Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 12:10 am GMT

PDB ID	:	4V1N
EMDB ID	:	EMD-2785
Title	:	Architecture of the RNA polymerase II-Mediator core transcription initiation complex
Authors	:	Plaschka, C.; Lariviere, L.; Wenzeck, L.; Hemann, M.; Tegunov, D.; Petrotchenko, E.V.; Borchers, C.H.; Baumeister, W.; Herzog, F.; Villa, E.; Cramer, P.
Deposited on	:	2014-09-29
Resolution	:	7.80 Å(reported)

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

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

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

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

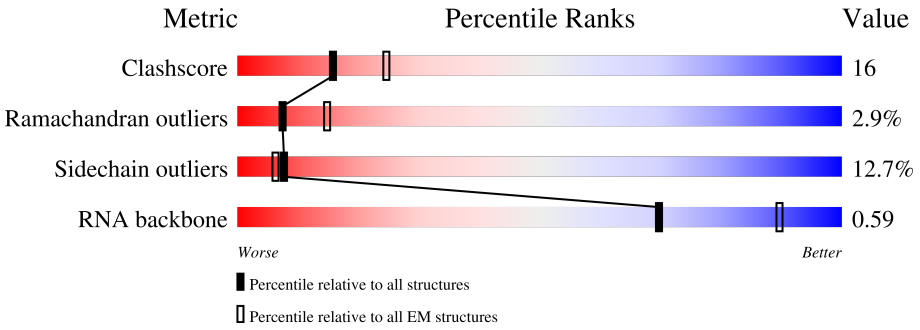
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 7.80 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	1733	7% 55% 23% 18%
2	B	1224	13% 62% 28% 6%
3	C	318	8% 61% 18% 16%
4	D	221	29% 55% 20% 5% 19%
5	E	215	7% 74% 22%
6	F	155	36% 16% 46%
7	G	171	28% 72% 25%

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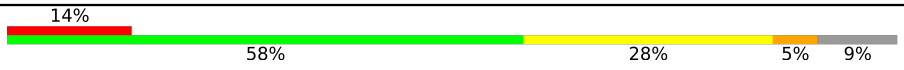
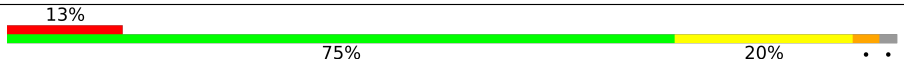
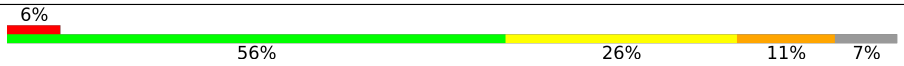
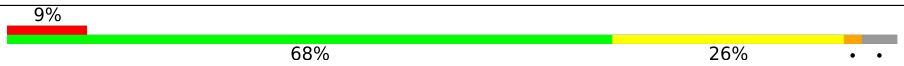
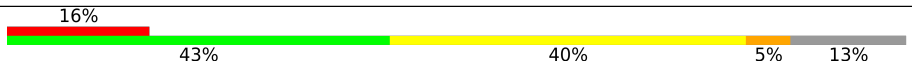
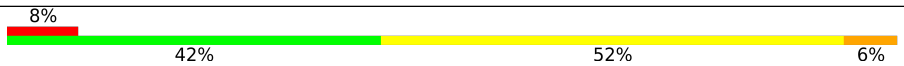
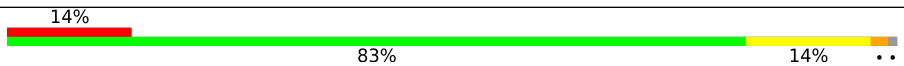
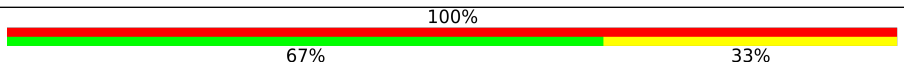
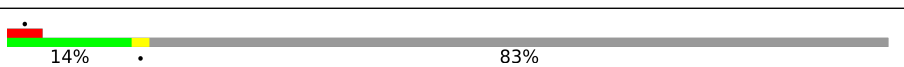
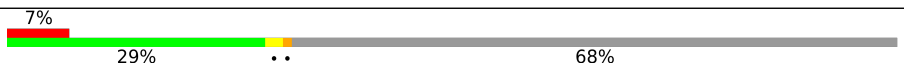
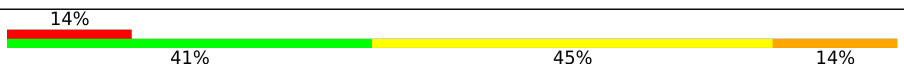
Mol	Chain	Length	Quality of chain
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	345	
14	N	50	
15	O	181	
16	P	6	
17	Q	734	
18	R	331	
19	T	58	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 38446 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	1422	11174	7036	1954	2122	62	0	0

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1156	9140	5781	1606	1697	56	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	266	2095	1317	348	417	13	0	0

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	178	1434	887	257	288	2	0	0

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	214	1752	1111	309	321	11	0	0

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	84	Total	C	N	O	S	0	0
			679	434	115	127	3		

- 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
			1340	861	222	249	8		

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1068	673	180	211	4		

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	119	Total	C	N	O	S	0	0
			971	596	179	186	10		

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	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	1
			920	590	157	171	2		

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			363	224	72	63	4		

- Molecule 13 is a protein called TRANSCRIPTION INITIATION FACTOR IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	300	Total	C	N	O	S	0	1
			2202	1384	380	423	15		

- Molecule 14 is a DNA chain called NONTEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	50	Total	C	N	O	P	0	0
			975	490	191	246	48		

- Molecule 15 is a protein called TATA-BOX-BINDING PROTEIN.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	60	MET	-	expression tag	UNP P13393

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	6	Total	C	N	O	P	0	0
			123	57	22	39	5		

- Molecule 17 is a protein called TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	122	Total	C	N	O	0	0
			606	362	122	122		

- Molecule 18 is a protein called TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT BETA.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	105	Total	C	N	O	0	0
			521	311	105	105		

- Molecule 19 is a DNA chain called TEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	58	Total	C	N	O	P	0	0
			1125	568	206	294	57		

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

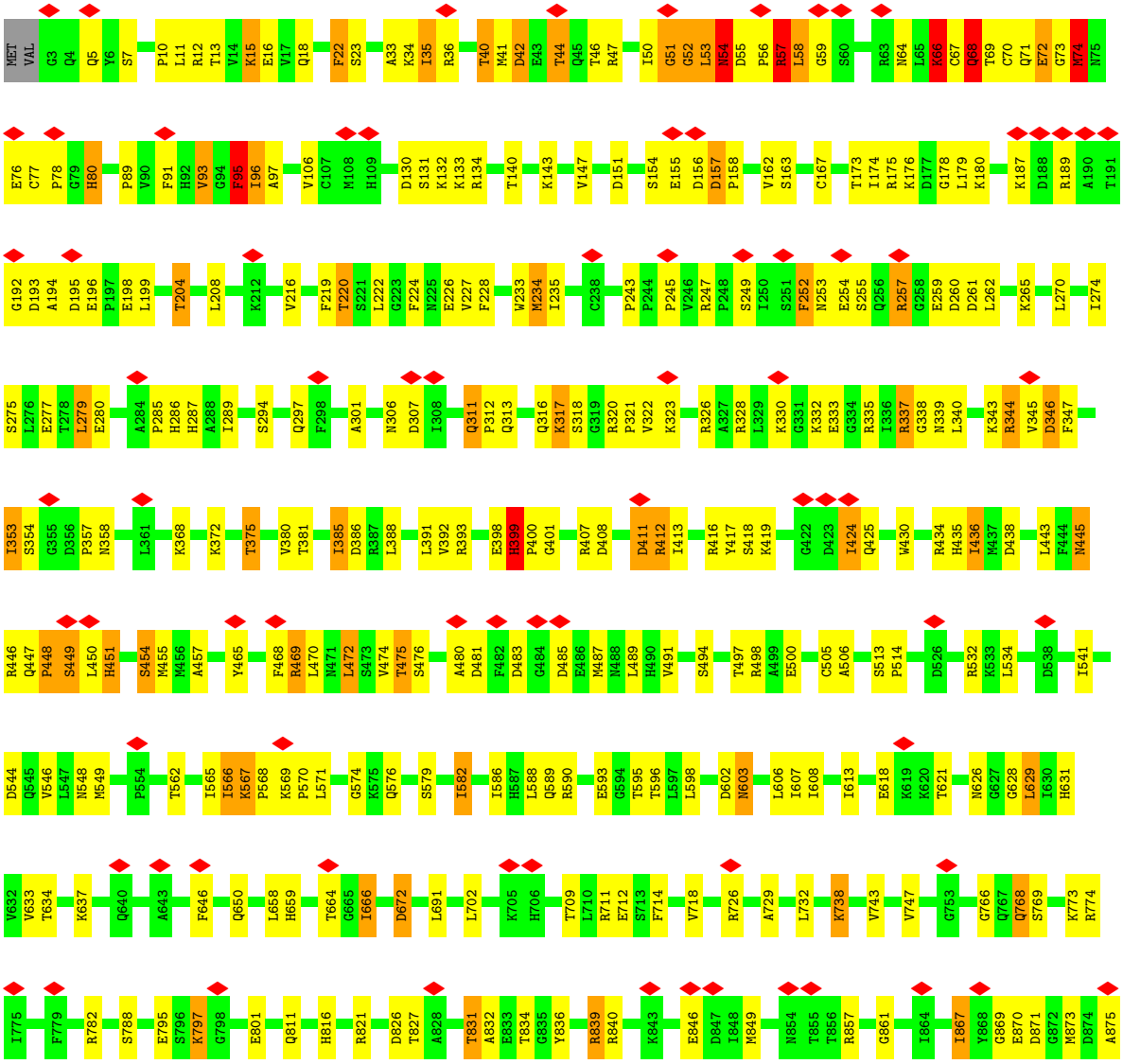
Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	Mg	0
			1	1	

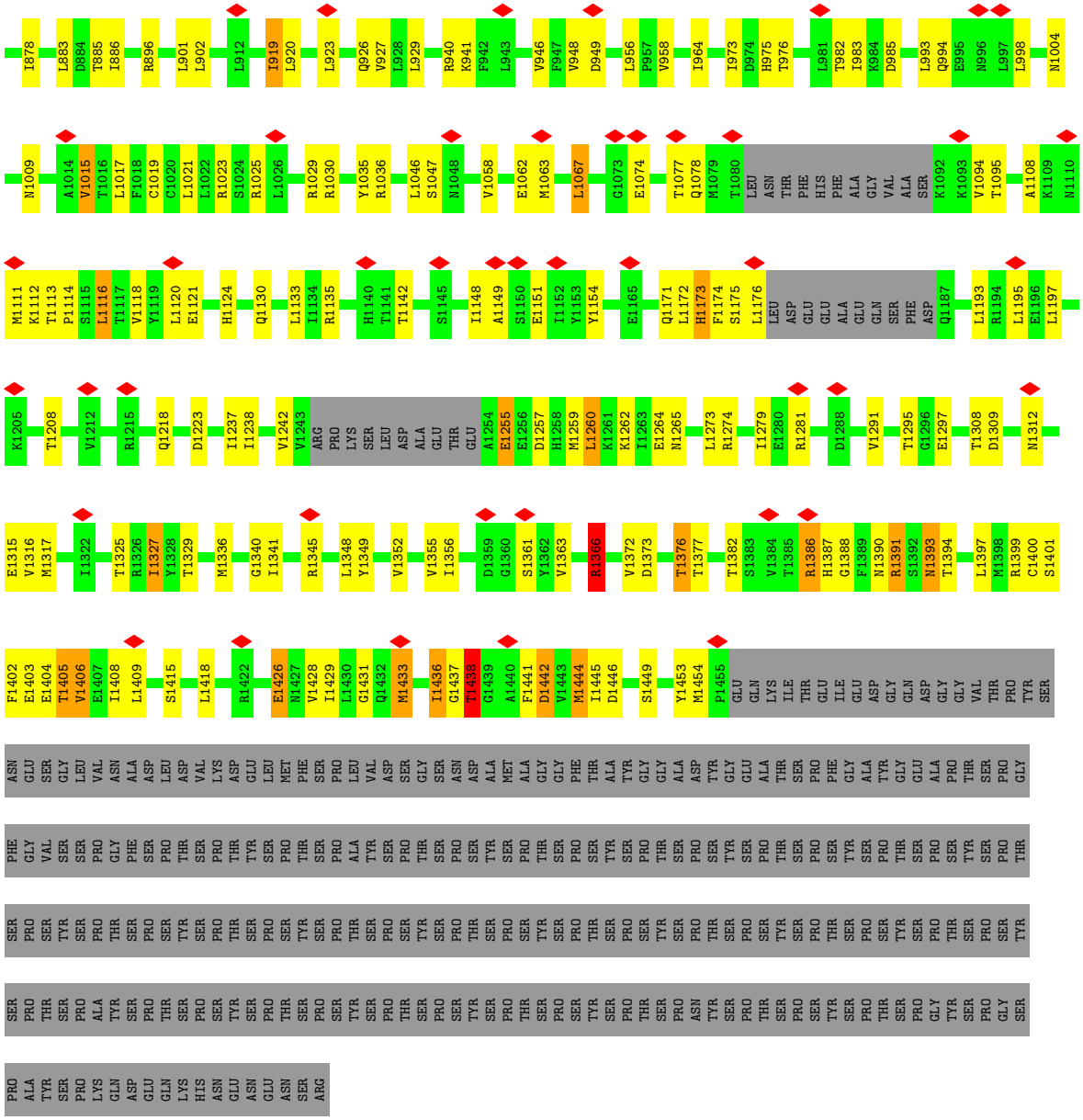
3 Residue-property plots (i)

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 II SUBUNIT RPB1

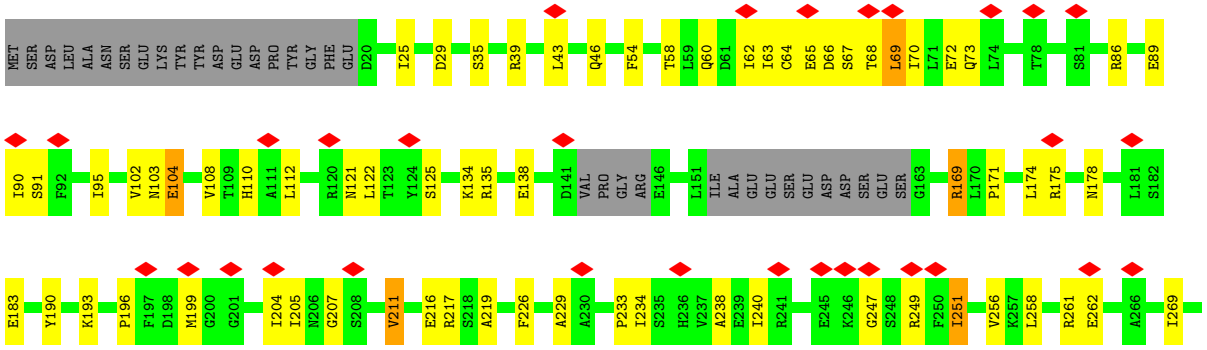
Chain A:

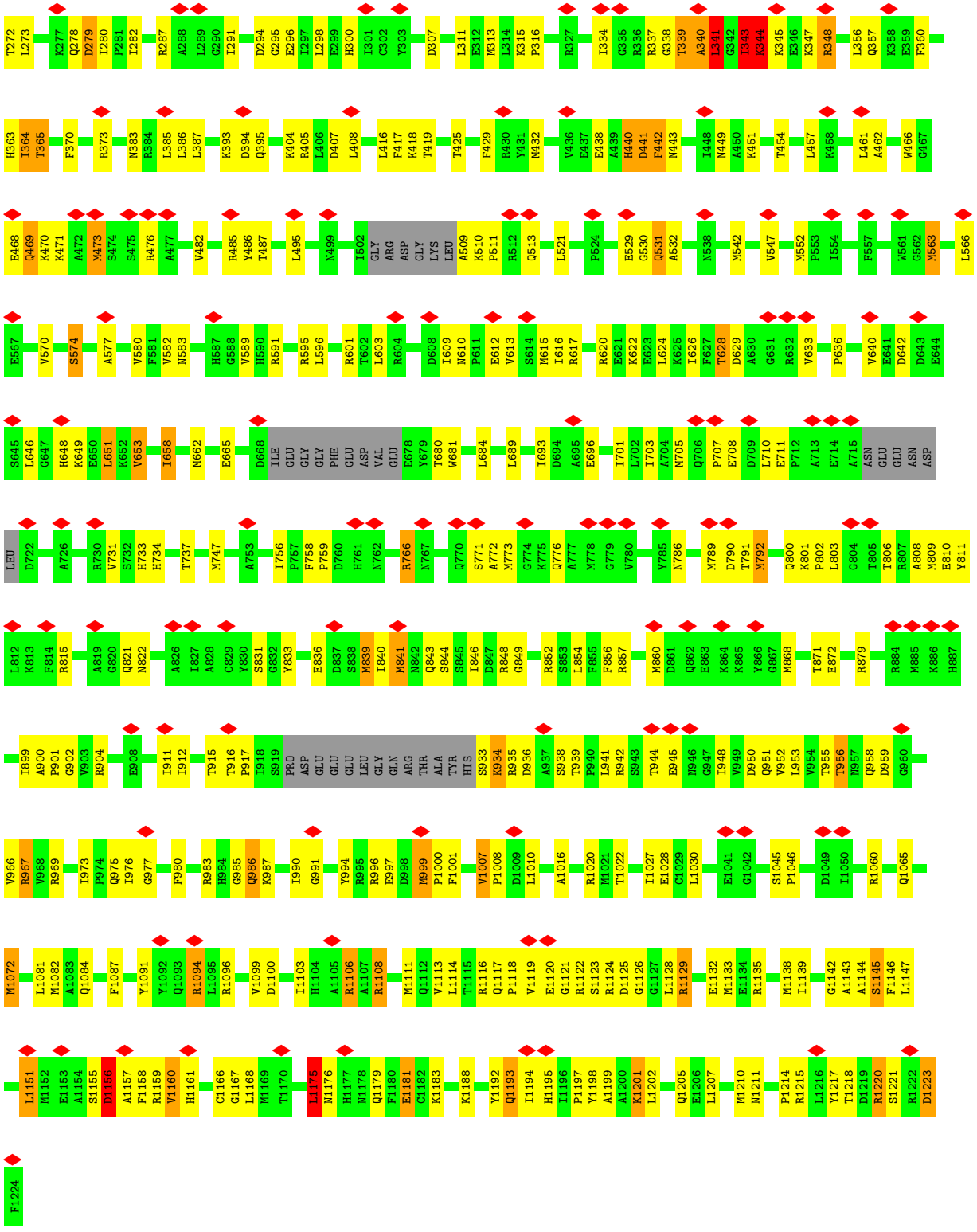




• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

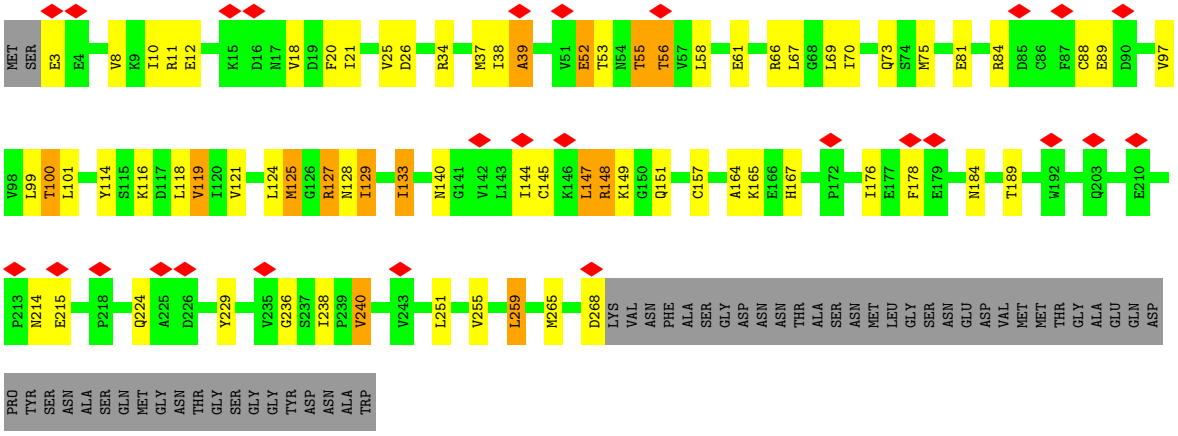
Chain B:



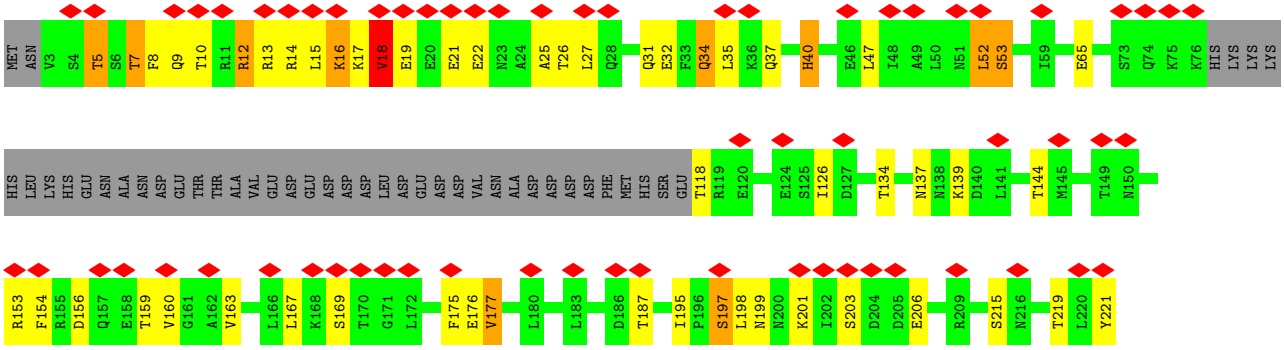


• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

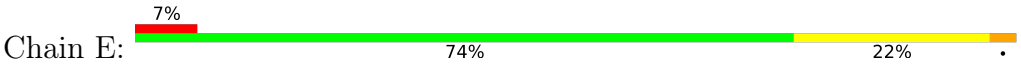
Chain C:

