Full wwPDB EM Validation Report ⓘ

Apr 30, 2024 – 09:24 pm BST

PDB ID	:	4V1O
EMDB ID	:	EMD-2786
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	:	9.70 Å(reported)

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

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

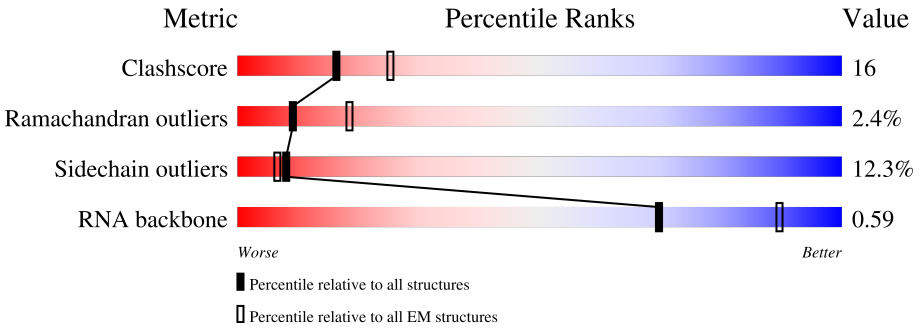
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 9.70 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1733	54% 23% 18%
2	B	1224	62% 29% 6%
3	C	318	60% 20% 16%
4	D	221	11% 51% 24% 5% 19%
5	E	215	74% 23%
6	F	155	33% 19% 46%
7	G	171	5% 69% 26% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	H	146	55% 30% 5% 9%
9	I	122	74% 20%
10	J	70	53% 29% 11% 7%
11	K	120	68% 27%
12	L	70	23% 27% 14% 34%
13	M	345	18% 43% 40% 5% 13%
14	N	50	18% 42% 52% 6%
15	O	181	34% 84% 14%
16	P	6	50% 67% 33%
17	Q	734	14% 83%
18	R	331	29% 68%
19	S	295	39% 7% 53%
20	T	58	14% 41% 45% 14%
21	U	222	62% 9% 29%
22	V	115	83% 14%
23	W	687	57% 39%
24	X	307	72% 24%
25	Y	209	91% 6%
26	Z	120	68% 5% 27%

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 45091 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 protein called MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	S	139	Total 691	C 413	N 139	O 139	0	0

- Molecule 20 is a DNA chain called TEMPLATE DNA.

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

- Molecule 21 is a protein called MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	158	Total 787	C 471	N 158	O 158	0	0

- Molecule 22 is a protein called MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 20.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	V	99	Total 491	C 293	N 99	O 99	0	0

- Molecule 23 is a protein called MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 11.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	W	419	Total 2085	C 1247	N 419	O 419	0	0

- Molecule 24 is a protein called MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 18.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	232	Total 1146	C 682	N 232	O 232	0	0

- Molecule 25 is a protein called MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 20.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	203	Total 1003	C 597	N 203	O 203	0	0

- Molecule 26 is a protein called MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 22.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Z	88	Total 442	C 266	N 88	O 88	1	0

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 28 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

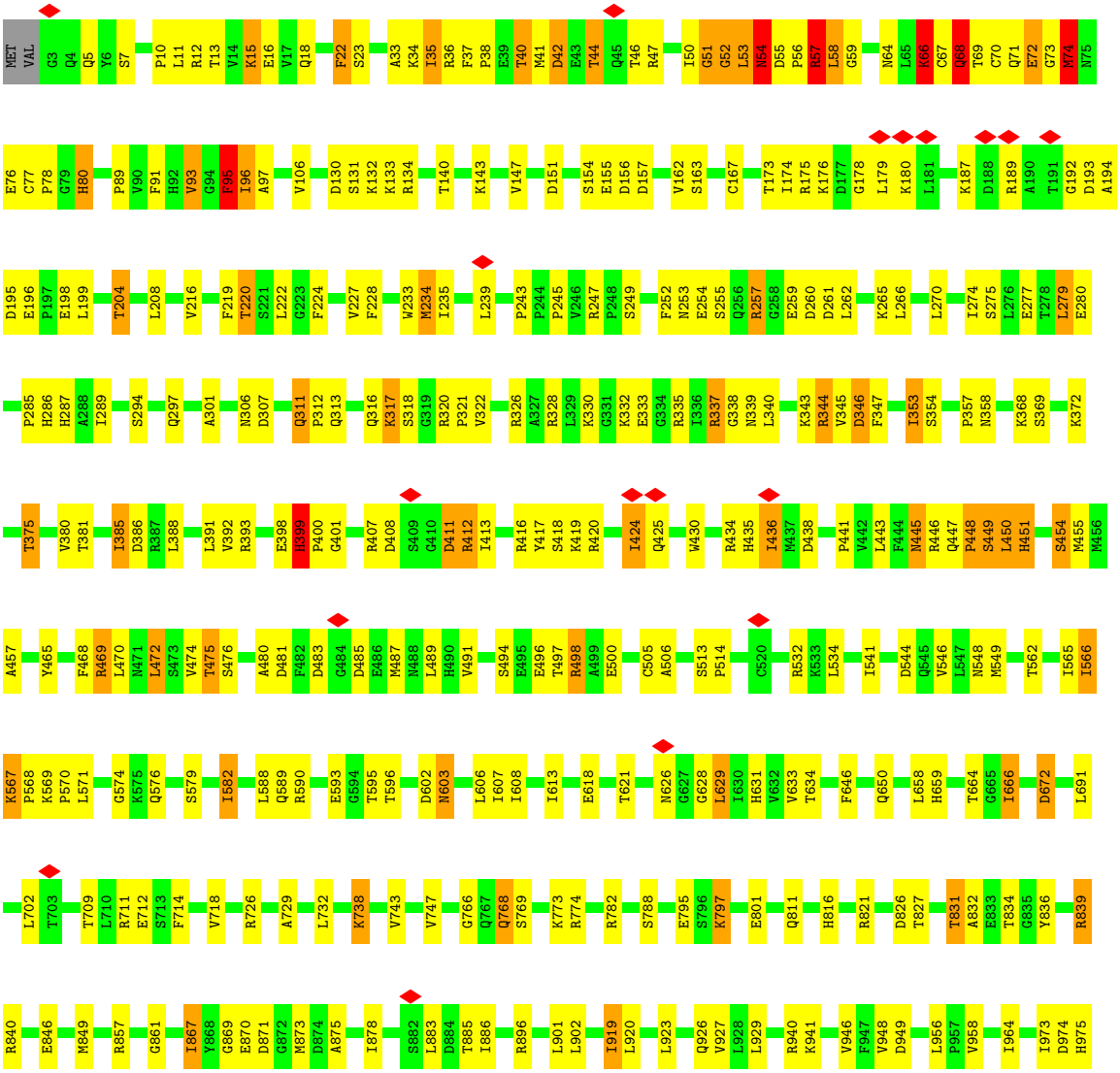
Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total 1	Mg 1	0

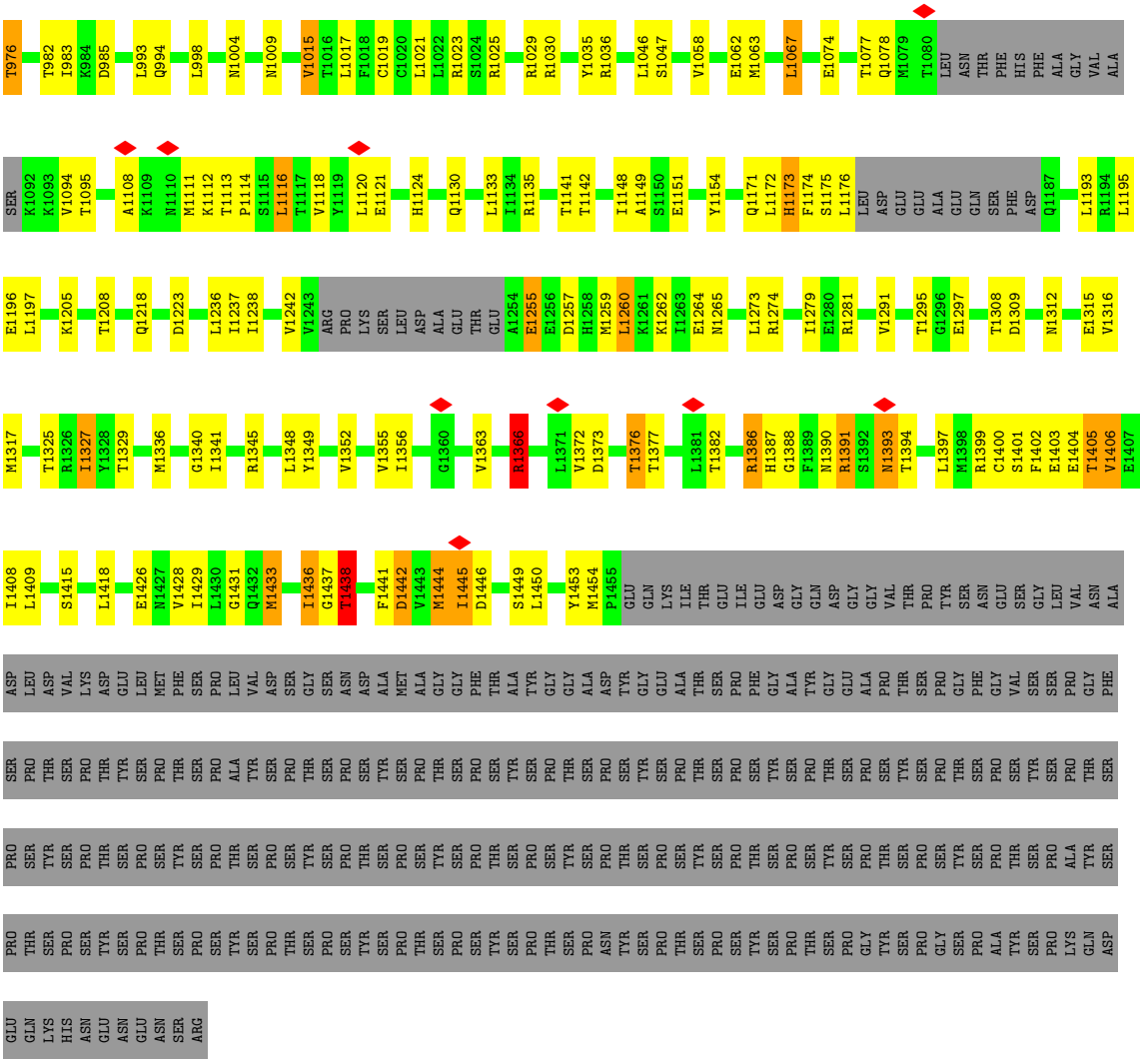
3 Residue-property plots (i)

