.17

*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 4.09 differs from the reported value 3.7 by more than 10 %

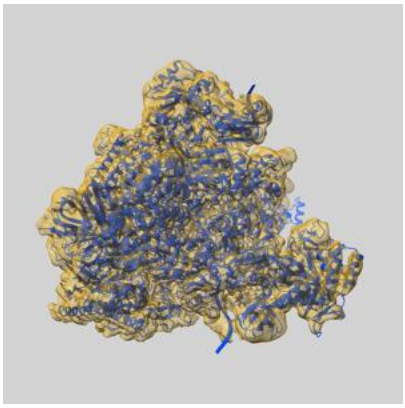
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3817 and PDB model 5OIK. Per-residue inclusion information can be found in section 3 on page 8.

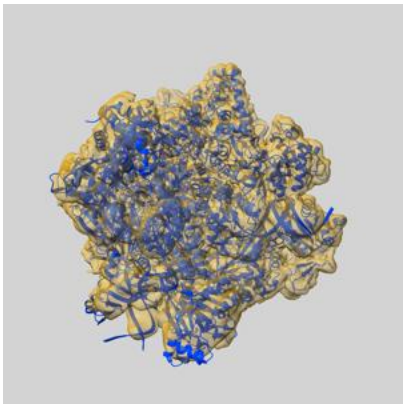
9.1 Map-model overlay



X



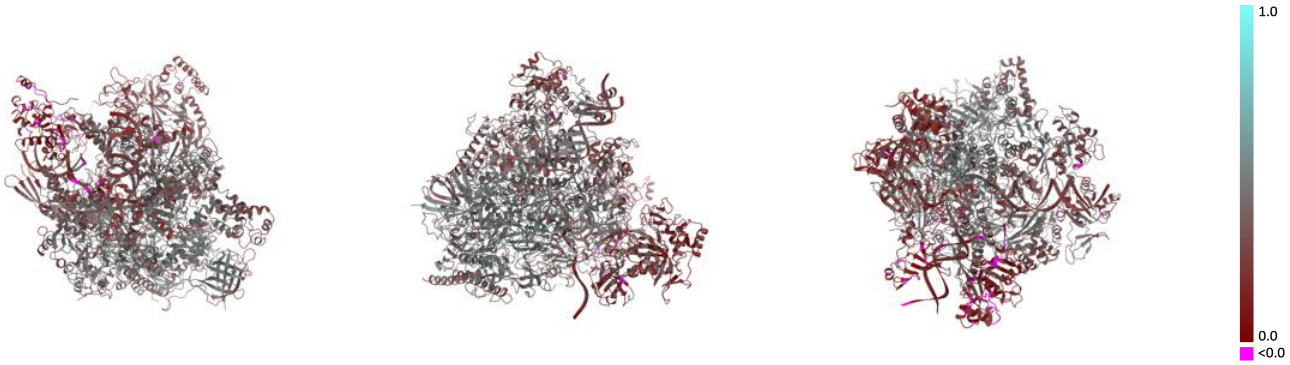
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022 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.

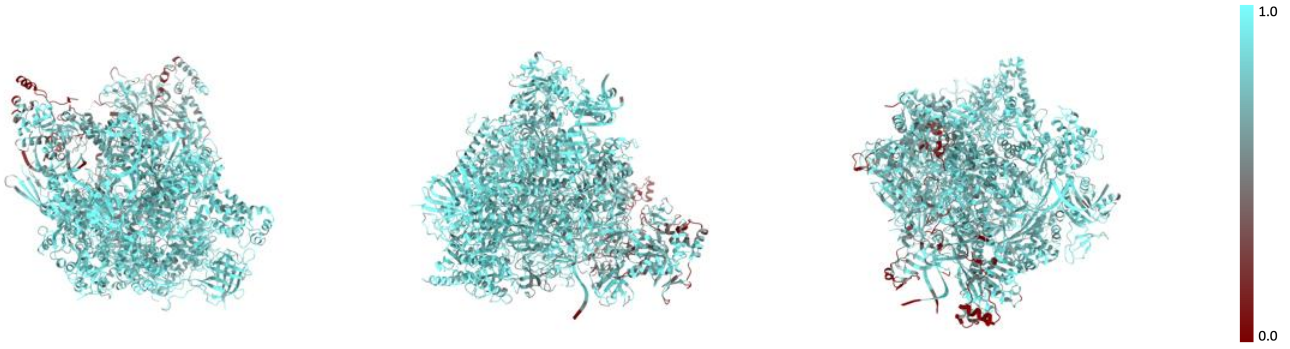
9.2 Q-score mapped to coordinate model (i)



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.