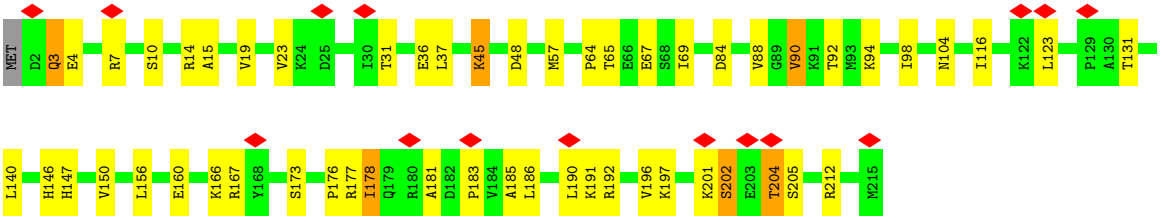


• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

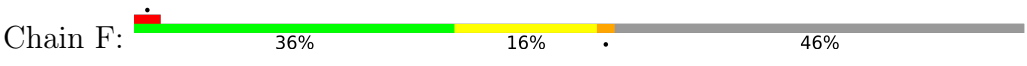


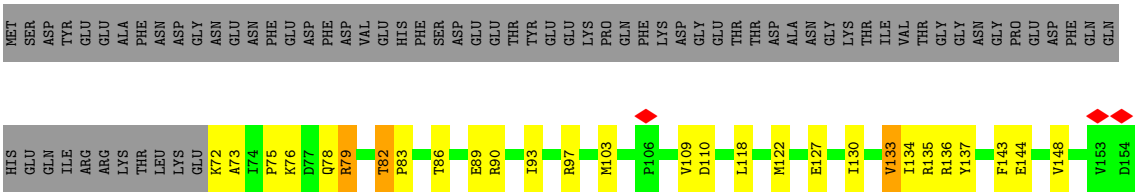
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1





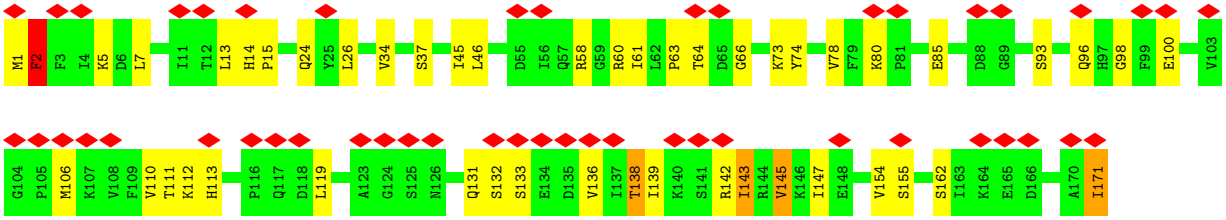
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2





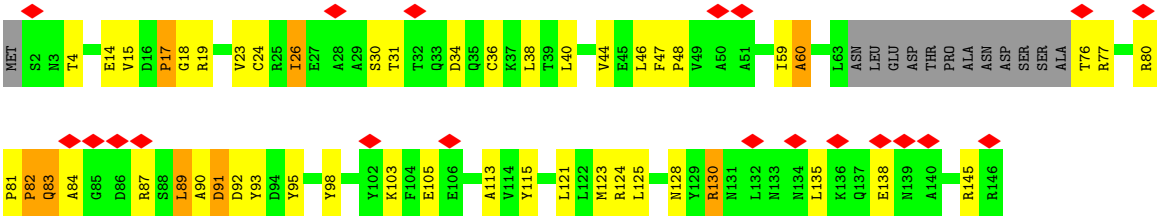
• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G:



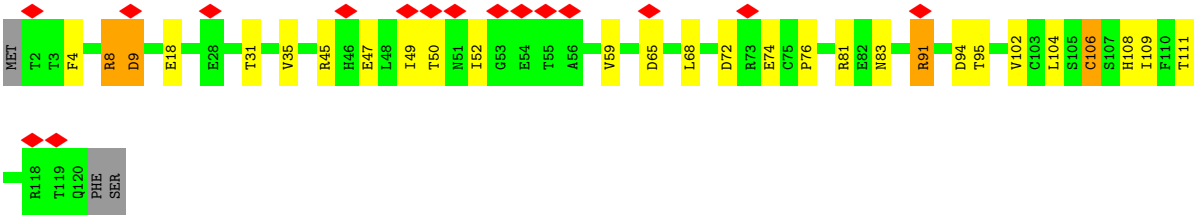
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H:



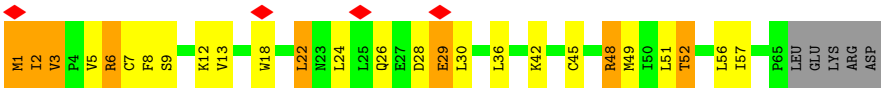
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

Chain I:



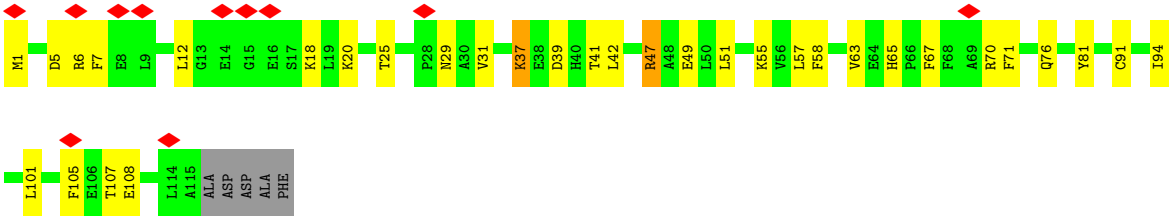
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J:

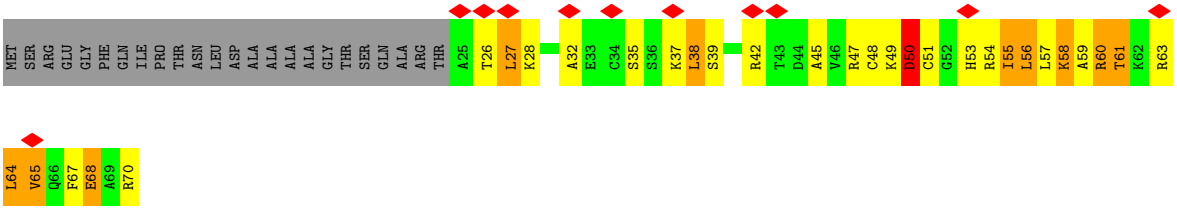


• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

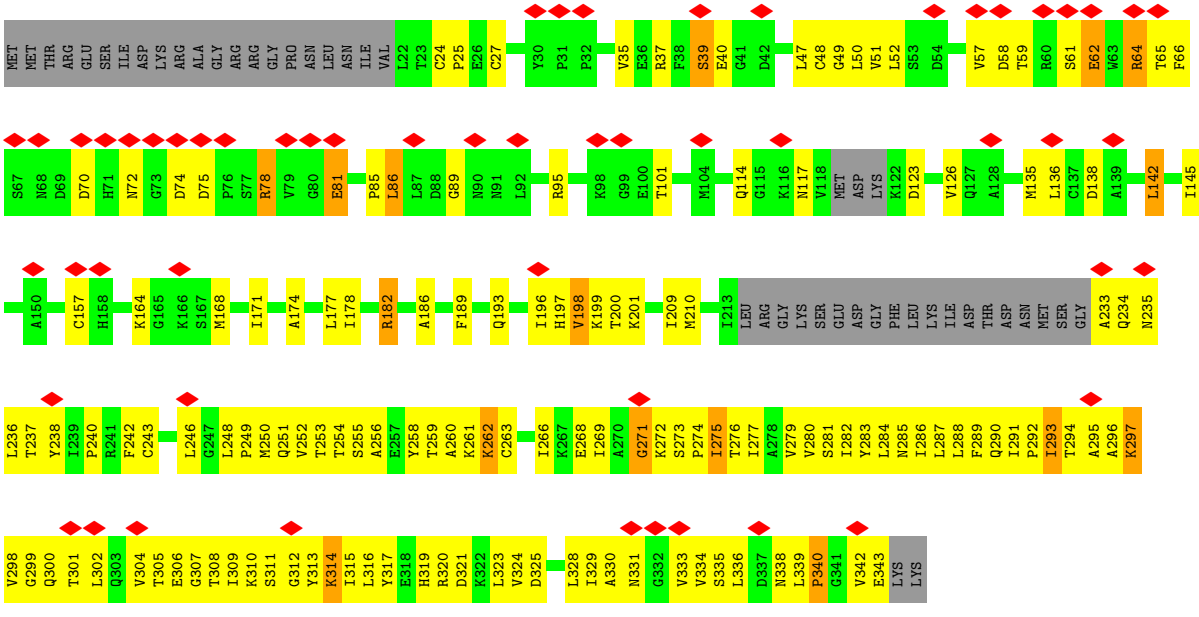
Chain K:



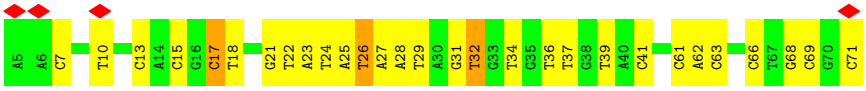
• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4



• Molecule 13: TRANSCRIPTION INITIATION FACTOR IIB

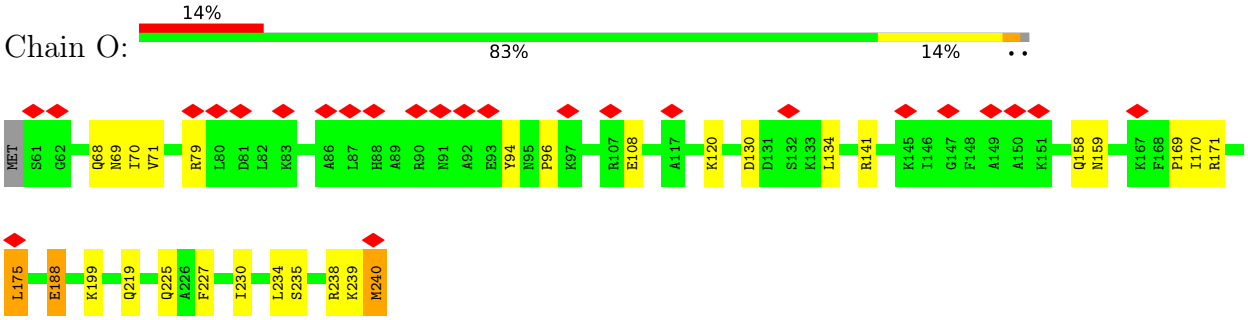


• Molecule 14: NONTEMPLATE DNA



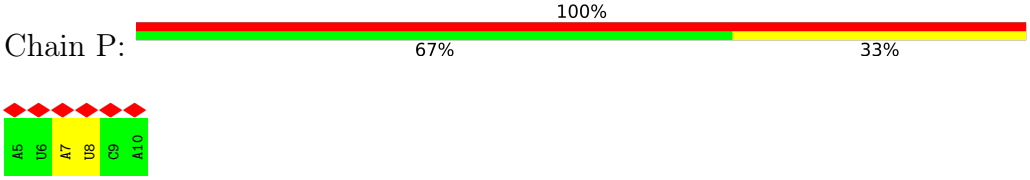
• Molecule 15: TATA-BOX-BINDING PROTEIN

Chain O:



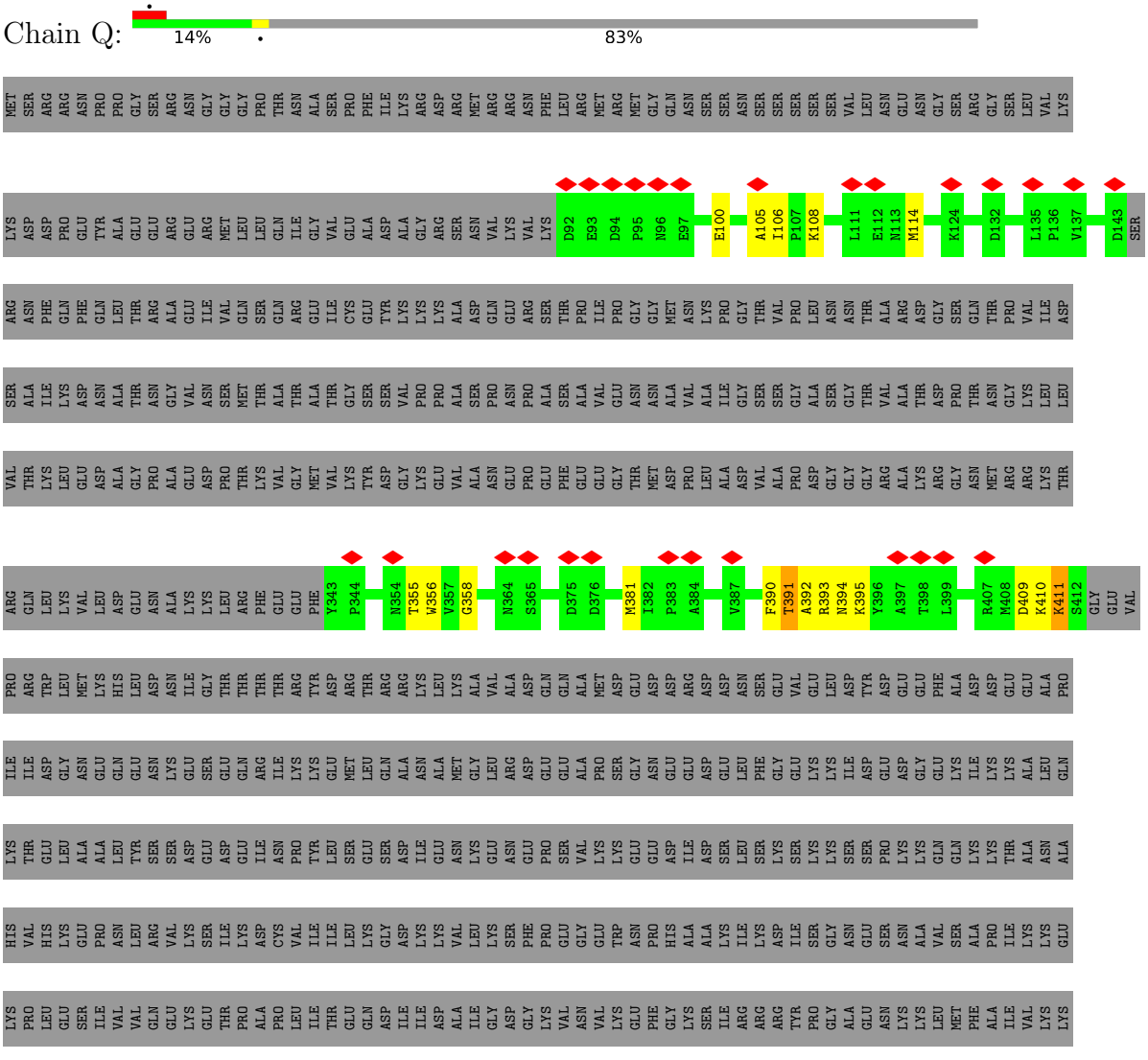
• Molecule 16: RNA

Chain P:

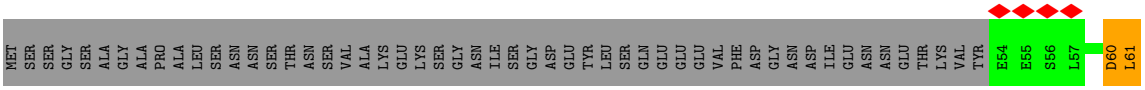


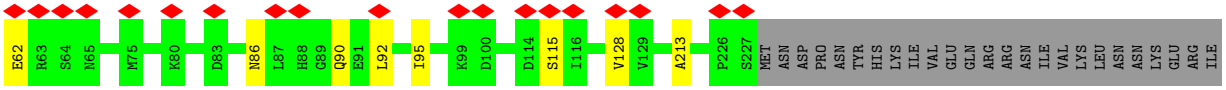
• Molecule 17: TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT ALPHA

Chain Q:

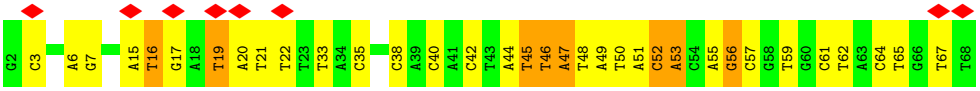


• Molecule 18: TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT BETA





• Molecule 19: TEMPLATE DNA



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	4439	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	37169	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.092	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0224	Depositor
Map size (Å)	378.0, 378.0, 378.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

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	0.56	4/11374 (0.0%)	0.81	11/15384 (0.1%)
2	B	0.49	1/9316 (0.0%)	0.74	4/12564 (0.0%)
3	C	0.49	0/2133	0.78	2/2891 (0.1%)
4	D	0.51	0/1444	0.83	2/1935 (0.1%)
5	E	0.48	0/1788	0.71	0/2406
6	F	0.62	0/691	0.81	0/933
7	G	0.52	0/1368	0.81	0/1844
8	H	0.50	0/1086	0.80	0/1470
9	I	0.47	0/989	0.78	0/1331
10	J	0.54	0/541	0.88	1/727 (0.1%)
11	K	0.47	0/938	0.71	0/1267
12	L	0.54	0/365	0.95	0/485
13	M	0.61	0/2232	0.77	1/3031 (0.0%)
14	N	1.13	14/1100 (1.3%)	1.31	5/1625 (0.3%)
15	O	0.58	0/1443	0.78	1/1942 (0.1%)
16	P	0.34	0/137	0.80	0/211
17	Q	0.95	0/604	1.19	3/840 (0.4%)
18	R	0.92	0/520	1.21	2/724 (0.3%)
19	T	1.22	18/1265 (1.4%)	1.44	15/1866 (0.8%)
All	All	0.60	37/39334 (0.1%)	0.85	47/53476 (0.1%)

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	2
2	B	0	1
17	Q	0	1
All	All	0	4

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1436	ILE	C-N	14.99	1.60	1.33
1	A	95	PHE	C-N	-14.47	1.00	1.34
19	T	53	DA	P-O5'	-11.71	1.48	1.59
1	A	234	MET	C-N	-11.62	1.07	1.34
19	T	47	DA	C1'-N9	-10.46	1.32	1.47
2	B	973	ILE	C-N	9.27	1.51	1.34
19	T	42	DC	P-O5'	-9.25	1.50	1.59
19	T	56	DG	C1'-N9	-6.65	1.38	1.47
19	T	61	DC	C1'-N1	6.24	1.57	1.49
1	A	1394	THR	C-N	-6.22	1.21	1.33
19	T	64	DC	C1'-N1	6.15	1.57	1.49
19	T	46	DT	C4'-C3'	-5.39	1.47	1.52
14	N	34	DT	C1'-N1	5.23	1.56	1.49
14	N	10	DT	C1'-N1	5.23	1.56	1.49
14	N	32	DT	C1'-N1	5.23	1.56	1.49
14	N	39	DT	C1'-N1	5.23	1.56	1.49
14	N	13	DC	C1'-N1	5.22	1.56	1.49
14	N	7	DC	C1'-N1	5.21	1.56	1.49
19	T	35	DC	C1'-N1	5.21	1.56	1.49
19	T	38	DC	C1'-N1	5.20	1.56	1.49
19	T	33	DT	C1'-N1	5.19	1.55	1.49
19	T	67	DT	C1'-N1	5.19	1.55	1.49
14	N	15	DC	C1'-N1	5.18	1.55	1.49
19	T	65	DT	C1'-N1	5.18	1.55	1.49
19	T	6	DA	O3'-P	-5.17	1.54	1.61
19	T	3	DC	C1'-N1	5.17	1.55	1.49
19	T	59	DT	C1'-N1	5.17	1.55	1.49
19	T	40	DC	C1'-N1	5.17	1.55	1.49
14	N	36	DT	C1'-N1	5.17	1.55	1.49
14	N	41	DC	C1'-N1	5.16	1.55	1.49
14	N	69	DC	C1'-N1	5.16	1.55	1.49
19	T	57	DC	C1'-N1	5.15	1.55	1.49
19	T	62	DT	C1'-N1	5.15	1.55	1.49
14	N	71	DC	C1'-N1	5.15	1.55	1.49
14	N	37	DT	C1'-N1	5.14	1.55	1.49
14	N	17	DC	C1'-N1	5.14	1.55	1.49
14	N	68	DG	O3'-P	-5.10	1.55	1.61

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	MET	O-C-N	-14.63	99.29	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	T	46	DT	O4'-C4'-C3'	-11.79	98.93	106.00
19	T	6	DA	O3'-P-O5'	-9.12	86.68	104.00
19	T	42	DC	O5'-P-OP1	-9.08	97.53	105.70
14	N	26	DT	O4'-C4'-C3'	-9.01	100.59	106.00
18	R	60	ASP	C-N-CA	8.73	143.52	121.70
1	A	95	PHE	C-N-CA	-8.00	101.69	121.70
1	A	234	MET	CA-C-N	7.99	134.79	117.20
1	A	346	ASP	O-C-N	-7.59	110.55	122.70
19	T	16	DT	O4'-C4'-C3'	-7.28	101.59	104.50
14	N	66	DC	C2-N1-C1'	7.26	126.78	118.80
19	T	45	DT	O4'-C4'-C3'	-7.25	101.60	104.50
1	A	399	HIS	N-CA-CB	7.23	123.62	110.60
14	N	68	DG	P-O3'-C3'	7.19	128.33	119.70
18	R	61	LEU	N-CA-C	6.92	129.69	111.00
1	A	234	MET	C-N-CA	6.61	138.22	121.70
19	T	46	DT	O4'-C1'-C2'	-6.47	100.73	105.90
4	D	25	ALA	C-N-CA	6.12	137.01	121.70
1	A	95	PHE	CA-C-N	-6.11	103.75	117.20
17	Q	411	LYS	CA-C-O	5.98	132.66	120.10
19	T	46	DT	C4-C5-C6	5.98	121.59	118.00
19	T	53	DA	N1-C6-N6	-5.88	115.07	118.60
17	Q	411	LYS	N-CA-C	5.82	126.70	111.00
14	N	66	DC	C6-N1-C1'	-5.82	113.82	120.80
1	A	58	LEU	CA-CB-CG	5.74	128.50	115.30
19	T	19	DT	O4'-C1'-N1	5.72	112.00	108.00
19	T	7	DG	C5-C6-O6	-5.71	125.17	128.60
2	B	340	ALA	C-N-CA	5.69	135.92	121.70
1	A	194	ALA	C-N-CA	5.64	135.79	121.70
19	T	6	DA	P-O3'-C3'	5.58	126.40	119.70
19	T	53	DA	P-O5'-C5'	5.51	129.71	120.90
4	D	26	THR	N-CA-C	-5.50	96.14	111.00
19	T	47	DA	O4'-C1'-N9	-5.47	104.17	108.00
13	M	340	PRO	C-N-CA	-5.46	110.83	122.30
3	C	39	ALA	N-CA-C	5.45	125.71	111.00
2	B	628	THR	C-N-CA	5.44	135.29	121.70
15	O	175	LEU	CA-CB-CG	5.44	127.80	115.30
3	C	89	GLU	N-CA-C	-5.29	96.73	111.00
1	A	1394	THR	C-N-CA	5.26	133.35	122.30
14	N	26	DT	P-O3'-C3'	5.20	125.94	119.70
2	B	1181	GLU	N-CA-C	5.16	124.94	111.00
19	T	52	DC	OP1-P-O3'	5.16	116.55	105.20
19	T	6	DA	O4'-C1'-N9	5.10	111.57	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Q	114	MET	C-N-CA	-5.10	108.95	121.70
10	J	5	VAL	N-CA-C	-5.03	97.42	111.00
2	B	1156	ASP	N-CA-C	5.03	124.57	111.00
1	A	346	ASP	CA-C-N	5.02	128.24	117.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	MET	Mainchain
1	A	95	PHE	Mainchain
2	B	43	LEU	Mainchain
17	Q	410	LYS	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	11174	0	11223	407	0
2	B	9140	0	9111	313	0
3	C	2095	0	2051	43	0
4	D	1434	0	1460	79	0
5	E	1752	0	1776	28	0
6	F	679	0	701	26	0
7	G	1340	0	1357	33	0
8	H	1068	0	1040	21	0
9	I	971	0	927	15	0
10	J	532	0	542	14	0
11	K	920	0	929	19	0
12	L	363	0	386	26	0
13	M	2202	0	2154	391	0
14	N	975	0	567	22	0
15	O	1416	0	1491	31	0
16	P	123	0	66	1	0
17	Q	606	0	256	30	0
18	R	521	0	216	5	0
19	T	1125	0	661	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	2	0	0	0	0
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	I	2	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
20	M	1	0	0	0	0
21	A	1	0	0	0	0
All	All	38446	0	36914	1219	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 16.