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

• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1

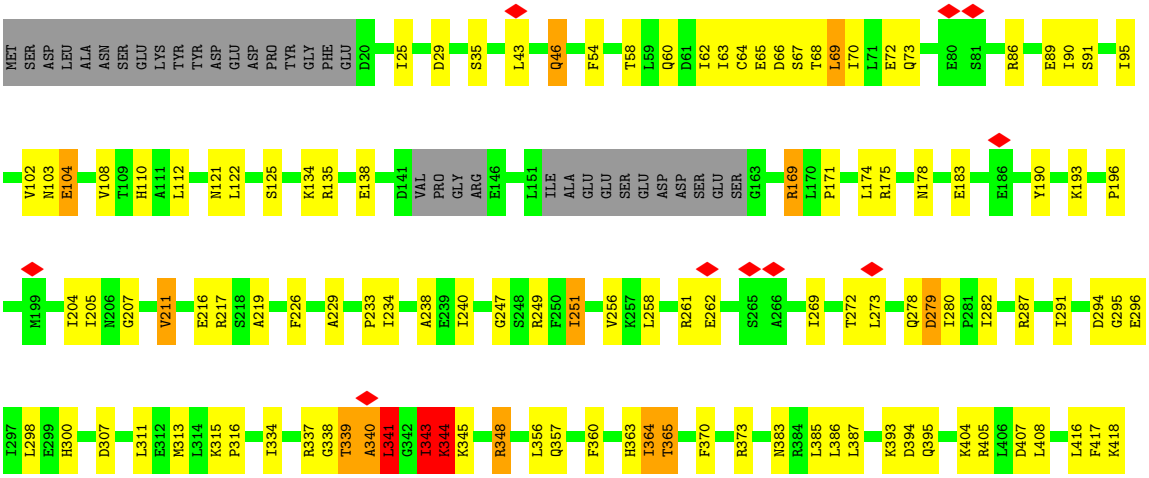
Chain A:

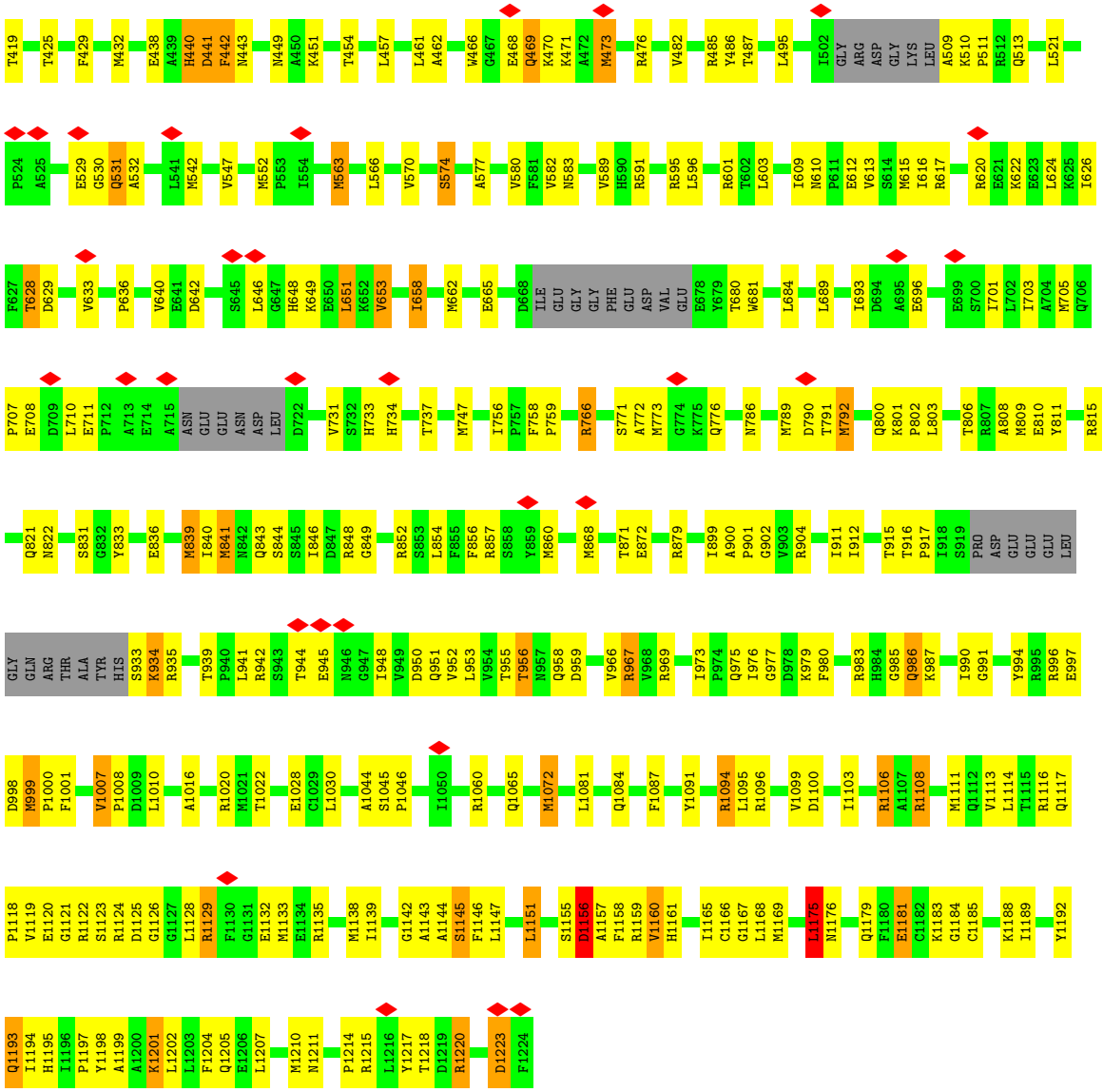




• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

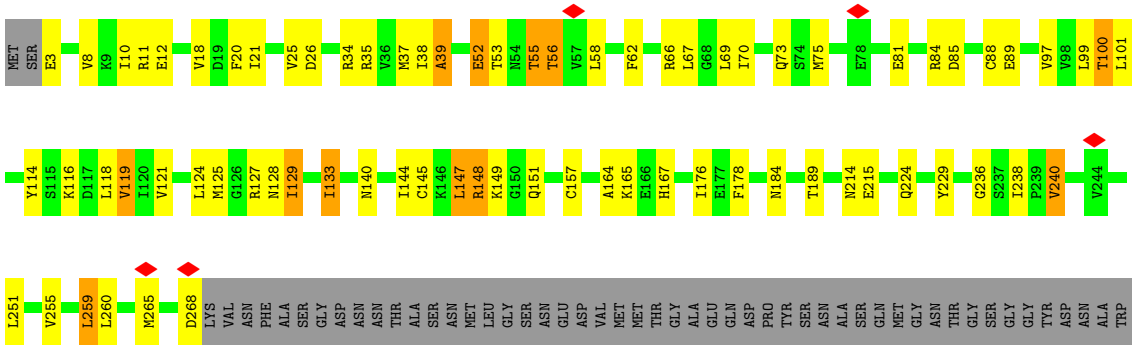
Chain B:





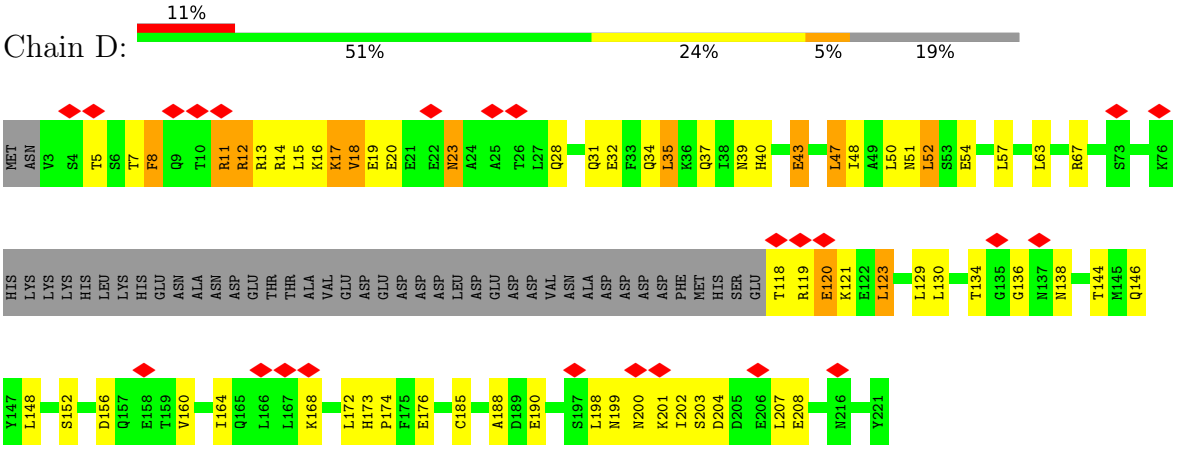
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C:



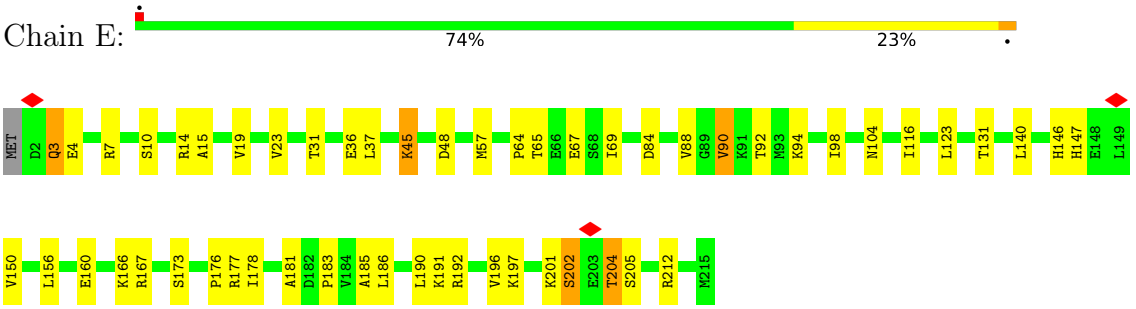
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

Chain D:



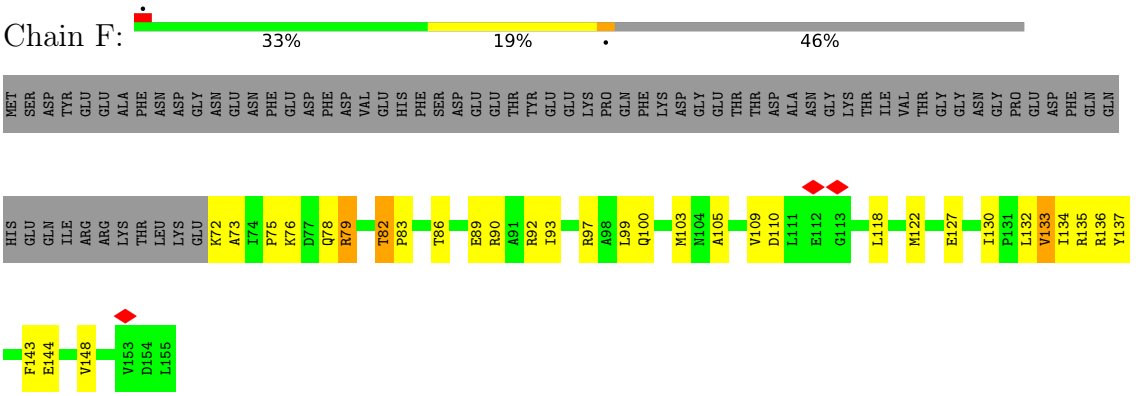
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

Chain E:



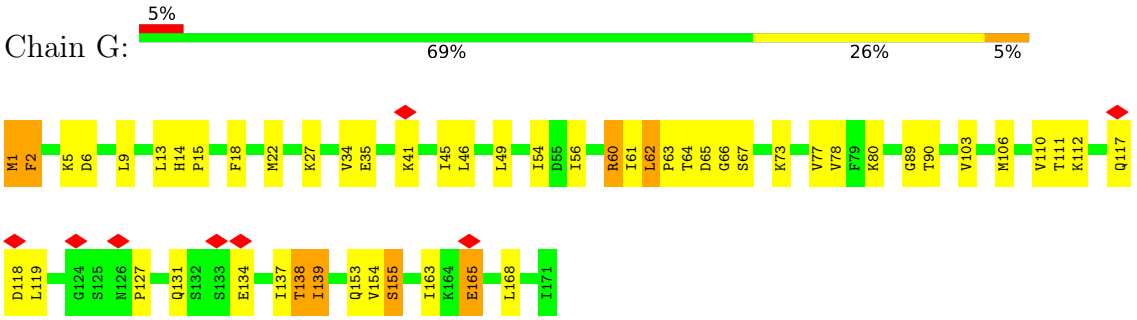
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F:



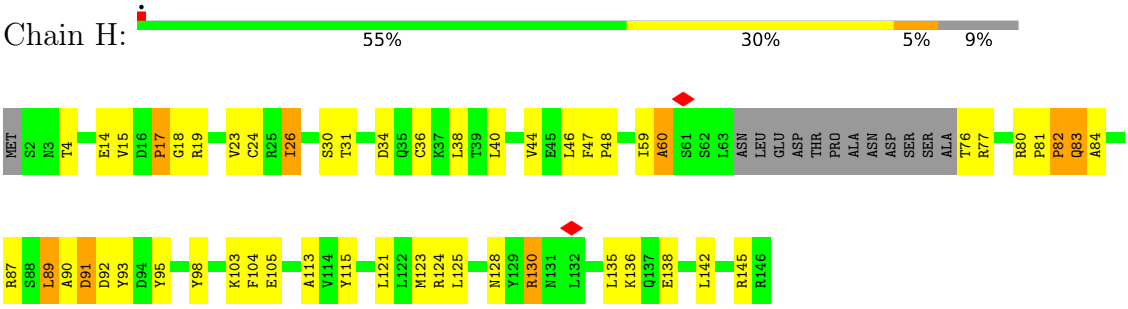
• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G:



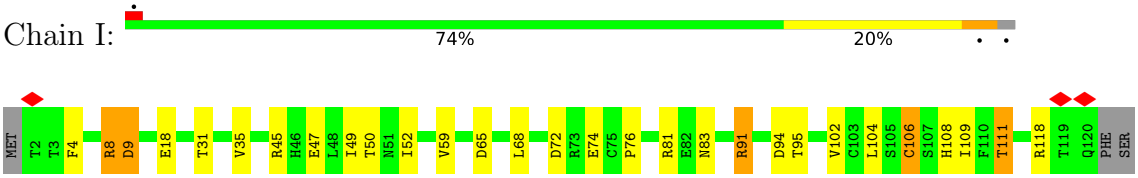
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H:



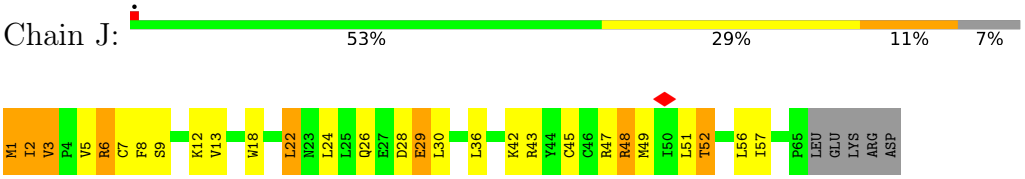
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

Chain I:



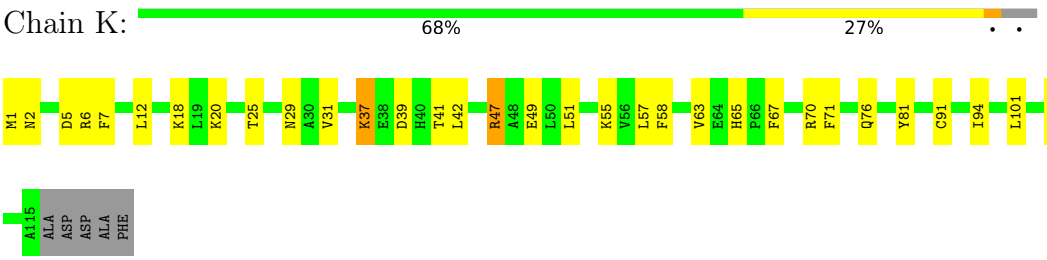
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J:



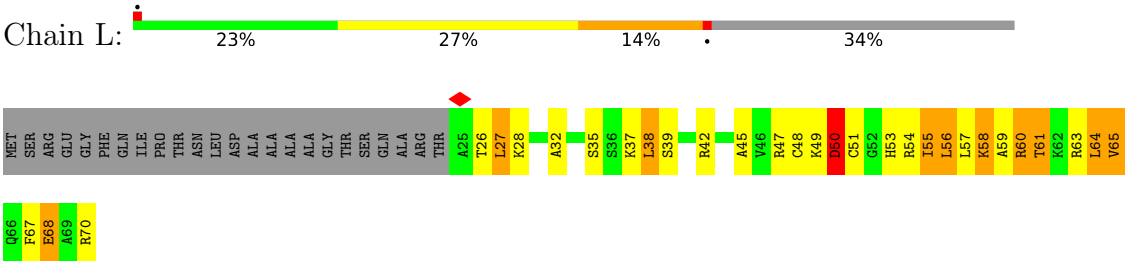
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K:



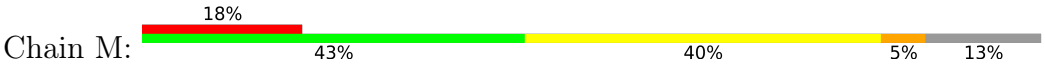
• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

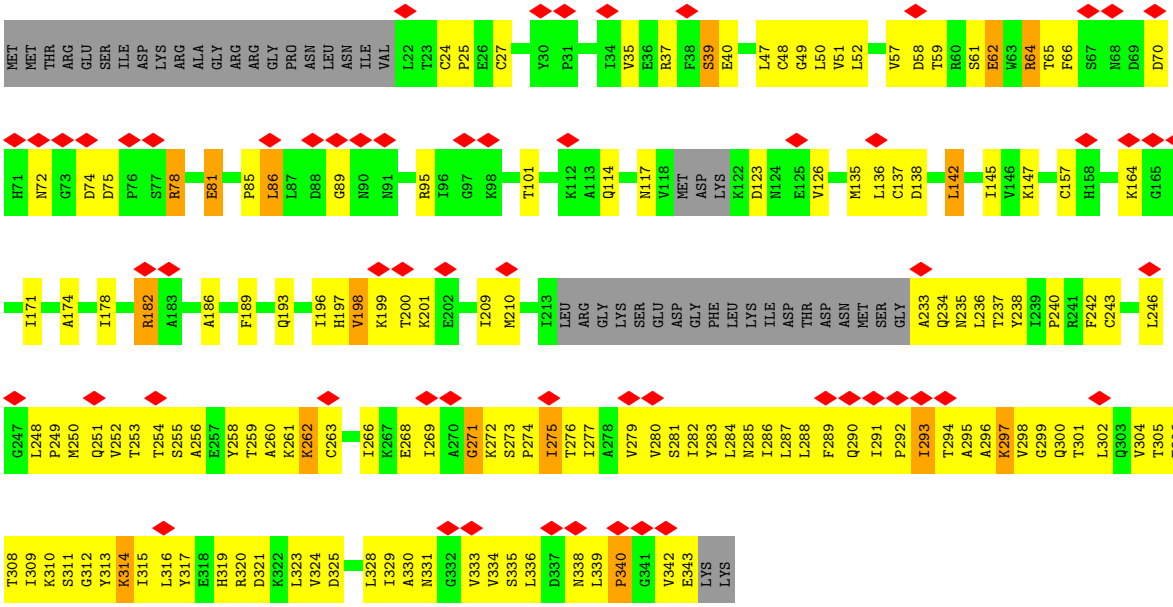
Chain L:



• Molecule 13: TRANSCRIPTION INITIATION FACTOR IIB

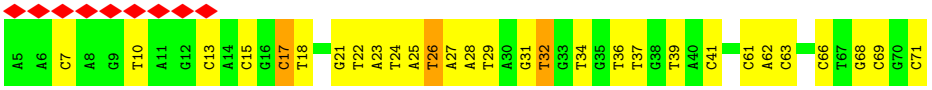
Chain M:





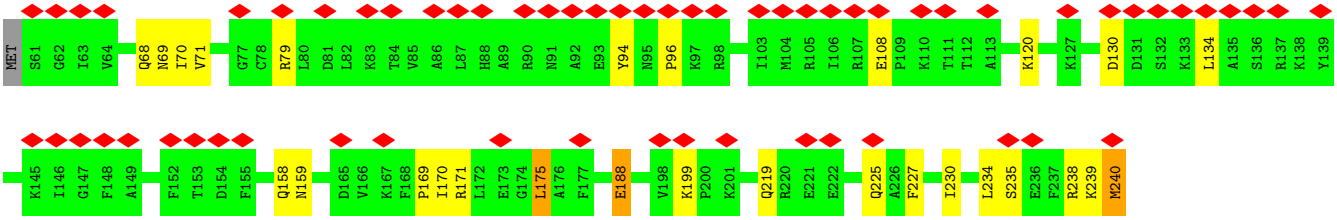
• Molecule 14: NONTEMPLATE DNA

Chain N:



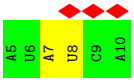
• Molecule 15: TATA-BOX-BINDING PROTEIN

Chain O:



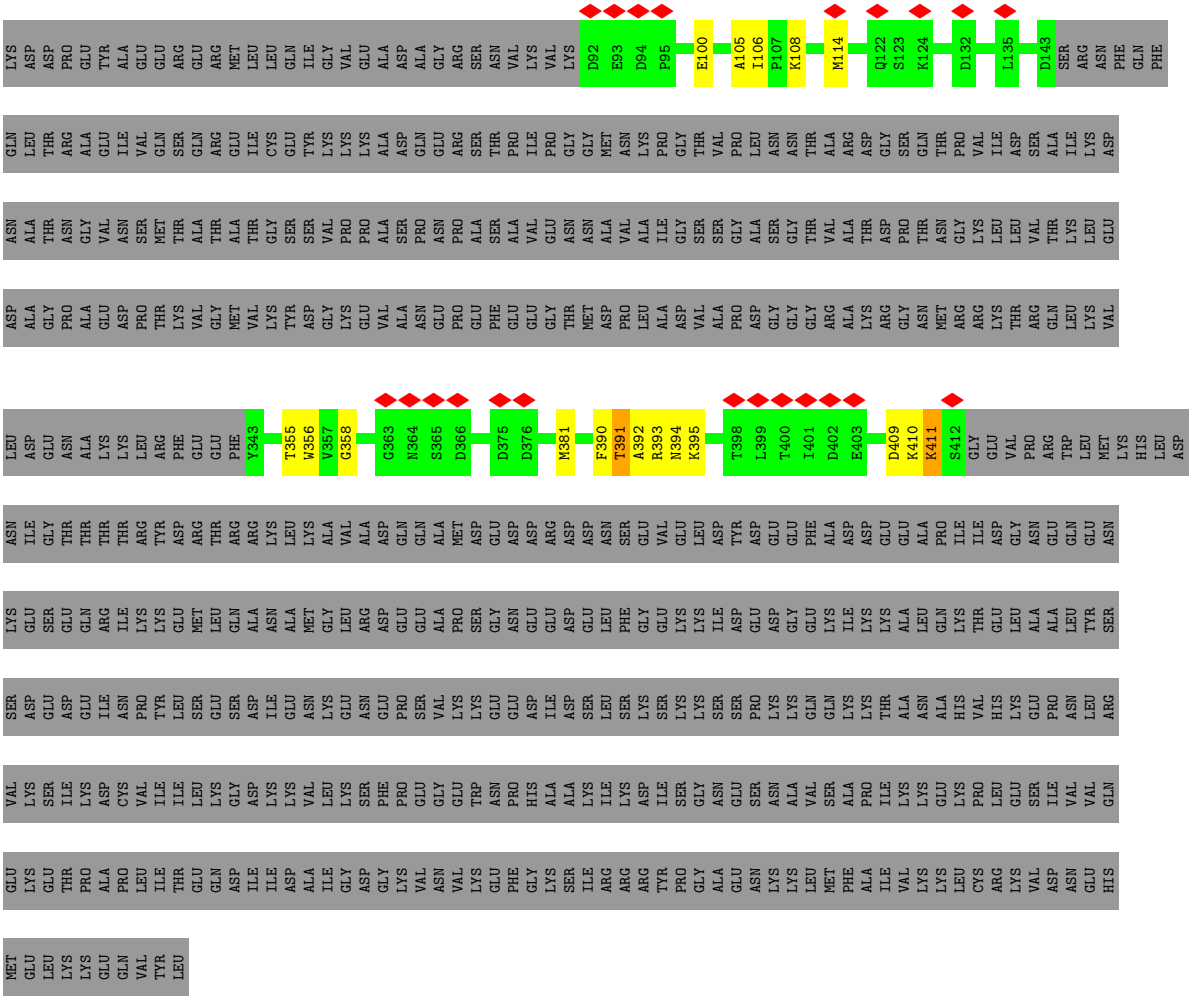
• Molecule 16: RNA

Chain P:



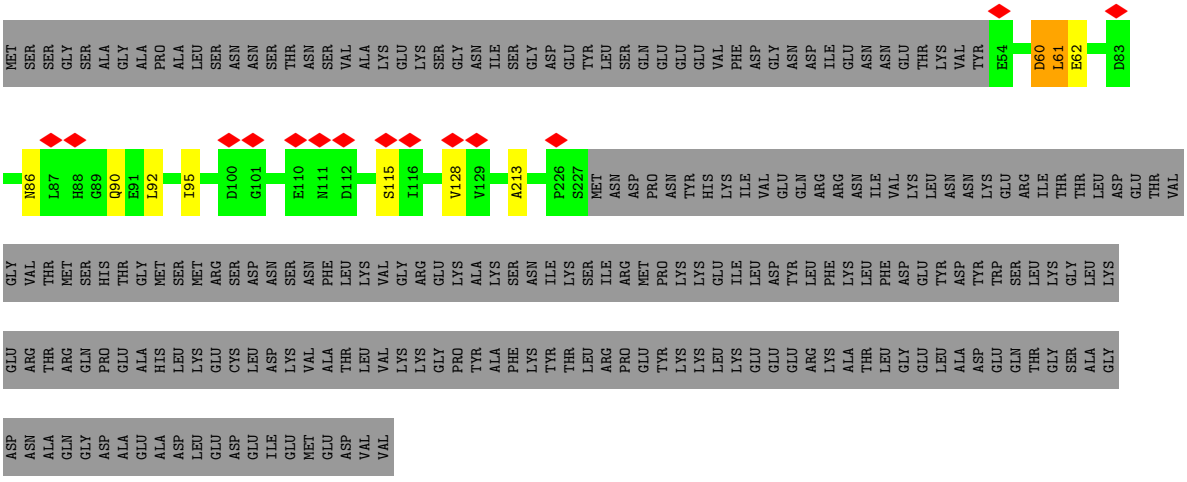
• Molecule 17: TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT ALPHA

Chain Q:



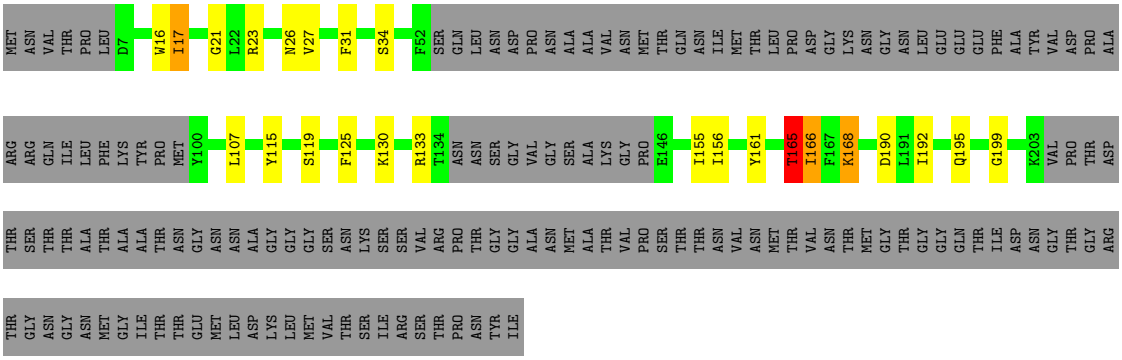
• Molecule 18: TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT BETA

Chain R:



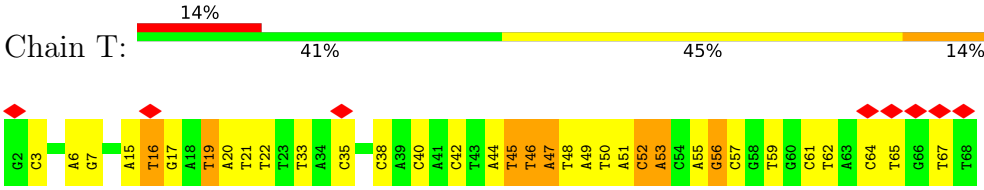
• Molecule 19: MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 6

Chain S:



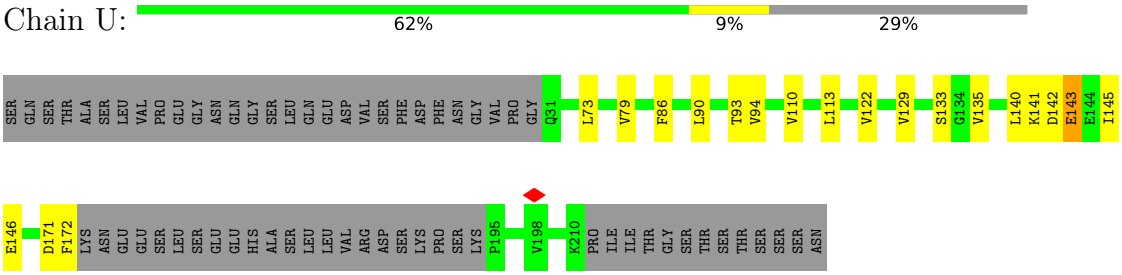
• Molecule 20: TEMPLATE DNA

Chain T:



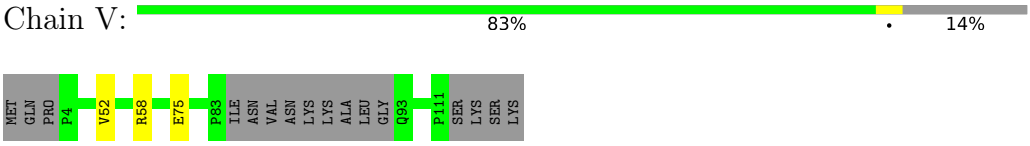
• Molecule 21: MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 8

Chain U:



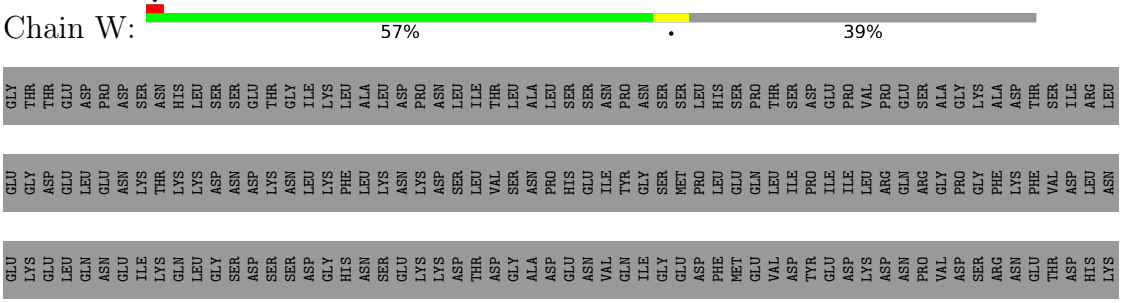
• Molecule 22: MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 20

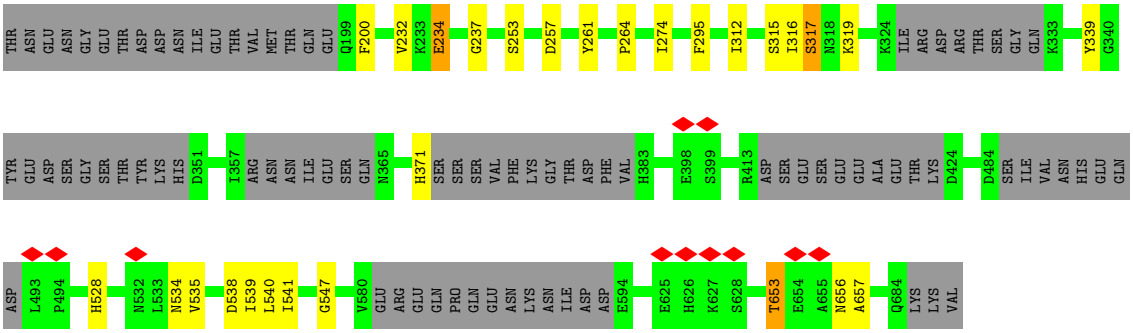
Chain V:



• Molecule 23: MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 11

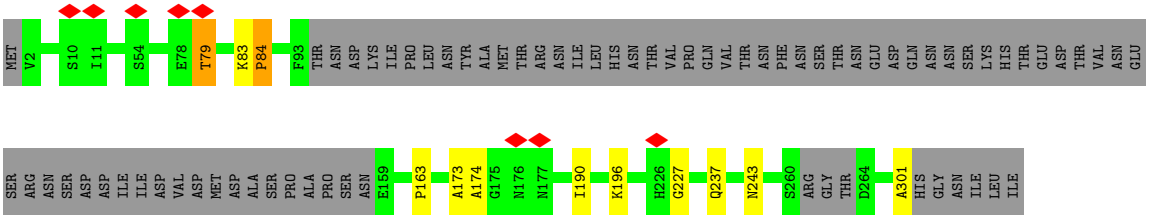
Chain W:





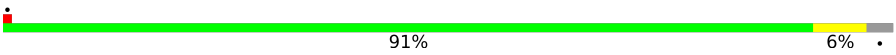
• Molecule 24: MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 18

Chain X:



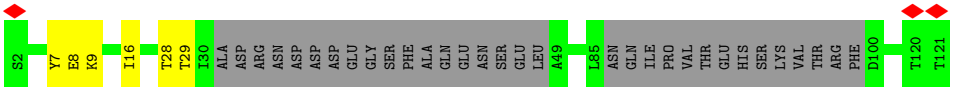
• Molecule 25: MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 20

Chain Y:



• Molecule 26: MEDIATOR OF RNA POLYMERASE II TRANSCRIPTION SUBUNIT 22

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	3267	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	0.055	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0135	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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.56	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	0.38	0/1444	0.59	0/1935
5	E	0.48	0/1788	0.71	0/2406
6	F	0.62	0/691	0.81	0/933
7	G	0.43	0/1368	0.61	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	15/1100 (1.4%)	1.32	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	S	0.53	0/688	1.40	15/956 (1.6%)
20	T	1.22	18/1265 (1.4%)	1.44	15/1866 (0.8%)
21	U	0.42	0/785	1.15	9/1094 (0.8%)
22	V	0.40	0/489	0.93	3/679 (0.4%)
23	W	0.40	0/2077	0.87	9/2889 (0.3%)
24	X	0.38	0/1143	0.76	2/1587 (0.1%)
25	Y	0.32	0/1001	0.69	2/1391 (0.1%)
26	Z	0.41	0/442	1.09	4/614 (0.7%)
All	All	0.58	38/45959 (0.1%)	0.85	89/62686 (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
19	S	0	1
21	U	0	2
23	W	0	4
All	All	0	11

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1436	ILE	C-N	14.98	1.60	1.33
1	A	95	PHE	C-N	-14.46	1.00	1.34
20	T	53	DA	P-O5'	-11.80	1.48	1.59
1	A	234	MET	C-N	-11.60	1.07	1.34
20	T	47	DA	C1'-N9	-10.47	1.32	1.47
2	B	973	ILE	C-N	9.29	1.51	1.34
20	T	42	DC	P-O5'	-9.23	1.50	1.59
20	T	56	DG	C1'-N9	-6.66	1.38	1.47
1	A	1394	THR	C-N	-6.24	1.21	1.33
20	T	61	DC	C1'-N1	6.22	1.57	1.49
20	T	64	DC	C1'-N1	6.16	1.57	1.49
20	T	46	DT	C4'-C3'	-5.36	1.47	1.52
14	N	32	DT	C1'-N1	5.27	1.56	1.49
14	N	34	DT	C1'-N1	5.26	1.56	1.49
20	T	33	DT	C1'-N1	5.25	1.56	1.49
20	T	3	DC	C1'-N1	5.25	1.56	1.49
14	N	7	DC	C1'-N1	5.23	1.56	1.49
20	T	38	DC	C1'-N1	5.22	1.56	1.49
14	N	39	DT	C1'-N1	5.22	1.56	1.49
14	N	10	DT	C1'-N1	5.21	1.56	1.49
14	N	41	DC	C1'-N1	5.20	1.56	1.49
20	T	35	DC	C1'-N1	5.20	1.56	1.49
20	T	65	DT	C1'-N1	5.19	1.55	1.49
20	T	62	DT	C1'-N1	5.19	1.55	1.49
14	N	68	DG	O3'-P	-5.17	1.54	1.61
14	N	37	DT	C1'-N1	5.17	1.55	1.49
14	N	15	DC	C1'-N1	5.17	1.55	1.49
14	N	13	DC	C1'-N1	5.17	1.55	1.49
20	T	6	DA	O3'-P	-5.17	1.54	1.61
14	N	17	DC	C1'-N1	5.16	1.55	1.49
14	N	36	DT	C1'-N1	5.16	1.55	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	T	59	DT	C1'-N1	5.16	1.55	1.49
20	T	67	DT	C1'-N1	5.15	1.55	1.49
20	T	40	DC	C1'-N1	5.14	1.55	1.49
20	T	57	DC	C1'-N1	5.12	1.55	1.49
14	N	69	DC	C1'-N1	5.12	1.55	1.49
14	N	71	DC	C1'-N1	5.11	1.55	1.49
14	N	66	DC	P-O5'	-5.02	1.54	1.59

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	MET	O-C-N	-14.65	99.26	122.70
19	S	192	ILE	CB-CA-C	-12.19	87.22	111.60
20	T	46	DT	O4'-C4'-C3'	-11.78	98.93	106.00
22	V	52	VAL	CB-CA-C	-9.98	92.44	111.40
20	T	42	DC	O5'-P-OP1	-9.11	97.50	105.70
20	T	6	DA	O3'-P-O5'	-9.11	86.69	104.00
14	N	26	DT	O4'-C4'-C3'	-8.93	100.64	106.00
18	R	60	ASP	C-N-CA	8.74	143.54	121.70
1	A	95	PHE	C-N-CA	-8.00	101.71	121.70
1	A	234	MET	CA-C-N	7.99	134.77	117.20
1	A	346	ASP	O-C-N	-7.57	110.59	122.70
20	T	16	DT	O4'-C4'-C3'	-7.36	101.56	104.50
20	T	45	DT	O4'-C4'-C3'	-7.34	101.56	104.50
26	Z	8	GLU	CB-CA-C	-7.33	95.74	110.40
14	N	66	DC	C2-N1-C1'	7.24	126.76	118.80
1	A	399	HIS	N-CA-CB	7.21	123.58	110.60
14	N	68	DG	P-O3'-C3'	7.20	128.34	119.70
25	Y	65	HIS	N-CA-C	-7.16	91.68	111.00
26	Z	7	TYR	CB-CA-C	-7.07	96.26	110.40
18	R	61	LEU	N-CA-C	6.92	129.67	111.00
19	S	166	ILE	N-CA-CB	6.74	126.30	110.80
19	S	161	TYR	CB-CA-C	6.69	123.79	110.40
21	U	122	VAL	CB-CA-C	-6.65	98.76	111.40
25	Y	53	VAL	N-CA-C	-6.65	93.04	111.00
1	A	234	MET	C-N-CA	6.61	138.22	121.70
20	T	46	DT	O4'-C1'-C2'	-6.50	100.70	105.90
21	U	171	ASP	CB-CA-C	6.47	123.33	110.40
19	S	130	LYS	N-CA-CB	6.43	122.18	110.60
19	S	156	ILE	CB-CA-C	-6.39	98.81	111.60
23	W	295	PHE	CB-CA-C	6.39	123.18	110.40
21	U	79	VAL	CB-CA-C	-6.37	99.30	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	S	133	ARG	CB-CA-C	-6.31	97.78	110.40
19	S	115	TYR	CB-CA-C	-6.14	98.11	110.40
1	A	95	PHE	CA-C-N	-6.13	103.72	117.20
19	S	168	LYS	CB-CA-C	6.12	122.65	110.40
23	W	232	VAL	CB-CA-C	-6.02	99.96	111.40
17	Q	411	LYS	CA-C-O	6.00	132.69	120.10
20	T	46	DT	C4-C5-C6	5.98	121.59	118.00
21	U	94	VAL	CB-CA-C	5.98	122.76	111.40
19	S	190	ASP	CB-CA-C	-5.95	98.50	110.40
23	W	274	ILE	CB-CA-C	-5.95	99.71	111.60
21	U	110	VAL	CB-CA-C	-5.91	100.17	111.40
20	T	53	DA	N1-C6-N6	-5.90	115.06	118.60
23	W	371	HIS	N-CA-CB	-5.88	100.02	110.60
17	Q	411	LYS	N-CA-C	5.81	126.68	111.00
14	N	66	DC	C6-N1-C1'	-5.80	113.83	120.80
19	S	107	LEU	CB-CA-C	5.78	121.19	110.20
20	T	7	DG	C5-C6-O6	-5.77	125.14	128.60
23	W	234	GLU	CB-CA-C	5.77	121.94	110.40
1	A	58	LEU	CA-CB-CG	5.74	128.50	115.30
2	B	340	ALA	C-N-CA	5.71	135.97	121.70
20	T	19	DT	O4'-C1'-N1	5.69	111.98	108.00
21	U	145	ILE	CB-CA-C	-5.66	100.27	111.60
19	S	16	TRP	N-CA-CB	5.66	120.79	110.60
1	A	194	ALA	C-N-CA	5.63	135.79	121.70
19	S	34	SER	CB-CA-C	5.59	120.72	110.10
20	T	6	DA	P-O3'-C3'	5.59	126.41	119.70
19	S	119	SER	N-CA-CB	5.56	118.83	110.50
22	V	75	GLU	CB-CA-C	-5.55	99.29	110.40
26	Z	16	ILE	CB-CA-C	-5.53	100.53	111.60
20	T	53	DA	P-O5'-C5'	5.53	129.75	120.90
13	M	340	PRO	C-N-CA	-5.49	110.78	122.30
20	T	47	DA	O4'-C1'-N9	-5.45	104.18	108.00
3	C	39	ALA	N-CA-C	5.44	125.70	111.00
2	B	628	THR	C-N-CA	5.43	135.29	121.70
15	O	175	LEU	CA-CB-CG	5.43	127.78	115.30
21	U	113	LEU	CB-CA-C	-5.41	99.93	110.20
21	U	172	PHE	CB-CA-C	5.40	121.20	110.40
23	W	339	TYR	CB-CA-C	-5.38	99.63	110.40
26	Z	9	LYS	CB-CA-C	-5.36	99.68	110.40
21	U	73	LEU	CB-CA-C	5.31	120.29	110.20
24	X	301	ALA	N-CA-C	5.30	125.32	111.00
24	X	79	THR	N-CA-C	-5.29	96.72	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	89	GLU	N-CA-C	-5.29	96.72	111.00
19	S	31	PHE	N-CA-CB	5.29	120.12	110.60
1	A	1394	THR	C-N-CA	5.28	133.38	122.30
23	W	200	PHE	CB-CA-C	5.27	120.95	110.40
19	S	17	ILE	CB-CA-C	-5.25	101.09	111.60
22	V	58	ARG	CB-CA-C	-5.20	100.01	110.40
14	N	26	DT	P-O3'-C3'	5.18	125.92	119.70
23	W	653	THR	N-CA-C	-5.17	97.04	111.00
2	B	1181	GLU	N-CA-C	5.17	124.95	111.00
20	T	52	DC	OP1-P-O3'	5.15	116.53	105.20
23	W	253	SER	N-CA-CB	5.12	118.18	110.50
17	Q	114	MET	C-N-CA	-5.08	109.00	121.70
20	T	6	DA	O4'-C1'-N9	5.06	111.54	108.00
10	J	5	VAL	N-CA-C	-5.02	97.44	111.00
2	B	1156	ASP	N-CA-C	5.01	124.53	111.00
1	A	346	ASP	CA-C-N	5.00	128.21	117.20