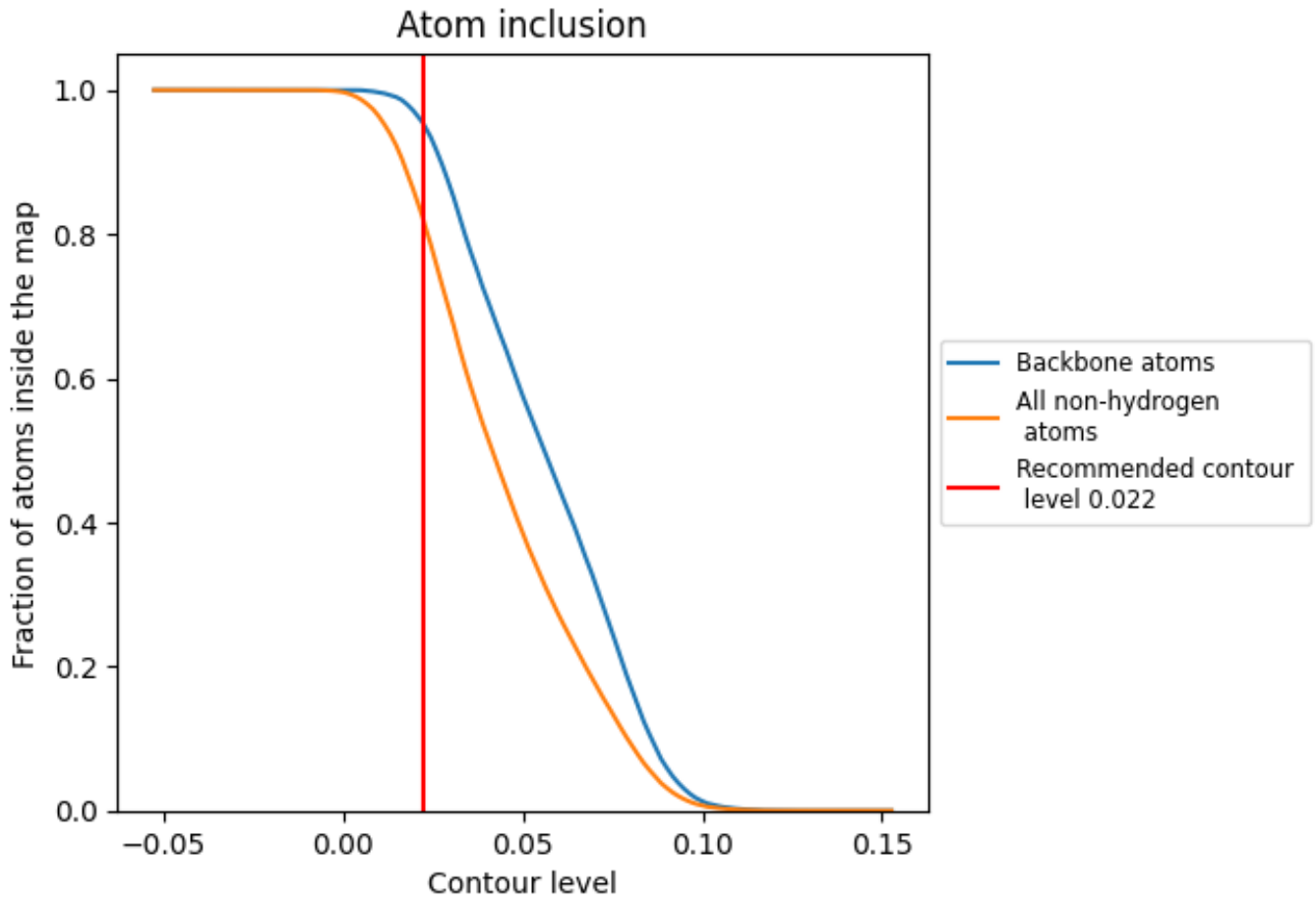
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.022).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 82% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8242	0.3730
A	0.8567	0.4130
B	0.8672	0.4300
C	0.9076	0.4500
D	0.5688	0.2090
E	0.8856	0.3890
F	0.8513	0.4310
G	0.7088	0.2920
H	0.8861	0.4230
I	0.8727	0.3670
J	0.8829	0.4490
K	0.8980	0.4390
L	0.8898	0.4150
N	0.8392	0.2270
P	0.8618	0.3150
T	0.8547	0.2910
Y	0.5354	0.1090
Z	0.6512	0.2050