All (1219) 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:868:MET:CE	13:M:182:ARG:HG2	1.34	1.54
1:A:867:ILE:CG1	1:A:867:ILE:CD1	1.83	1.53
17:Q:356:TRP:CA	17:Q:392:ALA:HA	1.06	1.52
2:B:1215:ARG:NH1	4:D:15:LEU:HD13	1.27	1.49
17:Q:356:TRP:HA	17:Q:392:ALA:CA	0.93	1.40
13:M:274:PRO:HD2	15:O:188:GLU:CD	1.38	1.40
2:B:1221:SER:HB3	4:D:12:ARG:CD	1.50	1.38
17:Q:390:PHE:HA	17:Q:391:THR:CB	1.44	1.38
13:M:274:PRO:CD	15:O:188:GLU:OE2	1.75	1.32
2:B:868:MET:HE1	13:M:182:ARG:CG	1.61	1.29
17:Q:355:THR:O	17:Q:393:ARG:N	1.61	1.28
1:A:344:ARG:NH2	2:B:1120:GLU:HG3	1.48	1.27
2:B:1221:SER:CB	4:D:12:ARG:HD2	1.62	1.27
13:M:273:SER:HB2	15:O:188:GLU:OE2	1.32	1.26
1:A:228:PHE:CZ	4:D:14:ARG:HB3	1.69	1.25
2:B:1215:ARG:CZ	4:D:15:LEU:HD13	1.67	1.24
17:Q:356:TRP:CB	17:Q:392:ALA:HB2	1.65	1.24
13:M:274:PRO:CD	15:O:188:GLU:CD	2.01	1.24
1:A:317:LYS:O	2:B:471:LYS:NZ	1.73	1.21
13:M:274:PRO:CD	15:O:188:GLU:OE1	1.89	1.20
2:B:1215:ARG:NH2	4:D:15:LEU:HD22	1.56	1.18
2:B:1215:ARG:NH1	4:D:15:LEU:CD1	2.07	1.17
14:N:24:DT:H2"	14:N:25:DA:H5'	1.25	1.16
13:M:248:LEU:HD11	13:M:286:ILE:HD12	1.22	1.16
2:B:104:GLU:OE2	12:L:54:ARG:HD3	1.44	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:868:MET:CE	13:M:182:ARG:CG	2.19	1.15
1:A:228:PHE:CE1	4:D:15:LEU:CB	2.31	1.13
13:M:295:ALA:HB1	13:M:309:ILE:HD11	1.28	1.12
17:Q:390:PHE:CA	17:Q:391:THR:CB	2.27	1.12
13:M:311:SER:HA	13:M:314:LYS:HE2	1.32	1.12
1:A:228:PHE:HZ	4:D:14:ARG:CB	1.62	1.11
1:A:228:PHE:HZ	4:D:14:ARG:HB3	0.95	1.11
1:A:836:TYR:OH	1:A:1403:GLU:OE2	1.69	1.10
1:A:419:LYS:NZ	13:M:48:CYS:HB3	1.65	1.09
13:M:288:LEU:HD21	13:M:339:LEU:HD11	1.35	1.08
1:A:89:PRO:HG2	1:A:204:THR:HB	1.35	1.07
1:A:78:PRO:O	2:B:1201:LYS:NZ	1.89	1.06
1:A:228:PHE:CE1	4:D:15:LEU:HB3	1.92	1.05
1:A:344:ARG:CZ	2:B:1120:GLU:HG3	1.88	1.03
2:B:451:LYS:HD2	13:M:138:ASP:OD2	1.59	1.03
1:A:317:LYS:O	2:B:471:LYS:CE	2.06	1.03
17:Q:356:TRP:CB	17:Q:392:ALA:CB	2.37	1.03
1:A:89:PRO:CG	1:A:204:THR:HB	1.88	1.02
13:M:279:VAL:HG23	13:M:298:VAL:HG22	1.38	1.02
17:Q:356:TRP:HA	17:Q:392:ALA:CB	1.88	1.02
17:Q:356:TRP:CA	17:Q:392:ALA:CA	1.86	1.01
1:A:228:PHE:CD1	4:D:15:LEU:CB	2.44	1.01
13:M:279:VAL:HB	13:M:302:LEU:HD22	1.39	1.01
2:B:902:GLY:O	12:L:65:VAL:HG11	1.59	1.00
13:M:272:LYS:HE3	19:T:53:DA:P	2.01	1.00
1:A:1386:ARG:NH1	1:A:1403:GLU:OE1	1.95	0.99
13:M:274:PRO:HD3	15:O:188:GLU:OE1	1.62	0.98
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.27	0.98
1:A:228:PHE:CD1	4:D:15:LEU:HB3	1.99	0.98
1:A:419:LYS:HB3	13:M:47:LEU:O	1.64	0.98
1:A:344:ARG:HD2	2:B:1118:PRO:O	1.64	0.98
17:Q:356:TRP:CA	17:Q:392:ALA:CB	2.40	0.97
1:A:228:PHE:CE1	4:D:15:LEU:HB2	1.99	0.96
13:M:259:THR:HG23	13:M:323:LEU:HB3	1.43	0.96
13:M:242:PHE:CE1	13:M:302:LEU:HA	2.01	0.96
13:M:186:ALA:HB1	13:M:237:THR:OG1	1.65	0.95
13:M:274:PRO:HD2	15:O:188:GLU:OE2	0.78	0.95
13:M:320:ARG:HE	13:M:336:LEU:HB3	1.32	0.94
17:Q:105:ALA:HB2	18:R:92:LEU:CB	1.98	0.93
13:M:283:TYR:CZ	13:M:287:LEU:HD11	2.04	0.93
13:M:286:ILE:HD13	13:M:293:ILE:CG2	1.98	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1221:SER:HB3	4:D:12:ARG:NE	1.85	0.92
13:M:248:LEU:CD1	13:M:286:ILE:HD12	2.00	0.92
13:M:269:ILE:HG12	13:M:315:ILE:HG21	1.48	0.91
13:M:279:VAL:CB	13:M:302:LEU:HD22	2.00	0.91
2:B:451:LYS:CE	13:M:138:ASP:OD2	2.19	0.91
13:M:238:TYR:HB3	13:M:242:PHE:CE2	2.06	0.90
13:M:288:LEU:CD2	13:M:339:LEU:HD11	2.02	0.90
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.52	0.89
13:M:242:PHE:HD1	13:M:301:THR:HG22	1.36	0.89
13:M:274:PRO:CG	15:O:188:GLU:OE1	2.21	0.89
2:B:451:LYS:CD	13:M:138:ASP:OD2	2.20	0.88
13:M:273:SER:CB	15:O:188:GLU:OE2	2.20	0.88
13:M:288:LEU:HG	13:M:339:LEU:HD21	1.56	0.88
13:M:298:VAL:HG22	13:M:302:LEU:HD13	1.54	0.88
17:Q:355:THR:O	17:Q:392:ALA:C	2.12	0.88
2:B:1221:SER:HB3	4:D:12:ARG:HD2	0.90	0.88
13:M:248:LEU:HD13	13:M:252:VAL:HG11	1.54	0.88
1:A:417:TYR:CE2	13:M:37:ARG:HD3	2.09	0.88
15:O:69:ASN:HB2	19:T:48:DT:O4’	1.74	0.88
1:A:832:ALA:HA	19:T:15:DA:O4’	1.73	0.87
1:A:419:LYS:HZ1	13:M:48:CYS:HB3	1.32	0.87
13:M:339:LEU:HB3	13:M:340:PRO:HD2	1.57	0.87
1:A:226:GLU:HG3	4:D:16:LYS:NZ	1.90	0.87
19:T:49:DA:C2’	19:T:50:DT:H5’	2.03	0.87
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.56	0.87
13:M:279:VAL:CG1	13:M:309:ILE:HG22	2.05	0.86
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.57	0.86
2:B:104:GLU:OE2	12:L:54:ARG:CD	2.22	0.86
1:A:91:PHE:HB3	1:A:96:ILE:HG13	1.56	0.86
10:J:48:ARG:HE	10:J:49:MET:HE2	1.39	0.86
1:A:417:TYR:CZ	13:M:37:ARG:HD3	2.09	0.86
1:A:228:PHE:HE1	4:D:15:LEU:CB	1.88	0.85
13:M:248:LEU:HD21	13:M:286:ILE:HD11	1.58	0.85
13:M:295:ALA:CB	13:M:309:ILE:HD11	2.06	0.85
13:M:295:ALA:HB1	13:M:306:GLU:HG3	1.56	0.85
1:A:228:PHE:CD1	4:D:15:LEU:HB2	2.08	0.85
13:M:234:GLN:HB2	13:M:236:LEU:CD2	2.07	0.85
13:M:310:LYS:HE3	13:M:342:VAL:HG22	1.59	0.85
1:A:11:LEU:HD11	2:B:1195:HIS:CD2	2.11	0.84
1:A:228:PHE:CZ	4:D:14:ARG:C	2.51	0.84
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:312:GLY:O	13:M:315:ILE:HG22	1.78	0.83
2:B:416:LEU:HD23	2:B:457:LEU:HD23	1.60	0.83
2:B:1215:ARG:NH2	4:D:15:LEU:CD2	2.39	0.83
13:M:295:ALA:CB	13:M:306:GLU:HG3	2.09	0.83
1:A:228:PHE:HA	4:D:15:LEU:HD23	1.60	0.83
13:M:311:SER:HA	13:M:314:LYS:CE	2.09	0.83
13:M:266:ILE:CD1	13:M:268:GLU:HB2	2.09	0.82
13:M:310:LYS:CE	13:M:342:VAL:HG22	2.09	0.82
3:C:148:ARG:H	3:C:151:GLN:HG3	1.43	0.82
13:M:238:TYR:HB3	13:M:242:PHE:CD2	2.14	0.82
13:M:279:VAL:HG23	13:M:298:VAL:CG2	2.09	0.82
6:F:103:MET:HE2	7:G:66:GLY:HA3	1.62	0.82
13:M:275:ILE:HD11	13:M:302:LEU:HB3	1.62	0.82
3:C:148:ARG:HD3	3:C:149:LYS:HG2	1.61	0.82
13:M:66:PHE:O	13:M:78:ARG:NH2	2.12	0.82
1:A:68:GLN:O	1:A:68:GLN:NE2	2.11	0.82
13:M:293:ILE:HD13	13:M:297:LYS:HG3	1.60	0.82
13:M:269:ILE:HD11	13:M:316:LEU:HD11	1.60	0.82
1:A:419:LYS:HZ2	13:M:48:CYS:HB3	1.41	0.81
14:N:24:DT:C2'	14:N:25:DA:H5'	2.09	0.81
13:M:269:ILE:HG23	13:M:272:LYS:HG2	1.61	0.81
13:M:273:SER:O	13:M:276:THR:HG22	1.79	0.81
17:Q:356:TRP:CB	17:Q:392:ALA:CA	2.58	0.81
1:A:53:LEU:HD23	1:A:54:ASN:H	1.44	0.81
13:M:315:ILE:CG2	13:M:316:LEU:HD12	2.10	0.81
2:B:868:MET:HE2	13:M:182:ARG:HG2	1.59	0.81
1:A:836:TYR:HH	1:A:1403:GLU:CD	1.83	0.81
1:A:55:ASP:HA	1:A:58:LEU:HB2	1.63	0.81
2:B:849:GLY:HA2	2:B:852:ARG:HD2	1.62	0.81
19:T:49:DA:H2"	19:T:50:DT:H5'	1.61	0.81
13:M:186:ALA:CB	13:M:237:THR:OG1	2.29	0.80
13:M:269:ILE:HG21	13:M:272:LYS:HB2	1.62	0.80
13:M:325:ASP:OD1	13:M:328:LEU:HB2	1.81	0.80
13:M:234:GLN:O	13:M:237:THR:HG22	1.81	0.80
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.63	0.80
13:M:269:ILE:CD1	13:M:316:LEU:HD11	2.12	0.80
2:B:451:LYS:NZ	13:M:138:ASP:OD1	2.15	0.79
13:M:279:VAL:CA	13:M:302:LEU:HD22	2.11	0.79
13:M:279:VAL:HG11	13:M:309:ILE:HG22	1.63	0.79
2:B:451:LYS:CE	13:M:138:ASP:CG	2.50	0.79
17:Q:356:TRP:C	17:Q:392:ALA:HA	2.03	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:VAL:HG13	13:M:240:PRO:HB2	1.64	0.79
13:M:315:ILE:HG23	13:M:316:LEU:HD12	1.64	0.79
13:M:248:LEU:HD23	13:M:291:ILE:CD1	2.13	0.79
13:M:336:LEU:HA	13:M:339:LEU:CD1	2.12	0.79
2:B:1217:TYR:CD2	4:D:14:ARG:CZ	2.65	0.78
13:M:305:THR:HG23	13:M:308:THR:H	1.46	0.78
13:M:286:ILE:HG21	13:M:293:ILE:HG22	1.65	0.78
13:M:310:LYS:CD	13:M:342:VAL:HG22	2.13	0.78
1:A:89:PRO:HB2	1:A:204:THR:CG2	2.13	0.78
13:M:286:ILE:HD13	13:M:293:ILE:HG22	1.64	0.78
13:M:296:ALA:O	13:M:300:GLN:HG3	1.83	0.78
13:M:287:LEU:HD13	13:M:340:PRO:HG3	1.65	0.78
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.64	0.78
2:B:451:LYS:NZ	13:M:138:ASP:CG	2.37	0.78
2:B:900:ALA:HB3	12:L:61:THR:HG23	1.64	0.78
13:M:269:ILE:HG21	13:M:277:ILE:CD1	2.14	0.78
2:B:1215:ARG:CZ	4:D:15:LEU:CD1	2.57	0.77
13:M:249:PRO:HD3	13:M:291:ILE:HD11	1.66	0.77
2:B:449:ASN:ND2	13:M:135:MET:HG3	1.99	0.77
2:B:451:LYS:HE3	13:M:138:ASP:CG	2.04	0.77
3:C:147:LEU:HB3	3:C:151:GLN:HB2	1.66	0.77
1:A:95:PHE:O	1:A:96:ILE:C	2.13	0.77
1:A:1444:MET:HG2	7:G:58:ARG:HB3	1.66	0.77
13:M:248:LEU:HD21	13:M:286:ILE:CD1	2.14	0.77
13:M:277:ILE:O	13:M:280:VAL:HG22	1.83	0.77
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.66	0.77
13:M:330:ALA:HB1	13:M:334:VAL:O	1.84	0.77
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.67	0.77
1:A:1433:MET:CE	2:B:1145:SER:OG	2.33	0.77
2:B:1215:ARG:HH12	4:D:15:LEU:CD1	1.98	0.76
19:T:47:DA:N7	19:T:48:DT:O4	2.19	0.76
1:A:22:PHE:HB2	2:B:1211:ASN:CG	2.06	0.76
19:T:48:DT:H2'	19:T:49:DA:C8	2.21	0.76
13:M:311:SER:CA	13:M:314:LYS:HE2	2.13	0.76
1:A:1390:ASN:O	1:A:1399:ARG:CD	2.34	0.75
1:A:419:LYS:HG2	13:M:48:CYS:HA	1.68	0.75
2:B:868:MET:HE1	13:M:182:ARG:HG2	0.77	0.75
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.66	0.75
13:M:320:ARG:NE	13:M:336:LEU:HB3	2.00	0.75
13:M:286:ILE:HD13	13:M:293:ILE:CB	2.16	0.75
1:A:418:SER:HA	13:M:48:CYS:C	2.07	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ARG:NH2	2:B:1120:GLU:CG	2.39	0.75
1:A:497:THR:HG22	2:B:1146:PHE:HD1	1.52	0.75
4:D:40:HIS:HB3	7:G:73:LYS:HE3	1.67	0.75
13:M:293:ILE:HD11	13:M:297:LYS:HB2	1.67	0.75
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.69	0.74
1:A:418:SER:CA	13:M:49:GLY:HA3	2.17	0.74
13:M:249:PRO:CD	13:M:291:ILE:HD11	2.18	0.74
13:M:290:GLN:NE2	13:M:291:ILE:HG23	2.02	0.74
13:M:290:GLN:CD	13:M:291:ILE:HG23	2.08	0.74
13:M:233:ALA:HB1	13:M:237:THR:HG21	1.70	0.74
2:B:792:MET:HE2	19:T:21:DT:OP1	1.87	0.74
2:B:868:MET:O	13:M:182:ARG:NH2	2.21	0.73
4:D:203:SER:HB3	4:D:206:GLU:HB2	1.70	0.73
13:M:275:ILE:CD1	13:M:302:LEU:HB3	2.19	0.73
13:M:335:SER:O	13:M:339:LEU:HD12	1.89	0.73
1:A:89:PRO:HG2	1:A:204:THR:CB	2.16	0.73
1:A:419:LYS:NZ	13:M:27:CYS:SG	2.62	0.73
13:M:274:PRO:CG	15:O:188:GLU:CD	2.57	0.73
1:A:91:PHE:HB3	1:A:96:ILE:CG1	2.18	0.72
1:A:836:TYR:CZ	1:A:1403:GLU:OE2	2.41	0.72
13:M:248:LEU:HA	13:M:291:ILE:HD11	1.69	0.72
2:B:952:VAL:O	12:L:58:LYS:HB2	1.89	0.72
1:A:35:ILE:HA	1:A:52:GLY:O	1.89	0.72
13:M:321:ASP:OD1	13:M:336:LEU:HD13	1.89	0.72
2:B:1125:ASP:OD2	13:M:39:SER:O	2.07	0.72
13:M:272:LYS:CE	19:T:53:DA:P	2.76	0.72
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.71	0.72
13:M:287:LEU:CD1	13:M:340:PRO:HG3	2.20	0.72
2:B:902:GLY:O	12:L:65:VAL:CG1	2.36	0.72
6:F:103:MET:HE1	7:G:66:GLY:N	2.05	0.72
13:M:286:ILE:HD13	13:M:293:ILE:HB	1.72	0.72
1:A:418:SER:HA	13:M:48:CYS:O	1.90	0.72
1:A:418:SER:HA	13:M:49:GLY:HA3	1.72	0.72
3:C:66:ARG:NH2	10:J:3:VAL:O	2.23	0.72
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.71	0.72
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.72	0.71
1:A:317:LYS:O	2:B:471:LYS:HE3	1.89	0.71
1:A:91:PHE:HB2	1:A:96:ILE:HD11	1.72	0.71
13:M:242:PHE:CD1	13:M:301:THR:HG22	2.24	0.71
13:M:275:ILE:HD12	13:M:304:VAL:CG2	2.20	0.71
13:M:342:VAL:HG13	13:M:343:GLU:N	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1198:TYR:CE2	2:B:1201:LYS:HE3	2.25	0.70
1:A:228:PHE:HE1	4:D:15:LEU:HB2	1.51	0.70
1:A:831:THR:HG23	19:T:15:DA:C5	2.27	0.70
19:T:46:DT:H2"	19:T:47:DA:O5'	1.91	0.70
1:A:346:ASP:OD1	2:B:1106:ARG:NE	2.21	0.70
2:B:1133:MET:SD	19:T:16:DT:H4'	2.32	0.70
13:M:243:CYS:SG	13:M:253:THR:HG22	2.32	0.70
13:M:286:ILE:CD1	13:M:293:ILE:HB	2.22	0.69
13:M:294:THR:H	13:M:297:LYS:HG3	1.57	0.69
17:Q:355:THR:O	17:Q:392:ALA:CA	2.39	0.69
13:M:274:PRO:HG3	15:O:188:GLU:OE1	1.92	0.69
2:B:429:PHE:HA	2:B:432:MET:HE2	1.73	0.69
1:A:417:TYR:CE2	13:M:37:ARG:CD	2.75	0.69
1:A:228:PHE:CE1	4:D:14:ARG:C	2.66	0.69
1:A:344:ARG:HA	2:B:1128:LEU:O	1.93	0.69
13:M:235:ASN:HD22	13:M:260:ALA:HB3	1.58	0.69
17:Q:358:GLY:HA2	17:Q:391:THR:CB	2.22	0.69
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.75	0.69
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.74	0.69
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.72	0.69
1:A:831:THR:CG2	19:T:15:DA:C5	2.75	0.69
1:A:50:ILE:O	1:A:52:GLY:N	2.23	0.69
1:A:53:LEU:CD2	1:A:54:ASN:H	2.06	0.69
2:B:563:MET:HE2	2:B:580:VAL:HB	1.75	0.69
2:B:868:MET:O	13:M:182:ARG:CZ	2.40	0.69
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.74	0.68
5:E:185:ALA:HA	5:E:190:LEU:HD12	1.74	0.68
1:A:228:PHE:HE1	4:D:15:LEU:N	1.90	0.68
1:A:412:ARG:HB3	13:M:51:VAL:CG1	2.24	0.68
17:Q:355:THR:O	17:Q:392:ALA:HB1	1.94	0.68
1:A:320:ARG:NH2	13:M:81:GLU:HG3	2.08	0.68
1:A:140:THR:HA	1:A:143:LYS:HE2	1.75	0.68
13:M:334:VAL:HA	13:M:338:ASN:ND2	2.09	0.68
7:G:1:MET:HE1	7:G:80:LYS:O	1.94	0.68
19:T:48:DT:H2'	19:T:49:DA:N7	2.08	0.68
13:M:334:VAL:HA	13:M:338:ASN:HD21	1.58	0.68
1:A:871:ASP:HB3	5:E:204:THR:HG23	1.76	0.68
2:B:792:MET:HE2	19:T:21:DT:P	2.33	0.68
7:G:138:THR:HG22	7:G:139:ILE:H	1.59	0.68
13:M:284:LEU:CD1	13:M:339:LEU:HD22	2.24	0.68
13:M:324:VAL:CG2	13:M:328:LEU:HD22	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:47:DA:C8	19:T:48:DT:O4	2.47	0.68
13:M:70:ASP:HB3	13:M:78:ARG:HD2	1.75	0.67
13:M:306:GLU:HA	13:M:309:ILE:HG12	1.76	0.67
13:M:269:ILE:HD11	13:M:316:LEU:CD1	2.23	0.67
13:M:283:TYR:O	13:M:287:LEU:HG	1.93	0.67
3:C:259:LEU:HD22	11:K:91:CYS:HB3	1.75	0.67
2:B:868:MET:CE	13:M:182:ARG:CD	2.73	0.67
1:A:419:LYS:NZ	13:M:48:CYS:CB	2.52	0.67
2:B:1215:ARG:HH22	4:D:15:LEU:HD22	1.60	0.66
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.75	0.66
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.59	0.66
1:A:15:LYS:NZ	2:B:1220:ARG:HE	1.93	0.66
2:B:872:GLU:HG2	2:B:916:THR:HG22	1.78	0.66
13:M:293:ILE:HG12	13:M:297:LYS:HD3	1.78	0.66
1:A:347:PHE:HE1	1:A:375:THR:HG22	1.60	0.66
13:M:261:LYS:HG3	13:M:262:LYS:N	2.09	0.66
13:M:272:LYS:HB3	13:M:276:THR:HG21	1.77	0.66
13:M:290:GLN:HB3	13:M:331:ASN:ND2	2.11	0.66
1:A:228:PHE:HA	4:D:15:LEU:CD2	2.25	0.66
1:A:419:LYS:HE3	13:M:47:LEU:C	2.15	0.66
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.26	0.66
13:M:243:CYS:CB	13:M:253:THR:HG22	2.26	0.66
13:M:269:ILE:HG21	13:M:277:ILE:HD11	1.76	0.66
1:A:204:THR:HG22	1:A:235:ILE:HG21	1.78	0.66
2:B:857:ARG:NH1	2:B:945:GLU:OE2	2.29	0.66
1:A:226:GLU:HG3	4:D:16:LYS:HZ1	1.58	0.65
1:A:311:GLN:HG3	1:A:312:PRO:HD2	1.77	0.65
1:A:1442:ASP:HB2	6:F:137:TYR:HE1	1.61	0.65
2:B:868:MET:HE1	13:M:182:ARG:CD	2.26	0.65
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.79	0.65
13:M:186:ALA:HB1	13:M:237:THR:HG1	1.60	0.65
1:A:57:ARG:O	1:A:68:GLN:HG2	1.96	0.65
13:M:269:ILE:CG1	13:M:315:ILE:HG21	2.25	0.65
13:M:242:PHE:O	13:M:246:LEU:HG	1.96	0.65
1:A:46:THR:HG22	1:A:47:ARG:H	1.61	0.65
1:A:388:LEU:O	1:A:392:VAL:HG23	1.96	0.65
17:Q:356:TRP:N	17:Q:392:ALA:HA	2.02	0.65
2:B:296:GLU:O	2:B:300:HIS:HD2	1.80	0.65
7:G:1:MET:CE	7:G:80:LYS:O	2.45	0.65
13:M:255:SER:OG	13:M:328:LEU:HD13	1.96	0.65
13:M:311:SER:O	13:M:314:LYS:HD3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LYS:HZ2	1:A:1415:SER:CB	2.09	0.65
13:M:286:ILE:HG12	13:M:292:PRO:HA	1.78	0.65
1:A:316:GLN:O	1:A:318:SER:N	2.30	0.65
13:M:269:ILE:HD12	13:M:277:ILE:HD12	1.79	0.64
13:M:283:TYR:CE2	13:M:287:LEU:HD11	2.31	0.64
1:A:226:GLU:HG3	4:D:16:LYS:CE	2.27	0.64
1:A:228:PHE:CE1	4:D:15:LEU:N	2.65	0.64
1:A:416:ARG:NH2	13:M:40:GLU:HG2	2.13	0.64
1:A:419:LYS:HZ2	13:M:48:CYS:CB	2.08	0.64
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.79	0.64
3:C:56:THR:HG21	3:C:145:CYS:SG	2.37	0.64
17:Q:409:ASP:HA	17:Q:411:LYS:O	1.97	0.64
2:B:868:MET:HE3	13:M:182:ARG:CG	2.25	0.64
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.79	0.64
1:A:832:ALA:HB2	19:T:15:DA:C8	2.32	0.64
13:M:279:VAL:HG13	13:M:309:ILE:HG22	1.78	0.64
19:T:49:DA:H2'	19:T:50:DT:H5'	1.80	0.64
12:L:28:LYS:HB2	12:L:39:SER:HA	1.80	0.64
13:M:269:ILE:CD1	13:M:277:ILE:HD12	2.28	0.64
13:M:275:ILE:HD13	13:M:275:ILE:O	1.97	0.64
19:T:21:DT:H2"	19:T:22:DT:H5'	1.80	0.64
2:B:806:THR:HG22	2:B:808:ALA:H	1.63	0.63
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.80	0.63
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.81	0.63
2:B:917:PRO:HA	2:B:934:LYS:HB3	1.80	0.63
1:A:89:PRO:CB	1:A:204:THR:HB	2.29	0.63
1:A:228:PHE:HZ	4:D:14:ARG:CA	2.11	0.63
1:A:447:GLN:NE2	19:T:17:DG:H4'	2.13	0.63
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.81	0.63
1:A:417:TYR:HE2	13:M:37:ARG:HG3	1.64	0.63
3:C:10:ILE:HD12	11:K:108:GLU:HB3	1.80	0.63
13:M:271:GLY:O	19:T:52:DC:H4'	1.99	0.63
13:M:235:ASN:ND2	13:M:260:ALA:HB3	2.13	0.63
2:B:841:MET:HB3	2:B:846:ILE:HD11	1.81	0.62
1:A:5:GLN:HG3	2:B:1175:LEU:HD11	1.81	0.62
2:B:68:THR:HG22	2:B:91:SER:HA	1.80	0.62
13:M:319:HIS:O	13:M:323:LEU:HG	2.00	0.62
13:M:335:SER:H	13:M:338:ASN:ND2	1.96	0.62
13:M:275:ILE:HD12	13:M:304:VAL:HG21	1.80	0.62
13:M:288:LEU:O	13:M:334:VAL:HG23	1.98	0.62
13:M:291:ILE:O	13:M:291:ILE:HG13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:CD1	2:B:1195:HIS:CD2	2.82	0.62
13:M:266:ILE:HD11	13:M:268:GLU:HB2	1.80	0.62
1:A:68:GLN:O	1:A:70:CYS:N	2.31	0.62
13:M:304:VAL:HG12	13:M:305:THR:N	2.15	0.62
13:M:242:PHE:CG	13:M:302:LEU:HG	2.34	0.62
18:R:60:ASP:CB	18:R:213:ALA:HA	2.29	0.62
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.82	0.61
1:A:66:LYS:HE2	1:A:68:GLN:H	1.65	0.61
1:A:91:PHE:CB	1:A:96:ILE:HD11	2.30	0.61
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.82	0.61
13:M:287:LEU:O	13:M:334:VAL:HG21	2.00	0.61
1:A:1390:ASN:O	1:A:1399:ARG:HG2	2.01	0.61
3:C:11:ARG:HH21	3:C:229:TYR:HD2	1.48	0.61
7:G:1:MET:SD	7:G:2:PHE:N	2.63	0.61
13:M:313:TYR:HD2	13:M:343:GLU:N	1.97	0.61
13:M:324:VAL:HG22	13:M:325:ASP:N	2.15	0.61
13:M:294:THR:H	13:M:297:LYS:CG	2.13	0.61
1:A:89:PRO:HB2	1:A:204:THR:HG21	1.83	0.61
2:B:1221:SER:CB	4:D:12:ARG:CD	2.43	0.61
13:M:256:ALA:HA	13:M:285:ASN:HD22	1.65	0.61
1:A:22:PHE:N	2:B:1211:ASN:O	2.32	0.61
1:A:226:GLU:CG	4:D:16:LYS:NZ	2.64	0.61
2:B:205:ILE:HD11	2:B:461:LEU:HD13	1.82	0.61
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.82	0.61
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.81	0.61
2:B:486:TYR:HB3	2:B:1096:ARG:CZ	2.31	0.61
17:Q:394:ASN:CB	17:Q:395:LYS:HA	2.30	0.61
1:A:228:PHE:CZ	4:D:14:ARG:CB	2.52	0.61
2:B:1217:TYR:CB	4:D:14:ARG:NH2	2.64	0.61
1:A:344:ARG:CZ	2:B:1120:GLU:CG	2.74	0.61
1:A:448:PRO:O	1:A:449:SER:HB2	2.01	0.61
2:B:911:ILE:HD11	2:B:941:LEU:HD12	1.82	0.61
4:D:176:GLU:OE2	4:D:197:SER:HB2	1.99	0.61
13:M:310:LYS:HD3	13:M:342:VAL:HG22	1.82	0.61
17:Q:105:ALA:HB3	18:R:90:GLN:O	2.01	0.61
1:A:95:PHE:C	1:A:97:ALA:N	2.54	0.60
1:A:412:ARG:HB3	13:M:51:VAL:HG11	1.83	0.60
2:B:249:ARG:HH12	2:B:418:LYS:HD2	1.66	0.60
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.84	0.60
1:A:132:LYS:NZ	1:A:1415:SER:CB	2.64	0.60
1:A:629:LEU:O	1:A:633:VAL:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.34	0.60
5:E:202:SER:HB3	5:E:205:SER:H	1.66	0.60
14:N:24:DT:H2"	14:N:25:DA:C5'	2.17	0.60
1:A:1063:MET:SD	1:A:1436:ILE:HB	2.42	0.60
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.83	0.60
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.83	0.60
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.82	0.60
13:M:255:SER:HB3	13:M:285:ASN:OD1	2.01	0.60
6:F:103:MET:CE	7:G:66:GLY:HA3	2.32	0.60
13:M:336:LEU:HA	13:M:339:LEU:HD13	1.83	0.60
1:A:53:LEU:HD23	1:A:54:ASN:N	2.15	0.60
8:H:82:PRO:C	8:H:84:ALA:H	2.05	0.60
13:M:294:THR:N	13:M:297:LYS:HG3	2.16	0.60
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.36	0.60
6:F:103:MET:CE	7:G:66:GLY:CA	2.80	0.60
13:M:324:VAL:HG23	13:M:328:LEU:HD22	1.83	0.60
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.83	0.60
2:B:976:ILE:O	2:B:990:ILE:HB	2.02	0.60
12:L:61:THR:HG21	12:L:63:ARG:HG2	1.84	0.60
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.83	0.59
1:A:22:PHE:CB	2:B:1211:ASN:OD1	2.50	0.59