There are no chirality outliers.

All (11) 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
19	S	165	THR	Peptide
21	U	135	VAL	Peptide
21	U	142	ASP	Peptide
23	W	316	ILE	Peptide
23	W	317	SER	Peptide
23	W	319	LYS	Peptide
23	W	540	LEU	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	426	0
2	B	9140	0	9108	326	0
3	C	2095	0	2051	44	0
4	D	1434	0	1460	106	0
5	E	1752	0	1776	27	0
6	F	679	0	701	52	0
7	G	1340	0	1357	71	0
8	H	1068	0	1040	22	0
9	I	971	0	927	17	0
10	J	532	0	542	15	0
11	K	920	0	929	19	0
12	L	363	0	386	26	0
13	M	2202	0	2154	388	0
14	N	975	0	567	23	0
15	O	1416	0	1491	29	0
16	P	123	0	66	1	0
17	Q	606	0	256	30	0
18	R	521	0	216	5	0
19	S	691	0	279	6	0
20	T	1125	0	661	62	0
21	U	787	0	330	5	0
22	V	491	0	201	0	0
23	W	2085	0	871	13	0
24	X	1146	0	489	25	0
25	Y	1003	0	467	6	0
26	Z	442	0	190	1	0
27	A	2	0	0	0	0
27	B	1	0	0	0	0
27	C	1	0	0	0	0
27	I	2	0	0	0	0
27	J	1	0	0	0	0
27	L	1	0	0	0	0
27	M	1	0	0	0	0
28	A	1	0	0	0	0
All	All	45091	0	39738	1340	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 (1340) 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	1.57
1:A:867:ILE:CG1	1:A:867:ILE:CD1	1.83	1.52
17:Q:356:TRP:CA	17:Q:392:ALA:HA	1.06	1.51
17:Q:356:TRP:HA	17:Q:392:ALA:CA	0.93	1.39
2:B:1215:ARG:CD	4:D:15:LEU:HD13	1.19	1.39
13:M:274:PRO:HD2	15:O:188:GLU:CD	1.38	1.39
3:C:85:ASP:OD1	25:Y:146:THR:CB	1.73	1.36
17:Q:390:PHE:HA	17:Q:391:THR:CB	1.44	1.35
13:M:274:PRO:CD	15:O:188:GLU:OE2	1.75	1.34
2:B:1217:TYR:CD2	4:D:13:ARG:NH1	1.97	1.32
17:Q:355:THR:O	17:Q:393:ARG:N	1.61	1.31
13:M:274:PRO:CD	15:O:188:GLU:CD	2.01	1.29
1:A:344:ARG:NH2	2:B:1120:GLU:HG3	1.48	1.26
2:B:868:MET:HE3	13:M:182:ARG:CG	1.63	1.25
17:Q:356:TRP:CB	17:Q:392:ALA:HB2	1.65	1.25
13:M:273:SER:HB2	15:O:188:GLU:OE2	1.32	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	1.21
23:W:528:HIS:O	24:X:227:GLY:HA2	1.41	1.19
13:M:248:LEU:HD11	13:M:286:ILE:HD12	1.22	1.18
1:A:420:ARG:NH2	24:X:174:ALA:H	1.44	1.16
1:A:420:ARG:NH1	24:X:174:ALA:HB2	1.60	1.15
2:B:1215:ARG:HD3	4:D:15:LEU:CD1	1.29	1.15
1:A:228:PHE:CZ	4:D:12:ARG:NH1	2.14	1.14
2:B:104:GLU:OE2	12:L:54:ARG:HD3	1.44	1.13
14:N:24:DT:H2"	14:N:25:DA:H5'	1.25	1.13
2:B:868:MET:CE	13:M:182:ARG:CG	2.19	1.13
7:G:1:MET:HE3	7:G:80:LYS:H	1.12	1.13
2:B:1217:TYR:CD2	4:D:13:ARG:CZ	2.17	1.12
1:A:419:LYS:NZ	13:M:48:CYS:HB3	1.65	1.12
17:Q:390:PHE:CA	17:Q:391:THR:CB	2.27	1.11
2:B:1166:CYS:HB2	4:D:15:LEU:HD12	1.23	1.11
1:A:420:ARG:HH22	24:X:174:ALA:N	1.48	1.10
1:A:227:VAL:HG13	4:D:14:ARG:NH2	1.64	1.09
13:M:295:ALA:HB1	13:M:309:ILE:HD11	1.28	1.09
1:A:89:PRO:HG2	1:A:204:THR:HB	1.35	1.08
2:B:1185:CYS:HA	4:D:17:LYS:HD3	1.32	1.08
1:A:836:TYR:OH	1:A:1403:GLU:OE2	1.69	1.08
1:A:496:GLU:CD	7:G:63:PRO:O	1.92	1.08
6:F:100:GLN:HG3	7:G:66:GLY:HA3	1.32	1.07
1:A:78:PRO:O	2:B:1201:LYS:NZ	1.89	1.06
13:M:311:SER:HA	13:M:314:LYS:HE2	1.32	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:PRO:CG	1:A:204:THR:HB	1.88	1.04
1:A:317:LYS:O	2:B:471:LYS:CE	2.06	1.04
13:M:279:VAL:HG23	13:M:298:VAL:HG22	1.39	1.03
13:M:288:LEU:HD21	13:M:339:LEU:HD11	1.35	1.03
2:B:1166:CYS:CB	4:D:15:LEU:HD12	1.89	1.02
17:Q:356:TRP:HA	17:Q:392:ALA:CB	1.88	1.02
2:B:451:LYS:HD2	13:M:138:ASP:OD2	1.59	1.02
2:B:1165:ILE:HG21	4:D:17:LYS:HA	1.35	1.02
17:Q:356:TRP:CB	17:Q:392:ALA:CB	2.37	1.02
1:A:228:PHE:HZ	4:D:12:ARG:NH1	1.56	1.02
6:F:99:LEU:HD21	7:G:65:ASP:HA	1.42	1.02
13:M:279:VAL:HB	13:M:302:LEU:HD22	1.39	1.01
1:A:344:ARG:CZ	2:B:1120:GLU:HG3	1.88	1.01
1:A:227:VAL:HG11	4:D:14:ARG:NE	1.75	1.01
13:M:272:LYS:HE3	20:T:53:DA:P	2.01	1.01
17:Q:356:TRP:CA	17:Q:392:ALA:CA	1.86	1.01
2:B:1166:CYS:HB3	4:D:15:LEU:O	1.61	1.00
23:W:535:VAL:O	23:W:539:ILE:N	1.93	1.00
2:B:902:GLY:O	12:L:65:VAL:HG11	1.59	1.00
1:A:1386:ARG:NH1	1:A:1403:GLU:OE1	1.95	0.99
17:Q:356:TRP:CA	17:Q:392:ALA:CB	2.40	0.99
1:A:344:ARG:HD2	2:B:1118:PRO:O	1.64	0.97
1:A:496:GLU:OE2	7:G:63:PRO:O	1.80	0.97
6:F:99:LEU:HD21	7:G:65:ASP:CA	1.95	0.96
6:F:132:LEU:HD22	7:G:61:ILE:HD12	1.47	0.96
13:M:274:PRO:HD3	15:O:188:GLU:OE1	1.62	0.96
13:M:259:THR:HG23	13:M:323:LEU:HB3	1.43	0.96
1:A:419:LYS:HB3	13:M:47:LEU:O	1.64	0.96
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.27	0.94
13:M:242:PHE:CE1	13:M:302:LEU:HA	2.01	0.94
13:M:274:PRO:HD2	15:O:188:GLU:OE2	0.78	0.94
13:M:186:ALA:HB1	13:M:237:THR:OG1	1.65	0.94
2:B:1185:CYS:CA	4:D:17:LYS:HD3	1.98	0.94
13:M:269:ILE:HG12	13:M:315:ILE:HG21	1.48	0.94
13:M:283:TYR:CZ	13:M:287:LEU:HD11	2.04	0.93