2:B:363:HIS:O	2:B:364:ILE:HB	2.02	0.59
12:L:47:ARG:HH21	12:L:54:ARG:HH21	1.50	0.59
13:M:197:HIS:H	13:M:198:VAL:HA	1.67	0.59
1:A:419:LYS:HE3	13:M:48:CYS:N	2.17	0.59
1:A:839:ARG:NH2	1:A:1401:SER:O	2.35	0.59
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.84	0.59
13:M:262:LYS:O	13:M:266:ILE:HG12	2.01	0.59
14:N:22:DT:C2'	14:N:23:DA:H5'	2.33	0.59
19:T:48:DT:C2'	19:T:49:DA:C8	2.86	0.59
5:E:4:GLU:HB3	5:E:7:ARG:NE	2.16	0.59
13:M:280:VAL:HG12	13:M:309:ILE:O	2.01	0.59
19:T:47:DA:H2'	19:T:48:DT:C5	2.38	0.59
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.83	0.59
1:A:418:SER:HA	13:M:49:GLY:CA	2.32	0.59
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.84	0.59
1:A:72:GLU:HB3	1:A:76:GLU:HB3	1.83	0.59
2:B:950:ASP:HB3	2:B:967:ARG:HG2	1.84	0.58
13:M:269:ILE:CG2	13:M:272:LYS:HB2	2.30	0.58
13:M:288:LEU:CG	13:M:339:LEU:HD21	2.30	0.58
13:M:293:ILE:HD11	13:M:297:LYS:CB	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ASP:HB2	2:B:987:LYS:HE3	1.84	0.58
1:A:857:ARG:HD3	1:A:861:GLY:O	2.03	0.58
2:B:1221:SER:OG	4:D:12:ARG:HD2	2.02	0.58
1:A:1387:HIS:O	1:A:1391:ARG:HG2	2.02	0.58
2:B:451:LYS:HE3	13:M:138:ASP:OD2	1.99	0.58
2:B:1217:TYR:CE2	4:D:14:ARG:CD	2.87	0.58
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.85	0.58
8:H:47:PHE:HB3	8:H:95:TYR:CD2	2.38	0.58
13:M:248:LEU:HD23	13:M:291:ILE:HD12	1.85	0.58
13:M:293:ILE:HD13	13:M:297:LYS:CG	2.29	0.58
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.85	0.58
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.85	0.58
1:A:1433:MET:HE2	2:B:1145:SER:OG	2.02	0.58
1:A:228:PHE:HZ	4:D:14:ARG:C	2.02	0.57
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.36	0.57
1:A:1390:ASN:O	1:A:1399:ARG:HD3	2.04	0.57
1:A:831:THR:CG2	19:T:15:DA:C6	2.87	0.57
3:C:184:ASN:HD21	3:C:189:THR:H	1.50	0.57
13:M:334:VAL:CA	13:M:338:ASN:HD21	2.17	0.57
1:A:836:TYR:CE1	1:A:1403:GLU:OE2	2.57	0.57
13:M:284:LEU:HD11	13:M:339:LEU:HD22	1.87	0.57
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.86	0.57
13:M:248:LEU:HD23	13:M:291:ILE:HD11	1.86	0.57
1:A:228:PHE:CZ	4:D:14:ARG:O	2.58	0.57
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.70	0.57
13:M:310:LYS:HE3	13:M:342:VAL:CG2	2.32	0.57
2:B:65:GLU:OE1	2:B:247:GLY:HA2	2.04	0.57
13:M:269:ILE:HG23	13:M:272:LYS:CG	2.33	0.57
14:N:61:DC:H2'	14:N:62:DA:C8	2.40	0.57
1:A:588:LEU:HD23	1:A:607:ILE:HD12	1.86	0.56
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.87	0.56
13:M:290:GLN:O	13:M:292:PRO:HD3	2.05	0.56
1:A:5:GLN:HG3	2:B:1175:LEU:CD1	2.35	0.56
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.87	0.56
2:B:1124:ARG:HD3	13:M:61:SER:HB3	1.87	0.56
1:A:93:VAL:HA	1:A:96:ILE:HD12	1.86	0.56
1:A:418:SER:CA	13:M:48:CYS:O	2.53	0.56
1:A:419:LYS:CB	13:M:47:LEU:O	2.48	0.56
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.87	0.56
4:D:40:HIS:HB3	7:G:73:LYS:CE	2.35	0.56
4:D:159:THR:O	4:D:163:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:237:THR:HG23	13:M:238:TYR:N	2.21	0.56
13:M:276:THR:O	13:M:280:VAL:HG13	2.06	0.56
13:M:305:THR:CG2	13:M:308:THR:HG23	2.36	0.56
13:M:334:VAL:HA	13:M:338:ASN:OD1	2.05	0.56
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.87	0.56
13:M:269:ILE:CG2	13:M:272:LYS:HG2	2.35	0.56
1:A:417:TYR:HE2	13:M:37:ARG:CG	2.19	0.56
13:M:263:CYS:SG	13:M:316:LEU:HG	2.45	0.56
13:M:284:LEU:HD12	13:M:339:LEU:CD2	2.36	0.56
4:D:7:THR:HG21	7:G:5:LYS:HZ1	1.70	0.56
4:D:18:VAL:HG22	4:D:19:GLU:HA	1.88	0.56
13:M:242:PHE:CZ	13:M:302:LEU:HA	2.40	0.56
1:A:74:MET:O	2:B:1116:ARG:NH2	2.39	0.56
4:D:167:LEU:HB3	4:D:177:VAL:HG22	1.87	0.56
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.88	0.56
2:B:810:GLU:HA	2:B:815:ARG:HH12	1.69	0.56
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.88	0.56
13:M:324:VAL:HG21	13:M:328:LEU:CD2	2.36	0.56
13:M:329:ILE:HG23	13:M:329:ILE:O	2.05	0.56
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.88	0.55
7:G:34:VAL:O	7:G:37:SER:HB3	2.06	0.55
13:M:242:PHE:CD2	13:M:302:LEU:HG	2.41	0.55
13:M:273:SER:HB2	13:M:274:PRO:HD2	1.86	0.55
1:A:67:CYS:SG	1:A:77:CYS:SG	3.04	0.55
1:A:227:VAL:N	4:D:16:LYS:HE3	2.08	0.55
6:F:118:LEU:O	6:F:122:MET:HG3	2.06	0.55
1:A:257:ARG:HH11	1:A:257:ARG:HB2	1.71	0.55
13:M:254:THR:CG2	13:M:258:TYR:HE2	2.19	0.55
15:O:169:PRO:HG2	15:O:240:MET:SD	2.47	0.55
1:A:10:PRO:HG2	2:B:1192:TYR:HA	1.89	0.55
1:A:34:LYS:H	1:A:57:ARG:HH11	1.55	0.55
17:Q:355:THR:O	17:Q:392:ALA:CB	2.54	0.55
19:T:50:DT:H2"	19:T:51:DA:H5'	1.88	0.55
2:B:54:PHE:HA	2:B:58:THR:HB	1.88	0.55
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.88	0.55
13:M:320:ARG:HE	13:M:336:LEU:CB	2.13	0.55
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.88	0.55
6:F:89:GLU:O	6:F:93:ILE:HD12	2.06	0.55
6:F:109:VAL:HG23	6:F:127:GLU:OE1	2.07	0.55
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.87	0.55
1:A:416:ARG:HH22	13:M:40:GLU:HG2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:ILE:O	2:B:344:LYS:HB2	2.07	0.55
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.89	0.55
2:B:815:ARG:HG3	2:B:815:ARG:HH11	1.72	0.55
13:M:272:LYS:HD2	19:T:52:DC:H3'	1.89	0.55
1:A:18:GLN:HG2	1:A:1418:LEU:HD13	1.89	0.55
1:A:275:SER:OG	13:M:117:ASN:OD1	2.24	0.55
2:B:451:LYS:NZ	13:M:138:ASP:OD2	2.40	0.55
2:B:792:MET:CE	19:T:21:DT:P	2.94	0.55
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.87	0.55
11:K:57:LEU:HB2	11:K:76:GLN:HG2	1.88	0.55
13:M:75:ASP:HB3	13:M:78:ARG:HB3	1.89	0.55
13:M:243:CYS:HB3	13:M:253:THR:HG22	1.89	0.55
13:M:279:VAL:HA	13:M:302:LEU:HD22	1.88	0.55
1:A:344:ARG:CA	2:B:1128:LEU:O	2.55	0.54
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.89	0.54
1:A:418:SER:CB	13:M:48:CYS:O	2.55	0.54
2:B:868:MET:HE3	13:M:182:ARG:CD	2.36	0.54
13:M:295:ALA:HA	13:M:298:VAL:HG12	1.87	0.54
1:A:338:GLY:HA2	2:B:1129:ARG:NH2	2.23	0.54
1:A:418:SER:OG	13:M:48:CYS:O	2.25	0.54
1:A:497:THR:HG23	2:B:1146:PHE:HA	1.89	0.54
1:A:1015:VAL:HG13	1:A:1019:CYS:SG	2.47	0.54
10:J:1:MET:HB2	10:J:56:LEU:HB2	1.89	0.54
1:A:1399:ARG:HB3	1:A:1408:ILE:HD13	1.89	0.54
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.40	0.54
13:M:272:LYS:HE3	19:T:53:DA:OP1	2.07	0.54
13:M:289:PHE:HA	13:M:331:ASN:OD1	2.07	0.54
2:B:486:TYR:HB3	2:B:1096:ARG:NH2	2.22	0.54
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.88	0.54
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.72	0.54
2:B:405:ARG:NH2	2:B:629:ASP:OD2	2.40	0.54
10:J:24:LEU:O	10:J:30:LEU:HB2	2.08	0.54
1:A:33:ALA:HA	1:A:57:ARG:HD3	1.90	0.54
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.88	0.54
2:B:338:GLY:CA	2:B:339:THR:HB	2.38	0.54
13:M:284:LEU:HD12	13:M:339:LEU:HD22	1.88	0.54
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.73	0.54
1:A:608:ILE:HD12	1:A:613:ILE:HD13	1.89	0.54
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.90	0.54
13:M:294:THR:H	13:M:297:LYS:CD	2.20	0.54
13:M:339:LEU:CB	13:M:340:PRO:HD2	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PHE:HD1	4:D:15:LEU:CB	2.13	0.54
1:A:204:THR:HG22	1:A:235:ILE:CG2	2.37	0.54
1:A:344:ARG:CD	2:B:1118:PRO:O	2.47	0.54
1:A:982:THR:HB	1:A:985:ASP:H	1.73	0.54
13:M:304:VAL:HG12	13:M:305:THR:H	1.72	0.54
3:C:73:GLN:O	3:C:129:ILE:HA	2.08	0.53
13:M:236:LEU:HD23	13:M:237:THR:N	2.23	0.53
2:B:295:GLY:HA2	2:B:298:LEU:HB2	1.91	0.53
2:B:510:LYS:HB2	2:B:513:GLN:OE1	2.08	0.53
13:M:268:GLU:HG2	13:M:316:LEU:HA	1.89	0.53
1:A:658:LEU:HD23	1:A:659:HIS:NE2	2.24	0.53
7:G:131:GLN:HG2	7:G:136:VAL:HG22	1.90	0.53
13:M:269:ILE:HG22	13:M:269:ILE:O	2.06	0.53
13:M:279:VAL:HB	13:M:302:LEU:CD2	2.27	0.53
17:Q:394:ASN:CB	17:Q:395:LYS:CA	2.86	0.53
1:A:179:LEU:HD13	1:A:297:GLN:HG3	1.91	0.53
1:A:227:VAL:CG1	4:D:16:LYS:N	2.70	0.53
1:A:412:ARG:CB	13:M:51:VAL:HG11	2.38	0.53
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.90	0.53
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.42	0.53
13:M:249:PRO:HD2	13:M:291:ILE:HD11	1.91	0.53
2:B:1100:ASP:OD2	11:K:1:MET:HB3	2.08	0.53
7:G:111:THR:HG22	7:G:113:HIS:H	1.72	0.53
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.74	0.53
1:A:228:PHE:HD1	4:D:15:LEU:HB2	1.69	0.53
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.90	0.53
2:B:1215:ARG:HH12	4:D:15:LEU:HD11	1.74	0.53
5:E:19:VAL:O	5:E:23:VAL:HG23	2.08	0.53
13:M:298:VAL:HG13	13:M:299:GLY:N	2.24	0.53
1:A:91:PHE:HD2	1:A:179:LEU:O	1.92	0.53
5:E:156:LEU:HD11	5:E:197:LYS:HB2	1.90	0.53
1:A:22:PHE:HB3	2:B:1211:ASN:OD1	2.09	0.53
1:A:320:ARG:HG2	1:A:321:PRO:HD2	1.89	0.53
13:M:58:ASP:O	13:M:62:GLU:HB2	2.08	0.53
1:A:12:ARG:NH1	2:B:1218:THR:OG1	2.42	0.52
1:A:42:ASP:OD1	1:A:46:THR:N	2.41	0.52
1:A:1397:LEU:HB3	1:A:1429:ILE:HD12	1.90	0.52
11:K:5:ASP:HB3	11:K:7:PHE:CE2	2.45	0.52
12:L:50:ASP:HA	13:M:250:MET:HE1	1.90	0.52
13:M:269:ILE:HG12	13:M:315:ILE:CG2	2.31	0.52
1:A:1431:GLY:HA3	2:B:1197:PRO:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:LEU:HD11	2:B:204:ILE:HG13	1.91	0.52
1:A:23:SER:HB2	1:A:233:TRP:CE2	2.44	0.52
1:A:646:PHE:O	1:A:650:GLN:HG2	2.10	0.52
1:A:1390:ASN:O	1:A:1399:ARG:CG	2.57	0.52
2:B:90:ILE:HD11	2:B:134:LYS:HE2	1.91	0.52
13:M:294:THR:H	13:M:297:LYS:HD2	1.74	0.52
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.44	0.52
1:A:412:ARG:CB	13:M:51:VAL:CG1	2.88	0.52
1:A:1108:ALA:HA	14:N:63:DC:OP1	2.09	0.52
2:B:1217:TYR:CD2	4:D:14:ARG:NE	2.78	0.52
7:G:119:LEU:HD12	7:G:132:SER:HB2	1.91	0.52
2:B:249:ARG:HH12	2:B:418:LYS:CD	2.22	0.52
2:B:449:ASN:HD22	13:M:135:MET:HG3	1.72	0.52
3:C:164:ALA:HA	3:C:167:HIS:O	2.09	0.52
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.45	0.52
13:M:317:TYR:HE1	13:M:339:LEU:HB2	1.73	0.52
1:A:33:ALA:HB2	1:A:57:ARG:HB2	1.90	0.52
1:A:494:SER:HB3	1:A:497:THR:OG1	2.10	0.52
2:B:291:ILE:HD12	2:B:291:ILE:H	1.74	0.52
6:F:134:ILE:HG22	6:F:136:ARG:HG3	1.91	0.52
15:O:69:ASN:CB	19:T:48:DT:O4’	2.54	0.52
1:A:412:ARG:HB3	13:M:51:VAL:HG12	1.92	0.52
2:B:1122:ARG:HB2	19:T:19:DT:OP1	2.10	0.52
3:C:52:GLU:HA	12:L:64:LEU:HD22	1.91	0.52
13:M:246:LEU:CD1	13:M:282:ILE:HG21	2.40	0.52
13:M:315:ILE:HG22	13:M:316:LEU:HD12	1.88	0.52
13:M:334:VAL:O	13:M:334:VAL:HG23	2.10	0.52
1:A:253:ASN:O	1:A:255:SER:N	2.38	0.52
13:M:271:GLY:HA3	19:T:52:DC:H5”	1.92	0.52
1:A:1444:MET:HB2	6:F:133:VAL:HG12	1.92	0.51
2:B:438:GLU:HG3	2:B:440:HIS:HB2	1.91	0.51
15:O:69:ASN:HB2	19:T:48:DT:C4’	2.40	0.51
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.08	0.51
1:A:228:PHE:HE1	4:D:15:LEU:CA	2.22	0.51
1:A:340:LEU:HD21	2:B:1199:ALA:HB3	1.91	0.51
1:A:1116:LEU:H	1:A:1308:THR:HB	1.73	0.51
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.92	0.51
2:B:449:ASN:HD21	13:M:135:MET:HG3	1.75	0.51
5:E:15:ALA:O	5:E:19:VAL:HG23	2.10	0.51
13:M:312:GLY:O	13:M:316:LEU:HD13	2.09	0.51
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:19:DT:H2'	19:T:20:DA:C8	2.46	0.51
1:A:472:LEU:O	1:A:475:THR:HB	2.10	0.51
2:B:530:GLY:O	2:B:532:ALA:N	2.44	0.51
13:M:310:LYS:HE3	13:M:342:VAL:O	2.09	0.51
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.93	0.51
2:B:773:MET:CE	2:B:985:GLY:HA2	2.40	0.51
8:H:89:LEU:C	8:H:91:ASP:H	2.14	0.51
1:A:831:THR:HG23	19:T:15:DA:C4	2.45	0.51
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.40	0.51
13:M:266:ILE:HD12	13:M:268:GLU:HB2	1.88	0.51
13:M:286:ILE:HG23	13:M:287:LEU:N	2.23	0.51
1:A:345:VAL:N	2:B:1128:LEU:O	2.39	0.51
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.11	0.51
13:M:266:ILE:HG13	13:M:268:GLU:H	1.75	0.51
2:B:70:ILE:HG22	2:B:89:GLU:HG2	1.93	0.51
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.93	0.51
2:B:868:MET:HE3	13:M:182:ARG:NE	2.25	0.51
2:B:1221:SER:CB	4:D:12:ARG:NE	2.69	0.51
5:E:64:PRO:HB2	5:E:69:ILE:HD11	1.93	0.51
6:F:73:ALA:HB2	6:F:143:PHE:CZ	2.45	0.51
1:A:343:LYS:HB2	2:B:1117:GLN:OE1	2.11	0.51
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.94	0.51
13:M:263:CYS:HA	13:M:266:ILE:HG12	1.93	0.51
14:N:22:DT:H2"	14:N:23:DA:H5'	1.93	0.51
1:A:55:ASP:HA	1:A:58:LEU:H	1.76	0.50
2:B:373:ARG:HG2	2:B:566:LEU:HD23	1.92	0.50
13:M:249:PRO:HD3	13:M:291:ILE:CD1	2.39	0.50
1:A:89:PRO:HB2	1:A:204:THR:HB	1.93	0.50
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.93	0.50
13:M:334:VAL:HA	13:M:338:ASN:CG	2.30	0.50
13:M:342:VAL:CG1	13:M:343:GLU:N	2.73	0.50
13:M:196:ILE:HG13	13:M:197:HIS:HB3	1.92	0.50
13:M:237:THR:CG2	13:M:238:TYR:CD2	2.95	0.50
2:B:471:LYS:HG2	13:M:95:ARG:NH2	2.26	0.50
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.93	0.50
14:N:23:DA:N6	19:T:51:DA:N6	2.60	0.50
1:A:714:PHE:O	1:A:718:VAL:HG23	2.12	0.50
1:A:870:GLU:HB2	5:E:204:THR:CG2	2.40	0.50
2:B:60:GLN:OE1	2:B:95:ILE:HG22	2.12	0.50
2:B:1221:SER:HB3	4:D:12:ARG:HE	1.69	0.50
13:M:307:GLY:O	13:M:310:LYS:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:940:ARG:HB3	1:A:941:LYS:HE2	1.92	0.50
2:B:338:GLY:HA2	2:B:339:THR:HB	1.94	0.50
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.94	0.50
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.77	0.50
2:B:1072:MET:HB3	2:B:1081:LEU:HD12	1.94	0.50
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.92	0.50
1:A:919:ILE:HG12	1:A:983:ILE:HD13	1.94	0.50
2:B:211:VAL:HG13	2:B:495:LEU:HD23	1.93	0.50
2:B:1201:LYS:HD3	2:B:1205:GLN:OE1	2.11	0.50
13:M:254:THR:CG2	13:M:258:TYR:CE2	2.94	0.50
13:M:320:ARG:HG3	13:M:321:ASP:N	2.26	0.50
1:A:245:PRO:O	2:B:1114:LEU:HD12	2.12	0.50
1:A:1095:THR:HG23	1:A:1113:THR:HG23	1.92	0.50
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.93	0.50
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.52	0.50
14:N:26:DT:H4'	15:O:158:GLN:O	2.12	0.50
2:B:806:THR:HB	2:B:809:MET:HG3	1.94	0.50
10:J:48:ARG:HE	10:J:49:MET:CE	2.20	0.50
1:A:260:ASP:OD1	1:A:328:ARG:NH2	2.42	0.49
2:B:792:MET:CE	19:T:21:DT:OP1	2.57	0.49
13:M:157:CYS:HB3	13:M:210:MET:HE2	1.93	0.49
1:A:67:CYS:O	1:A:70:CYS:HB3	2.11	0.49
13:M:306:GLU:O	13:M:309:ILE:HG12	2.12	0.49
1:A:40:THR:HG21	1:A:259:GLU:OE2	2.12	0.49
1:A:216:VAL:O	1:A:220:THR:HB	2.12	0.49
15:O:68:GLN:O	19:T:48:DT:H4'	2.12	0.49
1:A:418:SER:HA	13:M:49:GLY:N	2.27	0.49
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.12	0.49
1:A:7:SER:HG	2:B:1161:HIS:CE1	2.24	0.49
1:A:11:LEU:HA	2:B:1193:GLN:HG2	1.95	0.49
1:A:320:ARG:HH22	13:M:81:GLU:HG3	1.74	0.49
1:A:1095:THR:HG21	1:A:1112:LYS:HB2	1.93	0.49
7:G:1:MET:CG	7:G:2:PHE:N	2.76	0.49
13:M:283:TYR:CE2	13:M:287:LEU:CD1	2.94	0.49
1:A:1193:LEU:HB2	1:A:1260:LEU:CD2	2.42	0.49
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.94	0.49
2:B:948:ILE:HD13	12:L:67:PHE:HE2	1.77	0.49
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	1.94	0.49
15:O:71:VAL:HG21	19:T:47:DA:H2	1.77	0.49
1:A:22:PHE:CB	2:B:1211:ASN:CG	2.78	0.49
1:A:417:TYR:HE2	13:M:37:ARG:CD	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:ILE:HG21	2:B:417:PHE:HD2	1.78	0.49
13:M:333:VAL:HG12	13:M:333:VAL:O	2.11	0.49
1:A:1172:LEU:C	1:A:1174:PHE:H	2.16	0.49
2:B:35:SER:HA	2:B:811:TYR:HE1	1.77	0.49
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.95	0.49
8:H:80:ARG:HG2	11:K:57:LEU:HD22	1.95	0.49
19:T:51:DA:H2"	19:T:52:DC:C5	2.47	0.49
1:A:261:ASP:HB3	1:A:322:VAL:HG13	1.95	0.49
1:A:832:ALA:HB2	19:T:15:DA:H8	1.74	0.49
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.94	0.49
7:G:142:ARG:HB3	7:G:171:ILE:HD12	1.95	0.49
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.95	0.49
13:M:276:THR:HA	13:M:279:VAL:HG12	1.94	0.49
1:A:132:LYS:HZ2	1:A:1415:SER:HB3	1.77	0.49
13:M:237:THR:HG23	13:M:238:TYR:CD2	2.48	0.49
14:N:26:DT:H1'	15:O:159:ASN:HB2	1.93	0.49
1:A:497:THR:CG2	2:B:1146:PHE:HD1	2.23	0.48
13:M:262:LYS:O	13:M:266:ILE:HG23	2.13	0.48
13:M:286:ILE:HG13	13:M:291:ILE:O	2.14	0.48
13:M:294:THR:OG1	13:M:297:LYS:HG2	2.13	0.48
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.95	0.48
1:A:1004:ASN:CG	5:E:167:ARG:HD2	2.33	0.48
2:B:849:GLY:HA2	2:B:852:ARG:CD	2.40	0.48
13:M:271:GLY:O	19:T:52:DC:C4'	2.62	0.48
1:A:12:ARG:O	2:B:1194:ILE:HG22	2.12	0.48
1:A:411:ASP:CG	13:M:50:LEU:HD11	2.33	0.48
1:A:1402:PHE:CE1	1:A:1403:GLU:HG3	2.48	0.48
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.95	0.48
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.94	0.48
14:N:24:DT:H3'	14:N:24:DT:H6	1.78	0.48
1:A:285:PRO:O	1:A:287:HIS:N	2.46	0.48
2:B:486:TYR:HB3	2:B:1096:ARG:NE	2.28	0.48
2:B:574:SER:HB3	2:B:591:ARG:HE	1.77	0.48
13:M:313:TYR:CD2	13:M:343:GLU:N	2.80	0.48
2:B:441:ASP:O	2:B:443:ASN:N	2.47	0.48
8:H:115:TYR:CE1	8:H:124:ARG:HG3	2.49	0.48
1:A:568:PRO:HG2	8:H:46:LEU:HD12	1.95	0.48
2:B:693:ILE:HG21	2:B:701:ILE:HD13	1.95	0.48
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.94	0.48
15:O:170:ILE:HD13	15:O:234:LEU:HD22	1.96	0.48
1:A:227:VAL:HG11	4:D:16:LYS:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:LYS:HA	8:H:19:ARG:HH12	1.79	0.48
12:L:68:GLU:HB2	12:L:70:ARG:HD2	1.96	0.48
13:M:293:ILE:HD11	13:M:297:LYS:C	2.34	0.48
13:M:311:SER:HA	13:M:314:LYS:CD	2.44	0.48
1:A:956:LEU:HD21	1:A:1017:LEU:HG	1.96	0.48
1:A:1116:LEU:HG	1:A:1327:ILE:HD11	1.95	0.48
2:B:345:LYS:HA	2:B:348:ARG:HD2	1.96	0.48
11:K:63:VAL:HG12	11:K:71:PHE:HB3	1.96	0.48
13:M:250:MET:HG3	13:M:251:GLN:N	2.27	0.48
13:M:289:PHE:CG	13:M:290:GLN:N	2.82	0.48
1:A:418:SER:N	13:M:49:GLY:HA3	2.28	0.48
2:B:219:ALA:HB2	2:B:405:ARG:HG2	1.95	0.48
2:B:249:ARG:NH1	2:B:418:LYS:CD	2.76	0.48
2:B:451:LYS:NZ	13:M:147:LYS:NZ	2.61	0.48
13:M:249:PRO:HG2	13:M:252:VAL:HG23	1.94	0.48
13:M:324:VAL:HG21	13:M:328:LEU:HD22	1.93	0.48
19:T:50:DT:H3'	19:T:50:DT:H6	1.79	0.48
1:A:280:GLU:HG2	1:A:289:ILE:HD13	1.95	0.48
1:A:475:THR:HG21	2:B:836:GLU:OE2	2.14	0.48
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.95	0.48
13:M:293:ILE:HD13	13:M:294:THR:N	2.29	0.48
1:A:257:ARG:HB2	1:A:257:ARG:NH1	2.29	0.47
1:A:1433:MET:HE3	2:B:1145:SER:OG	2.14	0.47
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.96	0.47
6:F:103:MET:HE1	7:G:66:GLY:CA	2.42	0.47
14:N:22:DT:H2'	14:N:23:DA:H5'	1.96	0.47
15:O:171:ARG:HG3	15:O:239:LYS:HD3	1.95	0.47
1:A:226:GLU:CG	4:D:16:LYS:HZ1	2.24	0.47
2:B:705:MET:H	2:B:710:LEU:HD12	1.79	0.47
13:M:280:VAL:O	13:M:283:TYR:HB3	2.14	0.47
15:O:171:ARG:HD3	15:O:238:ARG:O	2.14	0.47
17:Q:394:ASN:H	17:Q:395:LYS:HA	1.79	0.47
1:A:929:LEU:HD21	1:A:983:ILE:HG21	1.96	0.47
2:B:640:VAL:HG22	2:B:651:LEU:HG	1.95	0.47
2:B:951:GLN:OE1	12:L:57:LEU:CD2	2.62	0.47
4:D:8:PHE:HZ	4:D:37:GLN:NE2	2.13	0.47
5:E:176:PRO:O	5:E:212:ARG:HA	2.14	0.47
7:G:85:GLU:HB3	7:G:147:ILE:HD12	1.96	0.47
12:L:27:LEU:HD13	12:L:37:LYS:HG2	1.95	0.47
19:T:47:DA:C8	19:T:48:DT:C4	3.02	0.47
2:B:840:ILE:HG21	2:B:994:TYR:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:237:THR:CG2	13:M:238:TYR:CE2	2.98	0.47
13:M:306:GLU:CA	13:M:309:ILE:HG12	2.43	0.47
16:P:7:A:H2'	16:P:8:U:O4'	2.14	0.47
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.50	0.47
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.95	0.47
2:B:122:LEU:HD22	2:B:958:GLN:HG2	1.96	0.47
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.96	0.47
17:Q:356:TRP:CB	17:Q:391:THR:C	2.74	0.47
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.96	0.47
13:M:238:TYR:HB3	13:M:242:PHE:HE2	1.75	0.47
13:M:246:LEU:HD22	13:M:293:ILE:HG13	1.96	0.47
13:M:285:ASN:O	13:M:288:LEU:HB2	2.14	0.47
1:A:91:PHE:CB	1:A:96:ILE:CG1	2.91	0.47
1:A:419:LYS:HE3	13:M:48:CYS:CA	2.44	0.47
1:A:832:ALA:HA	19:T:15:DA:C1'	2.45	0.47
1:A:832:ALA:CB	19:T:15:DA:C8	2.97	0.47
1:A:883:LEU:HD23	1:A:1021:LEU:HB2	1.97	0.47
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.95	0.47
2:B:542:MET:HG3	2:B:747:MET:HB3	1.95	0.47
2:B:792:MET:HE2	19:T:20:DA:O3'	2.14	0.47
8:H:38:LEU:HD11	8:H:123:MET:HE2	1.96	0.47
13:M:193:GLN:HG2	13:M:198:VAL:HG12	1.96	0.47
2:B:291:ILE:HD12	2:B:291:ILE:N	2.30	0.47
13:M:72:ASN:ND2	13:M:74:ASP:OD2	2.47	0.47
19:T:49:DA:C2'	19:T:50:DT:C5'	2.86	0.47
1:A:67:CYS:C	1:A:68:GLN:HG3	2.34	0.47
1:A:91:PHE:CD2	1:A:179:LEU:O	2.68	0.47
1:A:132:LYS:NZ	1:A:1415:SER:HB3	2.30	0.47
2:B:473:MET:SD	13:M:72:ASN:OD1	2.72	0.47
2:B:901:PRO:HG2	12:L:60:ARG:HA	1.97	0.47
8:H:40:LEU:HD13	8:H:123:MET:HG3	1.96	0.47
13:M:293:ILE:CD1	13:M:297:LYS:CG	2.93	0.47
1:A:275:SER:O	1:A:279:LEU:HD12	2.14	0.47
2:B:1113:VAL:HG22	13:M:57:VAL:HG11	1.96	0.47
8:H:23:VAL:HG11	8:H:121:LEU:HD22	1.95	0.47
1:A:89:PRO:HB2	1:A:204:THR:CB	2.44	0.46
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.97	0.46
13:M:276:THR:O	13:M:279:VAL:HG12	2.15	0.46
1:A:71:GLN:O	1:A:73:GLY:N	2.47	0.46
1:A:579:SER:HA	1:A:582:ILE:HG13	1.97	0.46
1:A:709:THR:HG22	1:A:711:ARG:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:CYS:HA	2:B:67:SER:HB3	1.98	0.46
2:B:108:VAL:HG13	13:M:240:PRO:CB	2.42	0.46
13:M:254:THR:HG22	13:M:258:TYR:CD2	2.51	0.46
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.97	0.46
9:I:106:CYS:SG	9:I:108:HIS:HB3	2.55	0.46
13:M:234:GLN:HB2	13:M:236:LEU:HD21	1.91	0.46
1:A:11:LEU:HD13	2:B:1195:HIS:NE2	2.31	0.46
1:A:227:VAL:CG1	4:D:16:LYS:H	2.27	0.46
1:A:399:HIS:O	1:A:401:GLY:N	2.48	0.46
1:A:448:PRO:O	1:A:449:SER:CB	2.62	0.46
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.45	0.46
2:B:471:LYS:HE3	13:M:95:ARG:HE	1.80	0.46
2:B:1215:ARG:HH22	4:D:15:LEU:CD2	2.18	0.46
3:C:58:LEU:HD21	10:J:57:ILE:HD12	1.97	0.46
4:D:5:THR:HG21	7:G:74:TYR:OH	2.15	0.46
13:M:136:LEU:HD21	13:M:196:ILE:HG22	1.96	0.46
2:B:365:THR:HG21	2:B:370:PHE:CG	2.51	0.46
2:B:662:MET:HA	2:B:665:GLU:HB2	1.97	0.46
17:Q:394:ASN:N	17:Q:395:LYS:HA	2.29	0.46
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.97	0.46
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.96	0.46
2:B:756:ILE:O	2:B:759:PRO:HD3	2.15	0.46
2:B:803:LEU:HG	10:J:52:THR:HG21	1.98	0.46
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.81	0.46
13:M:62:GLU:O	13:M:65:THR:OG1	2.30	0.46
19:T:19:DT:H2'	19:T:20:DA:H8	1.80	0.46
1:A:180:LYS:CE	1:A:294:SER:HB3	2.46	0.46
1:A:497:THR:HG22	2:B:1146:PHE:CD1	2.42	0.46
1:A:1074:GLU:O	1:A:1077:THR:HB	2.16	0.46
13:M:305:THR:HG22	13:M:308:THR:OG1	2.15	0.46
1:A:56:PRO:O	1:A:57:ARG:HG3	2.16	0.46
2:B:451:LYS:NZ	13:M:147:LYS:HZ1	2.14	0.46
13:M:234:GLN:HB2	13:M:236:LEU:HD22	1.91	0.46
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.97	0.46
2:B:193:LYS:NZ	12:L:32:ALA:O	2.48	0.46
13:M:286:ILE:HD11	13:M:293:ILE:HB	1.98	0.46
1:A:34:LYS:N	1:A:57:ARG:HH11	2.13	0.46
1:A:58:LEU:HD22	1:A:80:HIS:O	2.16	0.46
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.15	0.46
1:A:831:THR:HG23	19:T:15:DA:C6	2.49	0.45
9:I:102:VAL:HG22	9:I:109:ILE:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:85:PRO:HA	13:M:89:GLY:O	2.15	0.45
13:M:269:ILE:CG2	13:M:272:LYS:CG	2.94	0.45
13:M:280:VAL:HG11	13:M:312:GLY:HA3	1.99	0.45
1:A:565:ILE:O	1:A:570:PRO:HA	2.16	0.45
3:C:148:ARG:N	3:C:151:GLN:HG3	2.22	0.45
8:H:30:SER:HB3	8:H:36:CYS:HB3	1.98	0.45
14:N:17:DC:H2"	14:N:18:DT:H71	1.98	0.45
1:A:923:LEU:O	1:A:927:VAL:HG23	2.16	0.45
2:B:451:LYS:HZ2	13:M:138:ASP:CG	2.20	0.45
13:M:258:TYR:O	13:M:261:LYS:HG2	2.16	0.45
13:M:279:VAL:HG23	13:M:302:LEU:HD13	1.98	0.45
13:M:279:VAL:HG21	13:M:309:ILE:HG21	1.99	0.45
1:A:228:PHE:HD1	4:D:15:LEU:CD2	2.28	0.45
1:A:1151:GLU:HG2	9:I:45:ARG:HG3	1.98	0.45
2:B:1217:TYR:HB2	4:D:14:ARG:NH2	2.30	0.45
5:E:65:THR:O	5:E:69:ILE:HD12	2.16	0.45
9:I:50:THR:HG22	9:I:52:ILE:H	1.81	0.45
9:I:72:ASP:O	9:I:81:ARG:HG2	2.16	0.45
9:I:83:ASN:HA	9:I:104:LEU:HG	1.98	0.45
13:M:298:VAL:CG2	13:M:302:LEU:HD13	2.36	0.45
2:B:468:GLU:HG2	2:B:469:GLN:HB2	1.99	0.45
14:N:24:DT:H2'	14:N:25:DA:C8	2.51	0.45
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.98	0.45
2:B:451:LYS:HZ2	13:M:147:LYS:NZ	2.14	0.45
3:C:18:VAL:HG12	3:C:20:PHE:HD1	1.81	0.45
3:C:100:THR:HG22	3:C:119:VAL:HG22	1.97	0.45
6:F:103:MET:CE	7:G:66:GLY:N	2.78	0.45
13:M:282:ILE:O	13:M:286:ILE:HG22	2.16	0.45
13:M:331:ASN:O	13:M:334:VAL:HG22	2.16	0.45
14:N:23:DA:N6	19:T:51:DA:H61	2.15	0.45
1:A:70:CYS:O	1:A:72:GLU:HG2	2.17	0.45
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.52	0.45
1:A:534:LEU:O	1:A:574:GLY:HA3	2.17	0.45
13:M:248:LEU:HD13	13:M:252:VAL:CG1	2.37	0.45
13:M:293:ILE:CD1	13:M:297:LYS:CB	2.94	0.45
15:O:94:TYR:CZ	15:O:96:PRO:HG3	2.52	0.45
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.99	0.45
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.98	0.45
5:E:90:VAL:HG23	5:E:123:LEU:HD11	1.98	0.45
7:G:98:GLY:HA3	7:G:110:VAL:O	2.17	0.45
13:M:193:GLN:HG2	13:M:198:VAL:CG1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:55:DA:H2"	19:T:56:DG:C8	2.52	0.45
1:A:514:PRO:HG2	1:A:1067:LEU:HD11	1.98	0.45
1:A:548:ASN:HD21	11:K:47:ARG:HH21	1.65	0.45
1:A:743:VAL:O	1:A:747:VAL:HG23	2.17	0.45
1:A:1356:ILE:HG21	1:A:1363:VAL:HG23	1.99	0.45
4:D:31:GLN:O	4:D:34:GLN:HB2	2.17	0.45
11:K:65:HIS:HE1	11:K:67:PHE:CG	2.35	0.45
13:M:272:LYS:HB2	13:M:277:ILE:HD11	1.97	0.45
13:M:283:TYR:CE1	13:M:287:LEU:HD11	2.47	0.45
13:M:293:ILE:CD1	13:M:298:VAL:N	2.79	0.45
19:T:44:DA:H2'	19:T:45:DT:H71	1.99	0.45
1:A:11:LEU:CD1	2:B:1195:HIS:NE2	2.80	0.45
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.81	0.45
3:C:55:THR:HB	3:C:151:GLN:HA	1.98	0.45
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.78	0.45
14:N:25:DA:C8	14:N:25:DA:O5'	2.70	0.45
17:Q:108:LYS:CB	18:R:86:ASN:CB	2.95	0.45
1:A:130:ASP:HB3	1:A:133:LYS:HB2	2.00	0.44
1:A:449:SER:HA	1:A:454:SER:HB3	1.98	0.44
6:F:133:VAL:HG21	7:G:58:ARG:NH2	2.32	0.44
13:M:269:ILE:CD1	13:M:277:ILE:CD1	2.94	0.44
15:O:239:LYS:O	15:O:240:MET:HG3	2.16	0.44
1:A:95:PHE:O	1:A:97:ALA:N	2.49	0.44
1:A:228:PHE:HD1	4:D:15:LEU:HD22	1.83	0.44
1:A:832:ALA:CB	19:T:15:DA:H8	2.30	0.44
2:B:102:VAL:HG23	2:B:112:LEU:HD22	1.99	0.44
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.99	0.44
3:C:11:ARG:HE	3:C:21:ILE:HD11	1.82	0.44
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.99	0.44
14:N:27:DA:H2'	14:N:28:DA:C8	2.52	0.44
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.99	0.44
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.46	0.44
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.97	0.44
13:M:269:ILE:HD13	13:M:277:ILE:CD1	2.48	0.44
1:A:151:ASP:HA	1:A:163:SER:HA	1.99	0.44
1:A:446:ARG:HB2	1:A:487:MET:SD	2.57	0.44
19:T:47:DA:C5	19:T:48:DT:O4	2.70	0.44
1:A:22:PHE:HD2	2:B:1211:ASN:HA	1.83	0.44
2:B:617:ARG:HG3	2:B:624:LEU:HD12	2.00	0.44
4:D:7:THR:HG23	7:G:7:LEU:HD23	1.99	0.44
13:M:289:PHE:CE2	13:M:290:GLN:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LEU:HA	1:A:270:LEU:HD12	1.69	0.44
1:A:869:GLY:O	5:E:204:THR:HG21	2.18	0.44
2:B:451:LYS:HZ2	13:M:147:LYS:HZ3	1.65	0.44
2:B:831:SER:HG	2:B:994:TYR:HE2	1.63	0.44
13:M:289:PHE:CD2	13:M:290:GLN:HG3	2.52	0.44
1:A:33:ALA:HB1	1:A:56:PRO:HB2	2.00	0.44
1:A:42:ASP:O	1:A:44:THR:N	2.50	0.44
1:A:332:LYS:HA	1:A:337:ARG:HB2	2.00	0.44
1:A:875:ALA:HB2	1:A:1366:ARG:CD	2.48	0.44
1:A:1393:ASN:ND2	1:A:1393:ASN:H	2.15	0.44
2:B:86:ARG:HG2	2:B:138:GLU:HG3	1.98	0.44
13:M:269:ILE:CG2	13:M:272:LYS:CB	2.95	0.44
1:A:91:PHE:HB3	1:A:96:ILE:CD1	2.48	0.44
1:A:187:LYS:HE3	1:A:198:GLU:HB2	1.99	0.44
1:A:709:THR:HB	1:A:712:GLU:H	1.83	0.44
2:B:1158:PHE:HE2	2:B:1160:VAL:HG13	1.83	0.44
13:M:259:THR:HG23	13:M:323:LEU:CB	2.30	0.44
1:A:22:PHE:HB2	2:B:1211:ASN:O	2.18	0.43
1:A:589:GLN:HG2	1:A:606:LEU:HD13	1.99	0.43
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.53	0.43
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.82	0.43
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.99	0.43
8:H:4:THR:HA	8:H:60:ALA:HB2	2.00	0.43
15:O:69:ASN:HB2	19:T:48:DT:H5'	2.00	0.43
19:T:52:DC:H1'	19:T:53:DA:H5'	2.00	0.43
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.53	0.43
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	2.00	0.43
2:B:89:GLU:HB2	2:B:135:ARG:HB2	1.99	0.43
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.99	0.43
7:G:143:ILE:HG22	7:G:145:VAL:HG22	1.99	0.43
13:M:316:LEU:HD12	13:M:316:LEU:N	2.33	0.43
2:B:394:ASP:OD2	9:I:91:ARG:HD2	2.17	0.43
13:M:280:VAL:HG23	13:M:281:SER:N	2.33	0.43
13:M:289:PHE:CD2	13:M:290:GLN:N	2.82	0.43
1:A:78:PRO:C	2:B:1201:LYS:HZ3	2.13	0.43
1:A:227:VAL:HG11	4:D:14:ARG:O	2.18	0.43
1:A:337:ARG:NH1	2:B:1132:GLU:OE1	2.49	0.43
1:A:449:SER:HA	1:A:454:SER:CB	2.49	0.43
1:A:774:ARG:HH21	1:A:797:LYS:HB2	1.83	0.43
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.18	0.43
1:A:1436:ILE:O	2:B:1144:ALA:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:521:LEU:HD22	2:B:633:VAL:HG12	2.01	0.43
2:B:766:ARG:NH2	2:B:1020:ARG:HD3	2.33	0.43
2:B:901:PRO:O	12:L:60:ARG:HA	2.18	0.43
2:B:951:GLN:OE1	12:L:57:LEU:HD22	2.18	0.43
7:G:1:MET:HE3	7:G:80:LYS:O	2.17	0.43
1:A:1444:MET:CE	6:F:135:ARG:HB2	2.39	0.43
2:B:69:LEU:HD22	2:B:425:THR:HG23	2.00	0.43
2:B:104:GLU:CD	12:L:54:ARG:NE	2.71	0.43
2:B:935:ARG:H	2:B:935:ARG:HD2	1.83	0.43
13:M:339:LEU:HD12	13:M:339:LEU:H	1.84	0.43
14:N:29:DT:OP1	15:O:120:LYS:HG3	2.18	0.43
1:A:227:VAL:HG12	4:D:16:LYS:N	2.34	0.43
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.65	0.43
1:A:1154:TYR:CE1	9:I:18:GLU:HG3	2.53	0.43
2:B:125:SER:HA	2:B:171:PRO:HA	2.00	0.43
2:B:383:ASN:O	2:B:387:LEU:HB2	2.19	0.43
2:B:955:THR:HG22	2:B:956:THR:N	2.34	0.43
3:C:148:ARG:HG3	3:C:151:GLN:HG3	2.01	0.43
7:G:93:SER:OG	7:G:100:GLU:HB2	2.19	0.43
13:M:189:PHE:O	13:M:193:GLN:HG3	2.18	0.43
13:M:236:LEU:HD23	13:M:237:THR:H	1.82	0.43
13:M:263:CYS:CA	13:M:266:ILE:HG12	2.49	0.43
13:M:272:LYS:NZ	19:T:53:DA:P	2.91	0.43
19:T:48:DT:H2'	19:T:49:DA:C5	2.54	0.43
1:A:343:LYS:NZ	2:B:1156:ASP:HB2	2.33	0.43
1:A:832:ALA:HA	19:T:15:DA:C8	2.54	0.43
3:C:133:ILE:HG21	3:C:236:GLY:HA3	2.00	0.43
13:M:64:ARG:NH2	19:T:22:DT:O4	2.49	0.43
1:A:306:ASN:O	1:A:313:GLN:HG2	2.19	0.43
1:A:1025:ARG:O	1:A:1035:TYR:HE2	2.02	0.43
2:B:226:PHE:HA	2:B:395:GLN:CG	2.49	0.43
2:B:980:PHE:CD1	2:B:1094:ARG:HA	2.54	0.43
8:H:105:GLU:HB3	8:H:113:ALA:HB3	2.00	0.43
13:M:27:CYS:SG	13:M:48:CYS:HB3	2.57	0.43
13:M:275:ILE:CG2	13:M:276:THR:N	2.82	0.43
13:M:304:VAL:HG12	13:M:308:THR:OG1	2.19	0.43
3:C:184:ASN:ND2	3:C:189:THR:O	2.52	0.43
10:J:36:LEU:HD11	10:J:51:LEU:HB2	2.00	0.43
1:A:1148:ILE:HA	9:I:49:ILE:HD12	2.00	0.43
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.84	0.43
8:H:15:VAL:HG22	8:H:26:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ASN:HB2	11:K:65:HIS:HD2	1.84	0.42
2:B:171:PRO:HG2	2:B:461:LEU:HD12	2.01	0.42
2:B:900:ALA:CB	12:L:61:THR:HG23	2.42	0.42
3:C:165:LYS:O	11:K:6:ARG:NH1	2.46	0.42
5:E:10:SER:O	5:E:14:ARG:HG3	2.19	0.42
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.84	0.42
13:M:24:CYS:HA	13:M:25:PRO:HD3	1.87	0.42
13:M:286:ILE:CG2	13:M:287:LEU:N	2.82	0.42
13:M:335:SER:H	13:M:338:ASN:CG	2.23	0.42
1:A:481:ASP:OD1	1:A:485:ASP:OD1	2.37	0.42
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.20	0.42
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	2.01	0.42
3:C:99:LEU:HB3	3:C:118:LEU:HD22	2.02	0.42
1:A:78:PRO:C	2:B:1201:LYS:NZ	2.69	0.42
1:A:91:PHE:CB	1:A:96:ILE:CD1	2.96	0.42
1:A:469:ARG:NH2	2:B:991:GLY:O	2.52	0.42
2:B:1143:ALA:HB1	2:B:1146:PHE:HB3	2.01	0.42
5:E:181:ALA:HA	5:E:186:LEU:HD21	2.01	0.42
6:F:82:THR:HG22	6:F:83:PRO:HD2	2.01	0.42
13:M:237:THR:CG2	13:M:238:TYR:N	2.83	0.42
1:A:1438:THR:HB	2:B:1142:GLY:O	2.19	0.42
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.84	0.42
13:M:236:LEU:HD23	13:M:236:LEU:N	2.34	0.42
1:A:270:LEU:O	1:A:274:ILE:HG13	2.19	0.42
2:B:915:THR:O	2:B:917:PRO:HD3	2.19	0.42
2:B:1166:CYS:O	2:B:1168:LEU:N	2.42	0.42
13:M:276:THR:HG23	13:M:277:ILE:N	2.35	0.42
13:M:304:VAL:CG1	13:M:305:THR:N	2.83	0.42
2:B:854:LEU:HD23	2:B:854:LEU:HA	1.86	0.42
6:F:133:VAL:HG11	7:G:58:ARG:CZ	2.50	0.42
13:M:123:ASP:HA	13:M:126:VAL:HG23	2.02	0.42
17:Q:355:THR:C	17:Q:392:ALA:HB1	2.39	0.42
1:A:332:LYS:HA	1:A:337:ARG:CB	2.49	0.42
1:A:332:LYS:O	1:A:333:GLU:HB2	2.19	0.42
1:A:873:MET:HB3	1:A:878:ILE:HD11	2.01	0.42
3:C:34:ARG:HA	3:C:37:MET:HE2	2.01	0.42
8:H:125:LEU:HG	8:H:130:ARG:HH22	1.85	0.42
13:M:263:CYS:SG	13:M:316:LEU:CG	3.07	0.42
13:M:295:ALA:CA	13:M:309:ILE:HD11	2.50	0.42
13:M:298:VAL:CG1	13:M:299:GLY:N	2.82	0.42
13:M:339:LEU:HB3	13:M:340:PRO:CD	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:HG	1:A:328:ARG:NH2	2.35	0.42
1:A:562:THR:O	1:A:576:GLN:NE2	2.53	0.42
2:B:273:LEU:HD12	2:B:280:ILE:HD12	2.01	0.42
2:B:904:ARG:HG3	2:B:948:ILE:HG13	2.02	0.42
13:M:272:LYS:HZ1	19:T:53:DA:P	2.43	0.42
14:N:31:DG:H2"	14:N:32:DT:C6	2.54	0.42
19:T:49:DA:H2'	19:T:50:DT:C5'	2.48	0.42
1:A:541:ILE:HG21	1:A:549:MET:CE	2.49	0.42
2:B:169:ARG:HB2	2:B:454:THR:HG23	2.01	0.42
3:C:251:LEU:O	3:C:255:VAL:HG23	2.19	0.42
13:M:248:LEU:CD2	13:M:291:ILE:HG13	2.50	0.42
13:M:324:VAL:CG2	13:M:325:ASP:N	2.82	0.42
15:O:227:PHE:HA	15:O:230:ILE:HG22	2.01	0.42
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.02	0.42
1:A:340:LEU:CD2	2:B:1199:ALA:HB3	2.50	0.42
1:A:729:ALA:HA	1:A:732:LEU:HD12	2.01	0.42
2:B:311:LEU:HB3	9:I:4:PHE:HE2	1.85	0.42
2:B:856:PHE:CE2	2:B:969:ARG:HG3	2.55	0.42
13:M:268:GLU:HG3	13:M:315:ILE:HG12	2.00	0.42
13:M:269:ILE:CG1	13:M:315:ILE:CG2	2.95	0.42
1:A:11:LEU:HA	2:B:1193:GLN:O	2.19	0.41
1:A:626:ASN:O	1:A:631:HIS:ND1	2.53	0.41
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.01	0.41
14:N:25:DA:O5'	14:N:25:DA:H8	2.03	0.41
1:A:11:LEU:HD21	2:B:1195:HIS:CD2	2.55	0.41
1:A:399:HIS:HB3	1:A:400:PRO:HD3	2.02	0.41
2:B:65:GLU:HG3	2:B:66:ASP:H	1.85	0.41
2:B:216:GLU:OE2	2:B:404:LYS:HD2	2.20	0.41
2:B:936:ASP:OD1	2:B:938:SER:OG	2.25	0.41
12:L:27:LEU:HD22	12:L:37:LYS:HE3	2.02	0.41
1:A:11:LEU:HD21	2:B:1195:HIS:HD2	1.84	0.41
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.85	0.41
2:B:279:ASP:OD1	2:B:279:ASP:N	2.53	0.41
2:B:789:MET:HG3	2:B:953:LEU:HD21	2.02	0.41
2:B:986:GLN:OE1	2:B:1016:ALA:HB1	2.20	0.41
2:B:1198:TYR:HE2	2:B:1201:LYS:HE3	1.83	0.41
12:L:49:LYS:O	12:L:50:ASP:HB2	2.19	0.41
1:A:413:ILE:HD13	1:A:424:ILE:HD11	2.01	0.41
2:B:871:THR:HG22	2:B:872:GLU:O	2.21	0.41
2:B:955:THR:HG22	2:B:956:THR:H	1.85	0.41
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:38:LEU:HD13	8:H:125:LEU:HD13	2.02	0.41
13:M:142:LEU:HD12	13:M:142:LEU:HA	1.89	0.41
2:B:841:MET:HG2	2:B:1010:LEU:HD12	2.01	0.41
12:L:38:LEU:HD21	12:L:48:CYS:HA	2.02	0.41
13:M:199:LYS:O	13:M:201:LYS:N	2.54	0.41
13:M:269:ILE:HD12	13:M:277:ILE:HG23	2.02	0.41
1:A:58:LEU:HB3	1:A:59:GLY:H	1.25	0.41
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.84	0.41
2:B:211:VAL:CG1	2:B:495:LEU:HD23	2.51	0.41
2:B:315:LYS:N	2:B:316:PRO:HD2	2.36	0.41
2:B:848:ARG:HD2	10:J:8:PHE:O	2.20	0.41
2:B:969:ARG:HD2	3:C:61:GLU:OE2	2.21	0.41
2:B:1111:MET:O	13:M:57:VAL:HG12	2.21	0.41
2:B:1217:TYR:CG	4:D:14:ARG:CZ	3.03	0.41
13:M:269:ILE:CG1	13:M:316:LEU:HD11	2.50	0.41
13:M:283:TYR:HD2	13:M:313:TYR:CD1	2.38	0.41
1:A:66:LYS:CE	1:A:68:GLN:H	2.31	0.41
1:A:1094:VAL:HG22	1:A:1113:THR:HB	2.03	0.41
1:A:1426:GLU:H	1:A:1426:GLU:HG2	1.55	0.41
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.86	0.41
10:J:22:LEU:O	10:J:26:GLN:HG2	2.20	0.41
10:J:28:ASP:C	10:J:30:LEU:H	2.24	0.41
11:K:39:ASP:OD1	11:K:41:THR:HB	2.21	0.41
17:Q:106:ILE:HA	17:Q:381:MET:O	2.20	0.41
1:A:343:LYS:HA	2:B:1129:ARG:NH1	2.36	0.41
2:B:509:ALA:O	2:B:511:PRO:HD3	2.20	0.41
2:B:542:MET:HE3	2:B:636:PRO:HG2	2.02	0.41
3:C:99:LEU:HD12	3:C:118:LEU:HB3	2.02	0.41
3:C:255:VAL:HG21	11:K:94:ILE:HG21	2.03	0.41
5:E:178:ILE:HG12	5:E:185:ALA:HB2	2.03	0.41
13:M:254:THR:HG22	13:M:258:TYR:CE2	2.55	0.41
13:M:276:THR:CG2	13:M:277:ILE:N	2.82	0.41
13:M:279:VAL:HA	13:M:302:LEU:CD2	2.50	0.41
13:M:293:ILE:CD1	13:M:297:LYS:HB2	2.43	0.41
1:A:133:LYS:HE3	1:A:1391:ARG:HH12	1.85	0.41
1:A:157:ASP:HA	1:A:158:PRO:HD3	2.00	0.41
1:A:417:TYR:CE2	13:M:37:ARG:CG	3.01	0.41
1:A:497:THR:CG2	2:B:1146:PHE:CD1	3.02	0.41
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.83	0.41
1:A:1444:MET:HE1	6:F:135:ARG:NE	2.36	0.41
2:B:190:TYR:CE2	2:B:196:PRO:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:622:LYS:HE3	9:I:59:VAL:HG22	2.02	0.41
2:B:951:GLN:CD	12:L:57:LEU:HD22	2.41	0.41
3:C:125:MET:HB2	3:C:127:ARG:NE	2.36	0.41
5:E:156:LEU:HD23	5:E:160:GLU:HB3	2.03	0.41
11:K:12:LEU:HA	11:K:37:LYS:HG3	2.03	0.41
13:M:282:ILE:HD12	13:M:302:LEU:HD21	2.03	0.41
14:N:21:DG:C2'	14:N:22:DT:H5'	2.51	0.41
19:T:51:DA:H2"	19:T:52:DC:C6	2.55	0.41
1:A:255:SER:HB3	13:M:86:LEU:HD12	2.03	0.41
1:A:354:SER:O	1:A:469:ARG:HA	2.21	0.41
2:B:199:MET:SD	2:B:199:MET:N	2.90	0.41
2:B:681:TRP:HA	2:B:684:LEU:HD12	2.03	0.41
7:G:14:HIS:CD2	7:G:15:PRO:HD2	2.56	0.41
13:M:320:ARG:CD	13:M:336:LEU:HB3	2.51	0.41
15:O:141:ARG:HD2	15:O:141:ARG:HA	1.88	0.41
1:A:1356:ILE:HG23	1:A:1361:SER:HB2	2.03	0.40
2:B:642:ASP:HA	2:B:649:LYS:HA	2.02	0.40
2:B:1082:MET:HA	3:C:189:THR:HA	2.03	0.40
13:M:242:PHE:CE1	13:M:301:THR:O	2.74	0.40
13:M:279:VAL:CA	13:M:302:LEU:CD2	2.93	0.40
1:A:982:THR:H	1:A:985:ASP:HB2	1.86	0.40
2:B:1119:VAL:HG23	2:B:1126:GLY:HA2	2.03	0.40
1:A:34:LYS:HG2	1:A:36:ARG:NH1	2.36	0.40
1:A:252:PHE:HB3	1:A:253:ASN:H	1.74	0.40
1:A:567:LYS:HA	1:A:568:PRO:C	2.41	0.40
1:A:1404:GLU:HB3	1:A:1408:ILE:HG13	2.02	0.40
2:B:39:ARG:HE	2:B:665:GLU:HG2	1.86	0.40
2:B:344:LYS:HB3	2:B:347:LYS:HB2	2.04	0.40
2:B:610:ASN:HB3	2:B:613:VAL:HG23	2.03	0.40
9:I:8:ARG:O	9:I:9:ASP:CB	2.69	0.40
14:N:26:DT:C1'	15:O:159:ASN:HB2	2.51	0.40
1:A:228:PHE:CD1	4:D:15:LEU:CD2	3.05	0.40
1:A:586:ILE:HD11	1:A:637:LYS:HG2	2.03	0.40
2:B:577:ALA:HB1	2:B:589:VAL:HB	2.03	0.40
2:B:1221:SER:CB	4:D:12:ARG:HE	2.32	0.40
3:C:69:LEU:HD23	10:J:6:ARG:HB2	2.04	0.40
4:D:154:PHE:HB2	4:D:160:VAL:HG22	2.04	0.40
13:M:177:LEU:HD13	13:M:189:PHE:HD1	1.86	0.40
15:O:71:VAL:HG21	19:T:47:DA:C2	2.56	0.40
2:B:341:LEU:HD11	2:B:343:ILE:HB	2.02	0.40
2:B:758:PHE:CE2	2:B:1027:ILE:HG22	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:3:GLN:HB2	5:E:4:GLU:H	1.74	0.40
13:M:174:ALA:O	13:M:178:ILE:HG12	2.20	0.40
13:M:254:THR:O	13:M:258:TYR:CD2	2.75	0.40
13:M:273:SER:CA	15:O:188:GLU:OE2	2.69	0.40
17:Q:100:GLU:HA	18:R:95:ILE:O	2.21	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	1414/1733 (82%)	1248 (88%)	115 (8%)	51 (4%)	3 25
2	B	1140/1224 (93%)	1019 (89%)	85 (8%)	36 (3%)	4 26
3	C	264/318 (83%)	242 (92%)	20 (8%)	2 (1%)	19 60
4	D	174/221 (79%)	148 (85%)	18 (10%)	8 (5%)	2 21
5	E	212/215 (99%)	195 (92%)	13 (6%)	4 (2%)	8 38
6	F	82/155 (53%)	75 (92%)	7 (8%)	0	100 100
7	G	169/171 (99%)	158 (94%)	8 (5%)	3 (2%)	8 40
8	H	129/146 (88%)	106 (82%)	14 (11%)	9 (7%)	1 14
9	I	117/122 (96%)	98 (84%)	16 (14%)	3 (3%)	5 31
10	J	63/70 (90%)	51 (81%)	9 (14%)	3 (5%)	2 21
11	K	113/120 (94%)	109 (96%)	4 (4%)	0	100 100
12	L	44/70 (63%)	27 (61%)	9 (20%)	8 (18%)	0 3
13	M	294/345 (85%)	267 (91%)	24 (8%)	3 (1%)	15 55
15	O	178/181 (98%)	174 (98%)	4 (2%)	0	100 100
17	Q	118/734 (16%)	106 (90%)	11 (9%)	1 (1%)	19 60
18	R	103/331 (31%)	96 (93%)	3 (3%)	4 (4%)	3 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4614/6156 (75%)	4119 (89%)	360 (8%)	135 (3%)	7 29

All (135) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	MET
1	A	96	ILE
1	A	189	ARG
1	A	195	ASP
1	A	286	HIS
1	A	317	LYS
1	A	399	HIS
1	A	449	SER
1	A	628	GLY
1	A	1377	THR
1	A	1405	THR
2	B	229	ALA
2	B	307	ASP
2	B	344	LYS
2	B	442	PHE
2	B	466	TRP
2	B	473	MET
2	B	531	GLN
2	B	772	ALA
2	B	1046	PRO
2	B	1181	GLU
4	D	18	VAL
4	D	53	SER
4	D	199	ASN
9	I	9	ASP
9	I	95	THR
12	L	50	ASP
12	L	53	HIS
13	M	200	THR
17	Q	391	THR
18	R	128	VAL
1	A	40	THR
1	A	44	THR
1	A	51	GLY
1	A	52	GLY
1	A	57	ARG
1	A	66	LYS

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Mol	Chain	Res	Type
1	A	68	GLN
1	A	167	CYS
1	A	178	GLY
1	A	193	ASP
1	A	224	PHE
1	A	252	PHE
1	A	254	GLU
1	A	330	LYS
1	A	672	ASP
1	A	1175	SER
1	A	1281	ARG
2	B	262	GLU
2	B	282	ILE
2	B	339	THR
2	B	341	LEU
2	B	707	PRO
2	B	731	VAL
2	B	792	MET
2	B	1175	LEU
2	B	1176	ASN
4	D	16	LYS
4	D	52	LEU
4	D	169	SER
5	E	36	GLU
7	G	2	PHE
8	H	17	PRO
8	H	81	PRO
8	H	82	PRO
8	H	83	GLN
8	H	90	ALA
10	J	6	ARG
12	L	45	ALA
12	L	56	LEU
18	R	61	LEU
18	R	62	GLU
1	A	54	ASN
1	A	975	HIS
1	A	1173	HIS
2	B	340	ALA
2	B	343	ILE
2	B	711	GLU
2	B	1156	ASP

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Mol	Chain	Res	Type
2	B	1157	ALA
2	B	1167	GLY
4	D	22	GLU
5	E	45	LYS
5	E	48	ASP
7	G	154	VAL
8	H	18	GLY
12	L	59	ALA
18	R	115	SER
1	A	69	THR
1	A	72	GLU
1	A	465	TYR
1	A	569	LYS
1	A	846	GLU
1	A	958	VAL
1	A	1255	GLU
1	A	1438	THR
2	B	441	ASP
2	B	648	HIS
2	B	1108	ARG
2	B	1155	SER
3	C	88	CYS
9	I	91	ARG
10	J	29	GLU
12	L	26	THR
12	L	55	ILE
12	L	64	LEU
1	A	156	ASP
1	A	567	LYS
1	A	1171	GLN
1	A	1366	ARG
2	B	251	ILE
2	B	462	ALA
2	B	469	GLN
2	B	1223	ASP
4	D	21	GLU
8	H	60	ALA
8	H	128	ASN
10	J	2	ILE
1	A	35	ILE
1	A	155	GLU
1	A	885	THR

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Mol	Chain	Res	Type
3	C	214	ASN
13	M	164	LYS
13	M	271	GLY
1	A	196	GLU
1	A	1388	GLY
1	A	1437	GLY
5	E	90	VAL
7	G	63	PRO
2	B	364	ILE
1	A	192	GLY
2	B	1121	GLY
1	A	448	PRO
2	B	1214	PRO
8	H	59	ILE

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	1240/1520 (82%)	1065 (86%)	175 (14%)	3 16
2	B	985/1061 (93%)	868 (88%)	117 (12%)	5 20
3	C	234/274 (85%)	206 (88%)	28 (12%)	5 20
4	D	160/200 (80%)	129 (81%)	31 (19%)	1 8
5	E	196/197 (100%)	175 (89%)	21 (11%)	6 23
6	F	74/137 (54%)	67 (90%)	7 (10%)	8 27
7	G	152/152 (100%)	135 (89%)	17 (11%)	6 22
8	H	117/128 (91%)	103 (88%)	14 (12%)	5 20
9	I	113/116 (97%)	106 (94%)	7 (6%)	18 43
10	J	60/65 (92%)	49 (82%)	11 (18%)	1 10
11	K	99/102 (97%)	87 (88%)	12 (12%)	5 20
12	L	40/57 (70%)	27 (68%)	13 (32%)	0 2
13	M	231/299 (77%)	208 (90%)	23 (10%)	7 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	O	152/153 (99%)	140 (92%)	12 (8%)	12 35
All	All	3853/4461 (86%)	3365 (87%)	488 (13%)	8 18

All (488) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	15	LYS
1	A	22	PHE
1	A	41	MET
1	A	42	ASP
1	A	53	LEU
1	A	54	ASN
1	A	57	ARG
1	A	64	ASN
1	A	66	LYS
1	A	68	GLN
1	A	74	MET
1	A	80	HIS
1	A	93	VAL
1	A	106	VAL
1	A	131	SER
1	A	134	ARG
1	A	147	VAL
1	A	157	ASP
1	A	173	THR
1	A	174	ILE
1	A	175	ARG
1	A	176	LYS
1	A	199	LEU
1	A	204	THR
1	A	208	LEU
1	A	219	PHE
1	A	220	THR
1	A	222	LEU
1	A	249	SER
1	A	257	ARG
1	A	265	LYS
1	A	277	GLU
1	A	279	LEU
1	A	307	ASP
1	A	311	GLN

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Mol	Chain	Res	Type
1	A	323	LYS
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	353	ILE
1	A	375	THR
1	A	381	THR
1	A	385	ILE
1	A	386	ASP
1	A	393	ARG
1	A	398	GLU
1	A	408	ASP
1	A	411	ASP
1	A	412	ARG
1	A	424	ILE
1	A	425	GLN
1	A	434	ARG
1	A	436	ILE
1	A	438	ASP
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	454	SER
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	489	LEU
1	A	498	ARG
1	A	500	GLU
1	A	505	CYS
1	A	513	SER
1	A	532	ARG
1	A	544	ASP
1	A	566	ILE
1	A	571	LEU
1	A	582	ILE
1	A	593	GLU
1	A	596	THR

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Mol	Chain	Res	Type
1	A	602	ASP
1	A	603	ASN
1	A	618	GLU
1	A	629	LEU
1	A	634	THR
1	A	664	THR
1	A	666	ILE
1	A	672	ASP
1	A	691	LEU
1	A	702	LEU
1	A	738	LYS
1	A	768	GLN
1	A	769	SER
1	A	773	LYS
1	A	782	ARG
1	A	788	SER
1	A	795	GLU
1	A	797	LYS
1	A	801	GLU
1	A	811	GLN
1	A	821	ARG
1	A	826	ASP
1	A	827	THR
1	A	831	THR
1	A	834	THR
1	A	839	ARG
1	A	849	MET
1	A	867	ILE
1	A	886	ILE
1	A	896	ARG
1	A	919	ILE
1	A	920	LEU
1	A	948	VAL
1	A	949	ASP
1	A	964	ILE
1	A	973	ILE
1	A	976	THR
1	A	998	LEU
1	A	1009	ASN
1	A	1015	VAL
1	A	1029	ARG
1	A	1030	ARG

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Mol	Chain	Res	Type
1	A	1047	SER
1	A	1058	VAL
1	A	1062	GLU
1	A	1067	LEU
1	A	1078	GLN
1	A	1116	LEU
1	A	1118	VAL
1	A	1120	LEU
1	A	1121	GLU
1	A	1124	HIS
1	A	1135	ARG
1	A	1142	THR
1	A	1173	HIS
1	A	1176	LEU
1	A	1195	LEU
1	A	1208	THR
1	A	1218	GLN
1	A	1223	ASP
1	A	1237	ILE
1	A	1242	VAL
1	A	1255	GLU
1	A	1257	ASP
1	A	1260	LEU
1	A	1264	GLU
1	A	1265	ASN
1	A	1273	LEU
1	A	1274	ARG
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1309	ASP
1	A	1315	GLU
1	A	1317	MET
1	A	1325	THR
1	A	1327	ILE
1	A	1336	MET
1	A	1341	ILE
1	A	1355	VAL
1	A	1366	ARG
1	A	1376	THR
1	A	1382	THR
1	A	1386	ARG

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Mol	Chain	Res	Type
1	A	1391	ARG
1	A	1393	ASN
1	A	1400	CYS
1	A	1405	THR
1	A	1406	VAL
1	A	1426	GLU
1	A	1433	MET
1	A	1438	THR
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1453	TYR
1	A	1454	MET
2	B	25	ILE
2	B	46	GLN
2	B	63	ILE
2	B	69	LEU
2	B	72	GLU
2	B	73	GLN
2	B	103	ASN
2	B	104	GLU
2	B	110	HIS
2	B	169	ARG
2	B	175	ARG
2	B	178	ASN
2	B	183	GLU
2	B	211	VAL
2	B	240	ILE
2	B	251	ILE
2	B	261	ARG
2	B	272	THR
2	B	278	GLN
2	B	279	ASP
2	B	287	ARG
2	B	294	ASP
2	B	313	MET
2	B	337	ARG
2	B	341	LEU
2	B	343	ILE
2	B	344	LYS
2	B	348	ARG
2	B	357	GLN

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Mol	Chain	Res	Type
2	B	365	THR
2	B	393	LYS
2	B	408	LEU
2	B	419	THR
2	B	440	HIS
2	B	442	PHE
2	B	470	LYS
2	B	476	ARG
2	B	482	VAL
2	B	485	ARG
2	B	487	THR
2	B	529	GLU
2	B	531	GLN
2	B	547	VAL
2	B	552	MET
2	B	563	MET
2	B	570	VAL
2	B	574	SER
2	B	595	ARG
2	B	596	LEU
2	B	601	ARG
2	B	603	LEU
2	B	609	ILE
2	B	612	GLU
2	B	615	MET
2	B	616	ILE
2	B	620	ARG
2	B	646	LEU
2	B	651	LEU
2	B	653	VAL
2	B	658	ILE
2	B	680	THR
2	B	696	GLU
2	B	708	GLU
2	B	734	HIS
2	B	737	THR
2	B	766	ARG
2	B	771	SER
2	B	776	GLN
2	B	786	ASN
2	B	790	ASP
2	B	791	THR

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Mol	Chain	Res	Type
2	B	801	LYS
2	B	839	MET
2	B	841	MET
2	B	844	SER
2	B	860	MET
2	B	879	ARG
2	B	933	SER
2	B	934	LYS
2	B	939	THR
2	B	942	ARG
2	B	944	THR
2	B	956	THR
2	B	959	ASP
2	B	967	ARG
2	B	975	GLN
2	B	986	GLN
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1028	GLU
2	B	1045	SER
2	B	1060	ARG
2	B	1065	GLN
2	B	1072	MET
2	B	1084	GLN
2	B	1094	ARG
2	B	1106	ARG
2	B	1123	SER
2	B	1129	ARG
2	B	1138	MET
2	B	1145	SER
2	B	1147	LEU
2	B	1151	LEU
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1175	LEU
2	B	1179	GLN
2	B	1183	LYS
2	B	1188	LYS
2	B	1193	GLN
2	B	1201	LYS

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Mol	Chain	Res	Type
2	B	1202	LEU
2	B	1210	MET
2	B	1220	ARG
2	B	1223	ASP
3	C	3	GLU
3	C	12	GLU
3	C	25	VAL
3	C	26	ASP
3	C	52	GLU
3	C	53	THR
3	C	55	THR
3	C	56	THR
3	C	81	GLU
3	C	84	ARG
3	C	100	THR
3	C	101	LEU
3	C	119	VAL
3	C	121	VAL
3	C	124	LEU
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	147	LEU
3	C	148	ARG
3	C	215	GLU
3	C	224	GLN
3	C	238	ILE
3	C	240	VAL
3	C	259	LEU
3	C	265	MET
3	C	268	ASP
4	D	5	THR
4	D	7	THR
4	D	9	GLN
4	D	10	THR
4	D	12	ARG
4	D	13	ARG
4	D	17	LYS
4	D	18	VAL
4	D	27	LEU
4	D	32	GLU

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Mol	Chain	Res	Type
4	D	34	GLN
4	D	35	LEU
4	D	40	HIS
4	D	47	LEU
4	D	52	LEU
4	D	53	SER
4	D	65	GLU
4	D	118	THR
4	D	126	ILE
4	D	134	THR
4	D	137	ASN
4	D	139	LYS
4	D	153	ARG
4	D	156	ASP
4	D	177	VAL
4	D	187	THR
4	D	197	SER
4	D	201	LYS
4	D	215	SER
4	D	219	THR
4	D	221	TYR
5	E	3	GLN
5	E	31	THR
5	E	37	LEU
5	E	45	LYS
5	E	57	MET
5	E	67	GLU
5	E	84	ASP
5	E	92	THR
5	E	104	ASN
5	E	131	THR
5	E	140	LEU
5	E	146	HIS
5	E	166	LYS
5	E	173	SER
5	E	177	ARG
5	E	178	ILE
5	E	191	LYS
5	E	192	ARG
5	E	196	VAL
5	E	202	SER
5	E	204	THR

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Mol	Chain	Res	Type
6	F	72	LYS
6	F	79	ARG
6	F	82	THR
6	F	86	THR
6	F	90	ARG
6	F	110	ASP
6	F	133	VAL
7	G	2	PHE
7	G	13	LEU
7	G	24	GLN
7	G	26	LEU
7	G	60	ARG
7	G	61	ILE
7	G	64	THR
7	G	96	GLN
7	G	106	MET
7	G	112	LYS
7	G	133	SER
7	G	138	THR
7	G	143	ILE
7	G	145	VAL
7	G	155	SER
7	G	162	SER
7	G	171	ILE
8	H	14	GLU
8	H	26	ILE
8	H	31	THR
8	H	34	ASP
8	H	76	THR
8	H	77	ARG
8	H	83	GLN
8	H	89	LEU
8	H	91	ASP
8	H	92	ASP
8	H	103	LYS
8	H	130	ARG
8	H	135	LEU
8	H	138	GLU
9	I	8	ARG
9	I	31	THR
9	I	35	VAL
9	I	74	GLU

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Mol	Chain	Res	Type
9	I	94	ASP
9	I	106	CYS
9	I	111	THR
10	J	1	MET
10	J	2	ILE
10	J	3	VAL
10	J	7	CYS
10	J	12	LYS
10	J	13	VAL
10	J	22	LEU
10	J	29	GLU
10	J	42	LYS
10	J	48	ARG
10	J	52	THR
11	K	18	LYS
11	K	20	LYS
11	K	25	THR
11	K	29	ASN
11	K	31	VAL
11	K	37	LYS
11	K	42	LEU
11	K	47	ARG
11	K	51	LEU
11	K	70	ARG
11	K	101	LEU
11	K	107	THR
12	L	27	LEU
12	L	35	SER
12	L	38	LEU
12	L	42	ARG
12	L	50	ASP
12	L	51	CYS
12	L	55	ILE
12	L	56	LEU
12	L	58	LYS
12	L	60	ARG
12	L	61	THR
12	L	65	VAL
12	L	68	GLU
13	M	35	VAL
13	M	39	SER
13	M	52	LEU

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Mol	Chain	Res	Type
13	M	59	THR
13	M	62	GLU
13	M	64	ARG
13	M	78	ARG
13	M	81	GLU
13	M	86	LEU
13	M	101	THR
13	M	114	GLN
13	M	142	LEU
13	M	145	ILE
13	M	168	MET
13	M	171	ILE
13	M	182	ARG
13	M	198	VAL
13	M	209	ILE
13	M	262	LYS
13	M	275	ILE
13	M	293	ILE
13	M	297	LYS
13	M	314	LYS
15	O	70	ILE
15	O	79	ARG
15	O	108	GLU
15	O	130	ASP
15	O	134	LEU
15	O	175	LEU
15	O	188	GLU
15	O	199	LYS
15	O	219	GLN
15	O	225	GLN
15	O	235	SER
15	O	240	MET

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	399	HIS
1	A	425	GLN
1	A	545	GLN
1	A	548	ASN
1	A	603	ASN
1	A	966	ASN

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Mol	Chain	Res	Type
1	A	994	GLN
1	A	1106	ASN
1	A	1140	HIS
1	A	1173	HIS
1	A	1270	ASN
1	A	1393	ASN
2	B	300	HIS
2	B	325	GLN
2	B	357	GLN
2	B	449	ASN
2	B	842	ASN
2	B	975	GLN
2	B	1025	HIS
2	B	1193	GLN
2	B	1195	HIS
3	C	184	ASN
4	D	37	GLN
4	D	143	ASN
5	E	3	GLN
7	G	71	ASN
7	G	102	GLN
8	H	35	GLN
8	H	83	GLN
9	I	83	ASN
9	I	89	GLN
9	I	108	HIS
13	M	235	ASN
13	M	285	ASN
13	M	300	GLN
15	O	158	GLN
15	O	219	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 10 ligands modelled in this entry, 10 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
1	A	2
19	T	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	23:DT	O3'	33:DT	P	36.30
1	B	351:TYR	C	352:ALA	N	3.29
1	A	234:MET	C	235:ILE	N	1.07
1	A	95:PHE	C	96:ILE	N	1.00

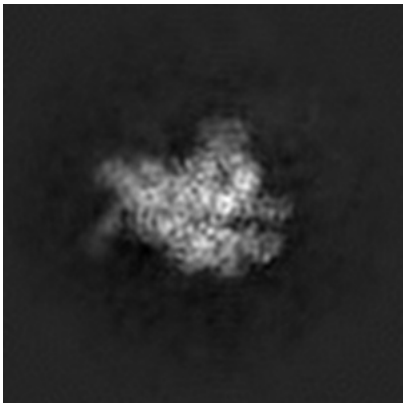
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2785. These allow visual inspection of the internal detail of the map and identification of artifacts.

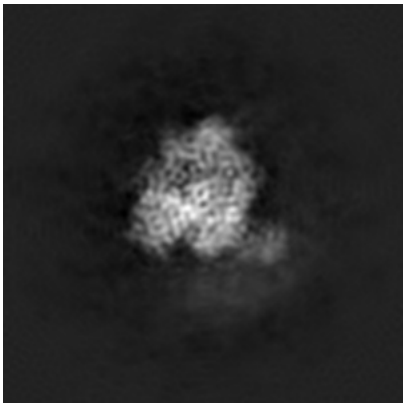
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

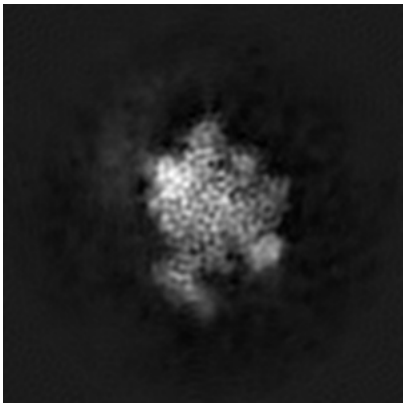
6.1.1 Primary map



X



Y

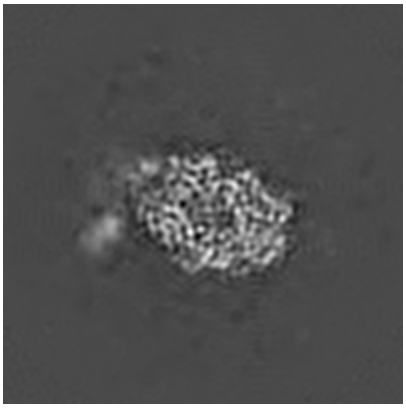


Z

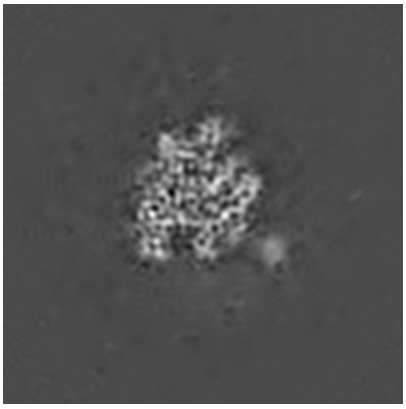
The images above show the map projected in three orthogonal directions.

6.2 Central slices

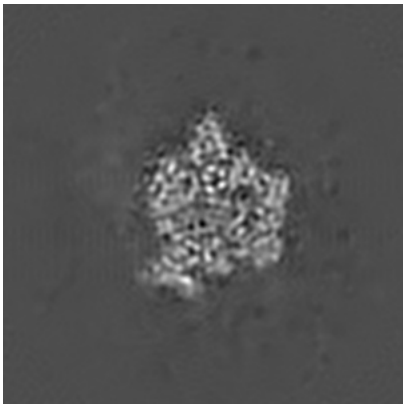
6.2.1 Primary map



X Index: 140



Y Index: 140

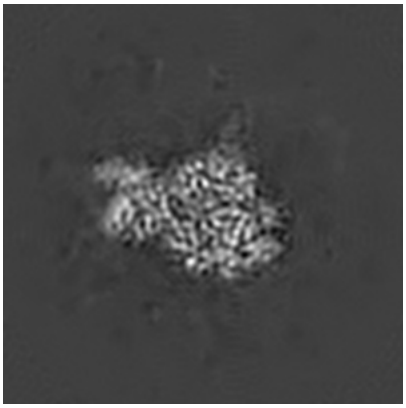


Z Index: 140

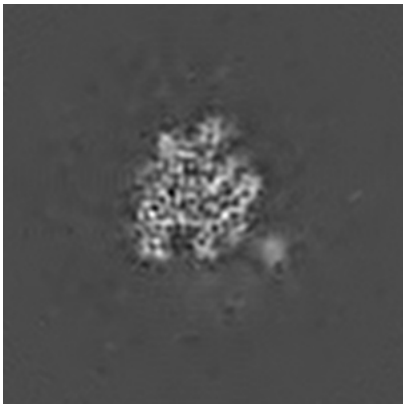
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

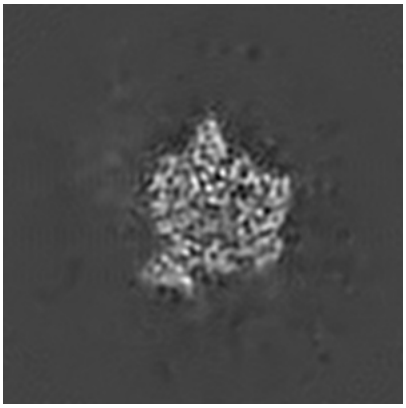
6.3.1 Primary map



X Index: 130



Y Index: 140

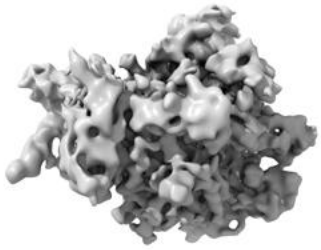


Z Index: 142

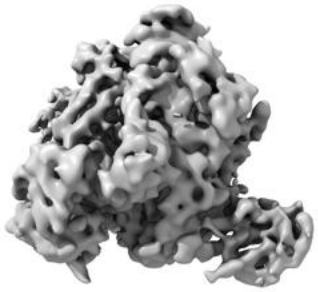
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

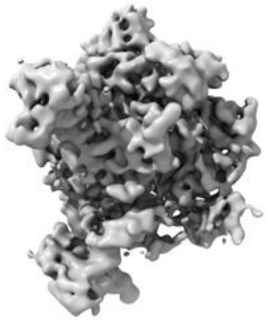
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0224. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

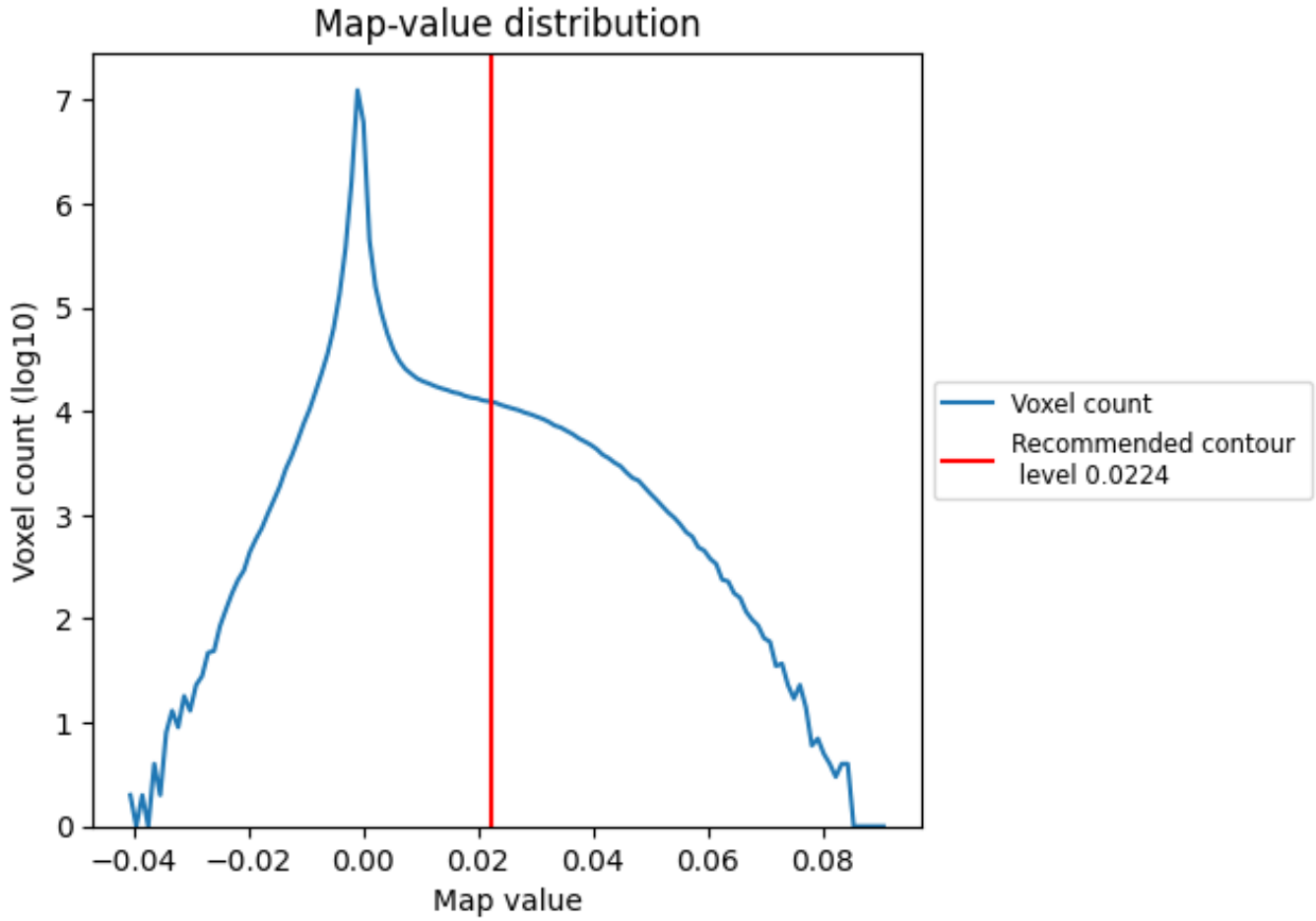
6.5 Mask visualisation (i)

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

7 Map analysis

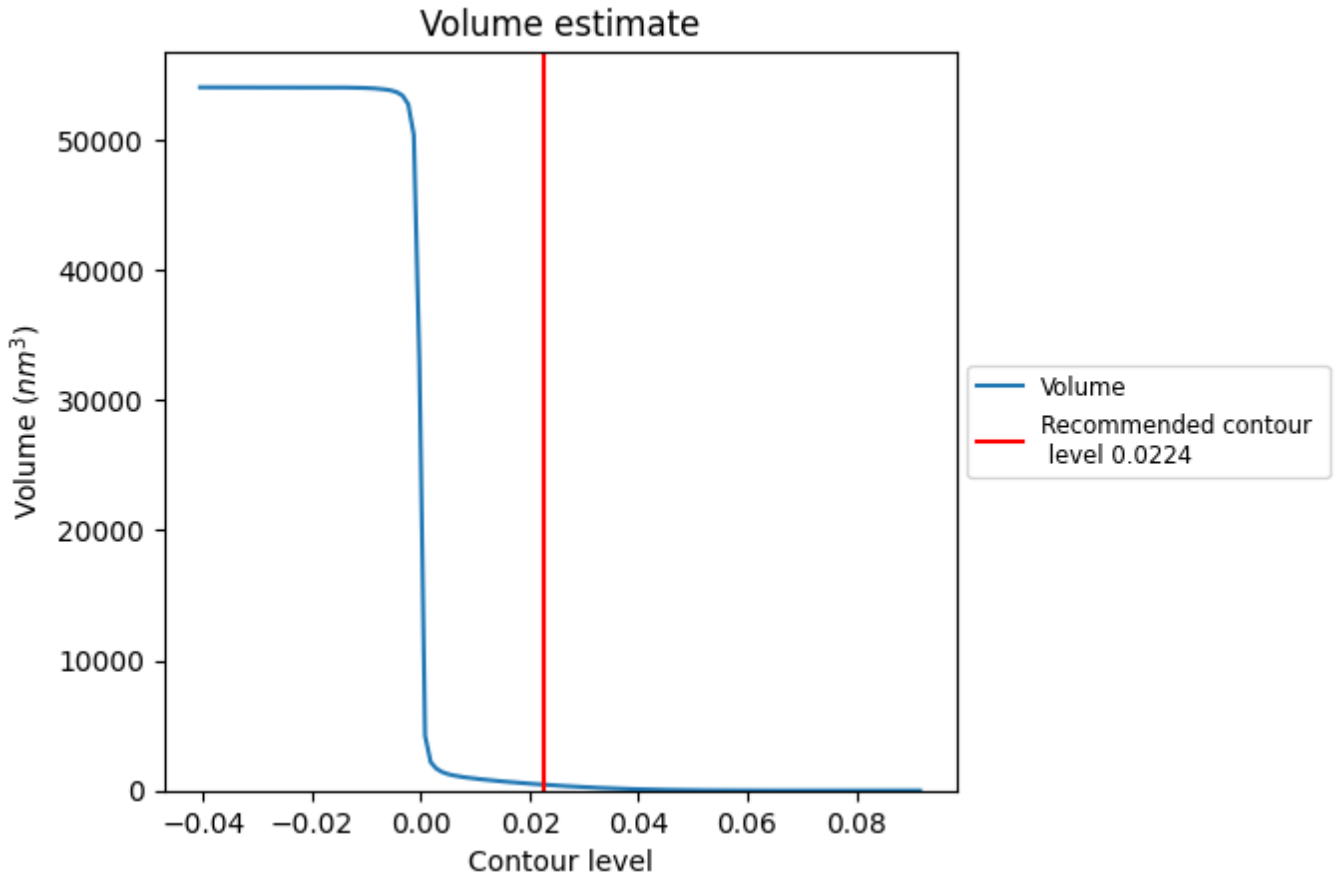
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

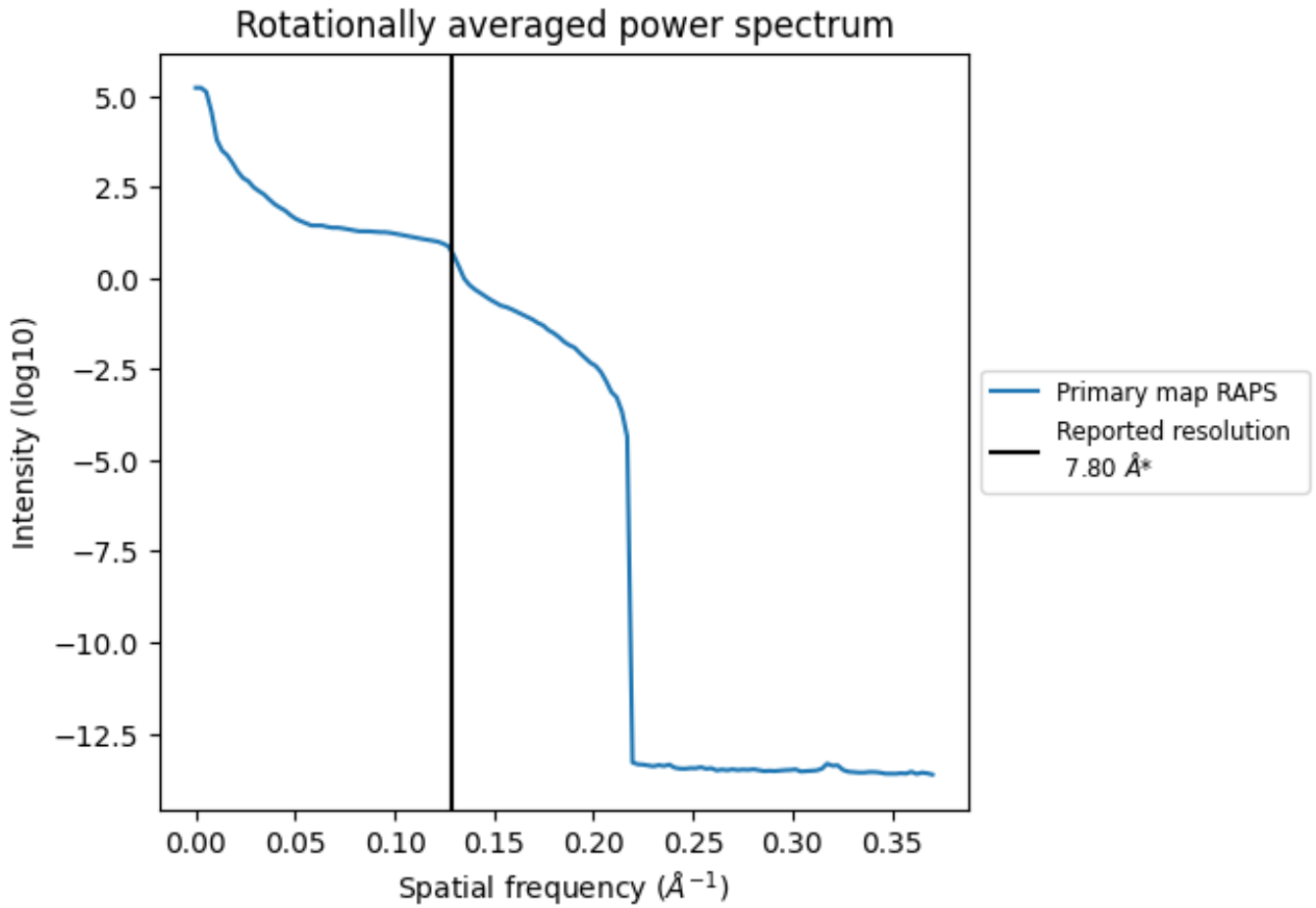
7.2 Volume estimate



The volume at the recommended contour level is 458 nm^3; this corresponds to an approximate mass of 414 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 0.128 $Å^{-1}$

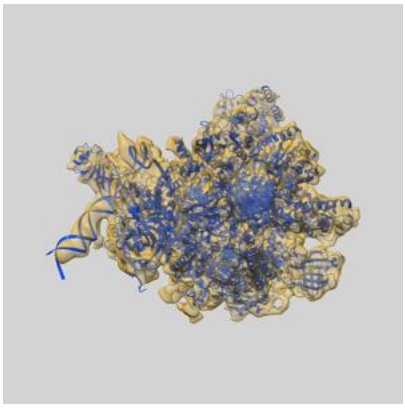
8 Fourier-Shell correlation (i)

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

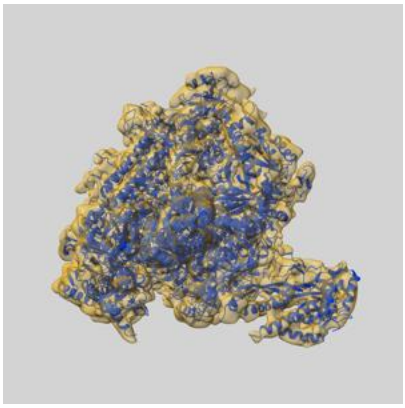
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2785 and PDB model 4V1N. Per-residue inclusion information can be found in section 3 on page 8.

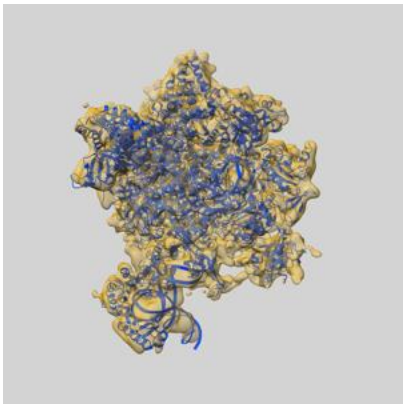
9.1 Map-model overlay



X



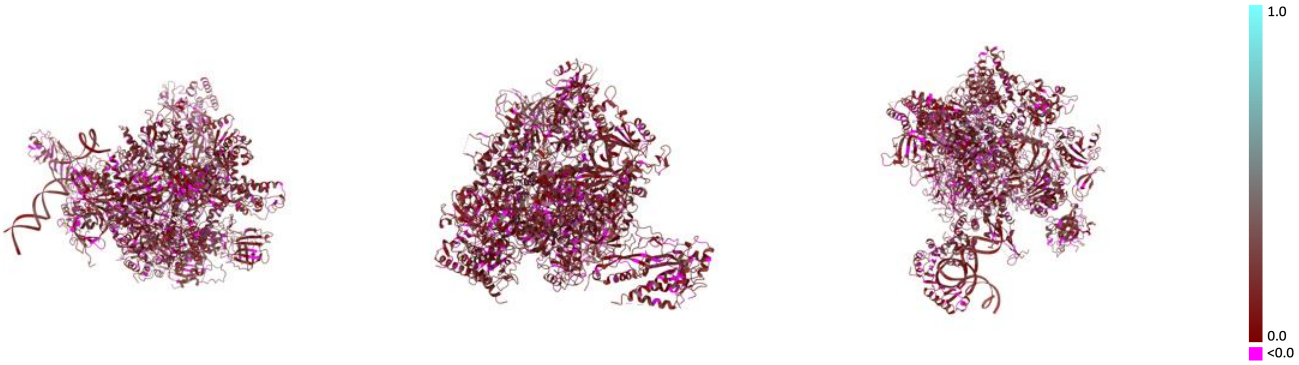
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0224 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.

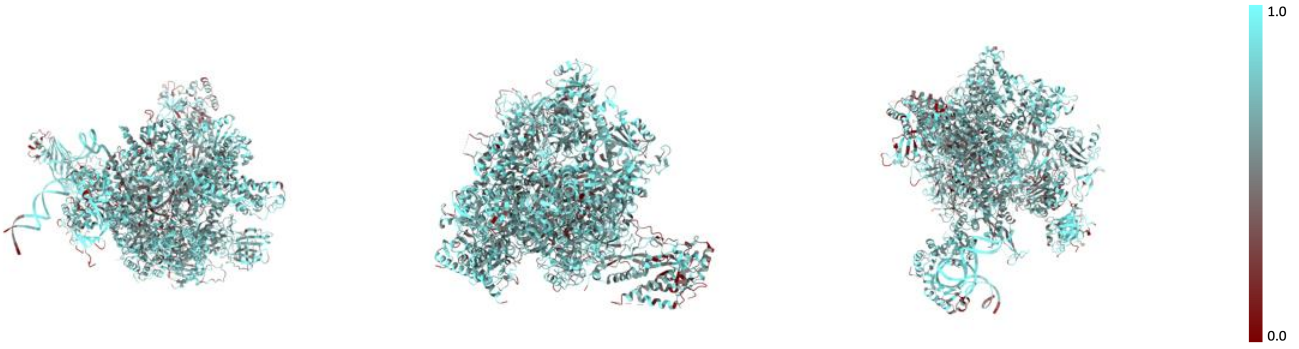
9.2 Q-score mapped to coordinate model (i)



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.

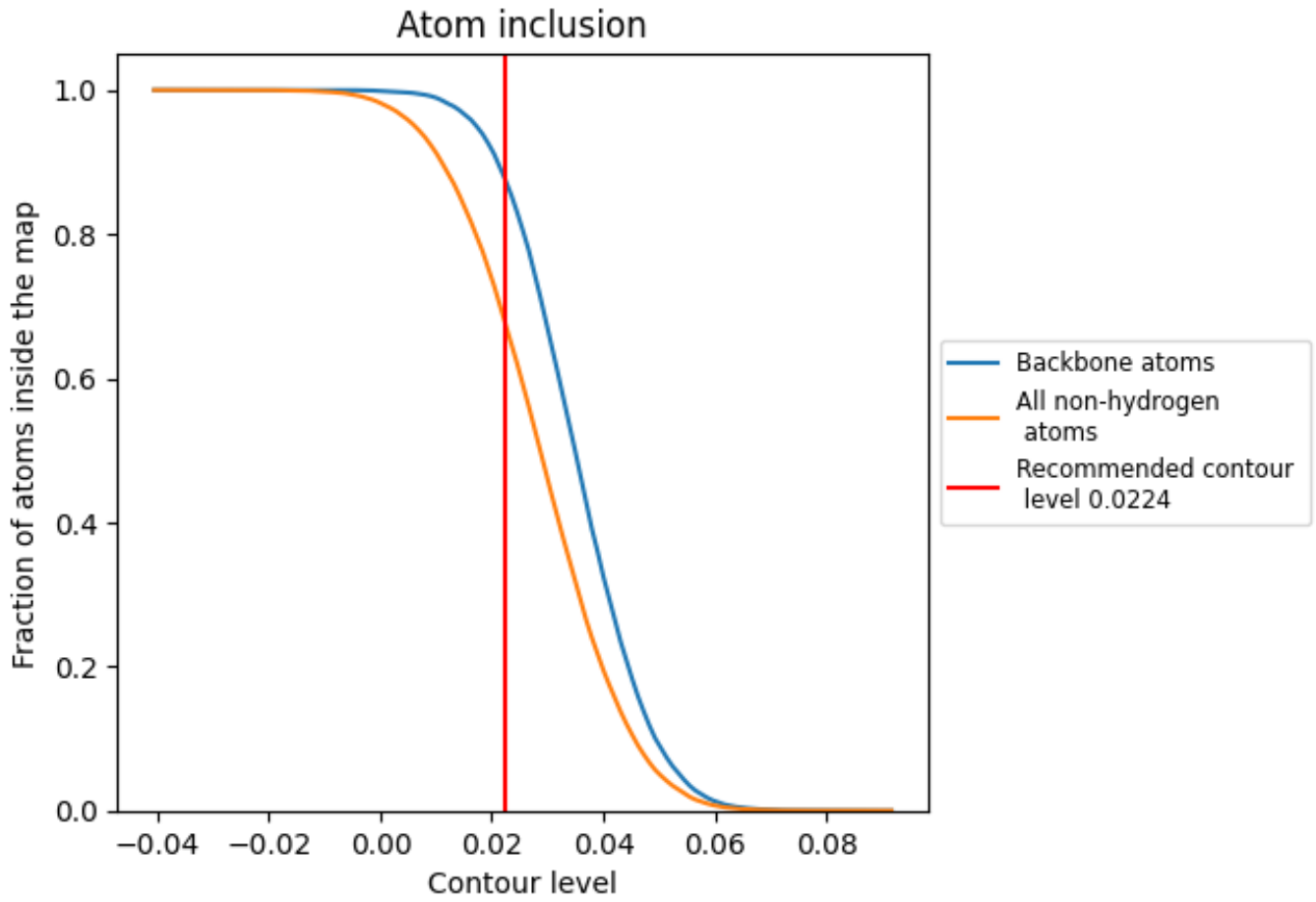
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0224).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 68% 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 (0.0224) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6769	0.1290
A	0.6896	0.1330
B	0.6552	0.1210
C	0.7220	0.1380
D	0.5327	0.1120
E	0.7226	0.1400
F	0.7186	0.1400
G	0.5681	0.1040
H	0.7067	0.1390
I	0.6839	0.1280
J	0.7215	0.1230
K	0.7122	0.1500
L	0.6125	0.1020
M	0.6207	0.1250
N	0.8062	0.1680
O	0.7010	0.1040
P	0.1545	0.0140
Q	0.7409	0.1820
R	0.7428	0.1360
T	0.7547	0.1400