6:F:99:LEU:CD2	7:G:64:THR:O	2.17	0.93
2:B:1215:ARG:CD	4:D:15:LEU:HB2	1.98	0.92
1:A:228:PHE:CE2	4:D:12:ARG:NH1	2.35	0.92
13:M:320:ARG:HE	13:M:336:LEU:HB3	1.32	0.92
17:Q:105:ALA:HB2	18:R:92:LEU:CB	1.98	0.92
1:A:420:ARG:NH1	24:X:174:ALA:CB	2.32	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:286:ILE:HD13	13:M:293:ILE:CG2	1.98	0.92
13:M:279:VAL:CB	13:M:302:LEU:HD22	2.00	0.91
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.52	0.91
1:A:419:LYS:HZ1	13:M:48:CYS:HB3	1.31	0.91
2:B:451:LYS:CE	13:M:138:ASP:OD2	2.19	0.90
13:M:238:TYR:HB3	13:M:242:PHE:CE2	2.06	0.90
13:M:248:LEU:CD1	13:M:286:ILE:HD12	2.00	0.90
13:M:248:LEU:HD13	13:M:252:VAL:HG11	1.54	0.90
2:B:1184:GLY:O	4:D:17:LYS:HD3	1.71	0.90
1:A:420:ARG:HH12	24:X:174:ALA:N	1.70	0.89
2:B:451:LYS:CD	13:M:138:ASP:OD2	2.20	0.89
13:M:273:SER:CB	15:O:188:GLU:OE2	2.20	0.89
23:W:528:HIS:O	24:X:227:GLY:CA	2.20	0.89
2:B:1217:TYR:HD2	4:D:13:ARG:NH1	1.69	0.89
13:M:298:VAL:HG22	13:M:302:LEU:HD13	1.54	0.89
1:A:832:ALA:HA	20:T:15:DA:O4'	1.73	0.88
1:A:420:ARG:HH22	24:X:174:ALA:H	0.89	0.88
13:M:288:LEU:CD2	13:M:339:LEU:HD11	2.02	0.88
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.56	0.88
1:A:417:TYR:CZ	13:M:37:ARG:HD3	2.09	0.88
2:B:1166:CYS:HB2	4:D:15:LEU:CD1	2.04	0.88
13:M:274:PRO:CG	15:O:188:GLU:OE1	2.21	0.88
1:A:420:ARG:HH12	24:X:174:ALA:CA	1.85	0.88
1:A:417:TYR:CE2	13:M:37:ARG:HD3	2.09	0.87
1:A:496:GLU:OE1	7:G:63:PRO:O	1.93	0.87
17:Q:355:THR:O	17:Q:392:ALA:C	2.12	0.87
13:M:242:PHE:HD1	13:M:301:THR:HG22	1.36	0.87
13:M:339:LEU:HB3	13:M:340:PRO:HD2	1.57	0.87
15:O:69:ASN:HB2	20:T:48:DT:O4'	1.74	0.87
6:F:100:GLN:CG	7:G:66:GLY:HA3	2.05	0.87
20:T:49:DA:C2'	20:T:50:DT:H5'	2.03	0.87
13:M:288:LEU:HG	13:M:339:LEU:HD21	1.56	0.87
2:B:104:GLU:OE2	12:L:54:ARG:CD	2.22	0.86
13:M:279:VAL:CG1	13:M:309:ILE:HG22	2.06	0.86
13:M:295:ALA:HB1	13:M:306:GLU:HG3	1.56	0.86
1:A:91:PHE:HB3	1:A:96:ILE:HG13	1.56	0.86
2:B:1215:ARG:HD3	4:D:15:LEU:HD12	1.55	0.86
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.57	0.85
1:A:11:LEU:HD11	2:B:1195:HIS:CD2	2.11	0.85
13:M:295:ALA:CB	13:M:309:ILE:HD11	2.06	0.85
2:B:1185:CYS:HA	4:D:17:LYS:CD	1.99	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:234:GLN:HB2	13:M:236:LEU:CD2	2.07	0.85
13:M:293:ILE:HD13	13:M:297:LYS:HG3	1.60	0.84
1:A:419:LYS:HZ2	13:M:48:CYS:HB3	1.41	0.84
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.59	0.84
13:M:248:LEU:HD21	13:M:286:ILE:HD11	1.58	0.84
1:A:68:GLN:O	1:A:68:GLN:NE2	2.11	0.83
2:B:1215:ARG:HD2	4:D:15:LEU:HB2	1.59	0.83
1:A:420:ARG:NH2	24:X:174:ALA:N	2.15	0.83
13:M:295:ALA:CB	13:M:306:GLU:HG3	2.09	0.83
2:B:416:LEU:HD23	2:B:457:LEU:HD23	1.61	0.83
13:M:279:VAL:HG23	13:M:298:VAL:CG2	2.09	0.83
13:M:311:SER:HA	13:M:314:LYS:CE	2.09	0.83
13:M:66:PHE:O	13:M:78:ARG:NH2	2.12	0.83
13:M:269:ILE:HG23	13:M:272:LYS:HG2	1.61	0.83
13:M:310:LYS:HE3	13:M:342:VAL:HG22	1.58	0.83
13:M:312:GLY:O	13:M:315:ILE:HG22	1.78	0.83
6:F:99:LEU:HD21	7:G:64:THR:O	1.78	0.83
1:A:53:LEU:HD23	1:A:54:ASN:H	1.44	0.83
13:M:266:ILE:CD1	13:M:268:GLU:HB2	2.09	0.82
1:A:344:ARG:NH2	2:B:1120:GLU:CG	2.40	0.82
13:M:269:ILE:HD11	13:M:316:LEU:HD11	1.60	0.82
13:M:273:SER:O	13:M:276:THR:HG22	1.79	0.82
3:C:148:ARG:H	3:C:151:GLN:HG3	1.43	0.82
13:M:275:ILE:HD11	13:M:302:LEU:HB3	1.61	0.82
20:T:49:DA:H2"	20:T:50:DT:H5'	1.61	0.82
23:W:534:ASN:O	23:W:538:ASP:CB	2.28	0.82
13:M:310:LYS:CE	13:M:342:VAL:HG22	2.09	0.82
3:C:148:ARG:HD3	3:C:149:LYS:HG2	1.61	0.81
13:M:315:ILE:CG2	13:M:316:LEU:HD12	2.10	0.81
17:Q:356:TRP:CB	17:Q:392:ALA:CA	2.58	0.81
13:M:269:ILE:HG21	13:M:272:LYS:HB2	1.62	0.81
13:M:238:TYR:HB3	13:M:242:PHE:CD2	2.14	0.81
14:N:24:DT:C2'	14:N:25:DA:H5'	2.09	0.81
2:B:1217:TYR:CE1	4:D:13:ARG:HB2	2.16	0.81
6:F:103:MET:CE	7:G:65:ASP:HB2	2.10	0.81
23:W:535:VAL:O	23:W:539:ILE:CA	2.27	0.81
2:B:849:GLY:HA2	2:B:852:ARG:HD2	1.62	0.81
7:G:1:MET:HE3	7:G:80:LYS:N	1.95	0.81
13:M:234:GLN:O	13:M:237:THR:HG22	1.81	0.81
13:M:305:THR:HG23	13:M:308:THR:H	1.46	0.81
13:M:186:ALA:CB	13:M:237:THR:OG1	2.28	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:279:VAL:CA	13:M:302:LEU:HD22	2.11	0.80
13:M:269:ILE:CD1	13:M:316:LEU:HD11	2.12	0.80
10:J:48:ARG:HE	10:J:49:MET:HE2	1.46	0.80
13:M:279:VAL:HG11	13:M:309:ILE:HG22	1.63	0.80
13:M:336:LEU:HA	13:M:339:LEU:CD1	2.12	0.80
6:F:100:GLN:HG3	7:G:66:GLY:CA	2.10	0.79
1:A:420:ARG:NH1	24:X:174:ALA:N	2.31	0.79
1:A:836:TYR:HH	1:A:1403:GLU:CD	1.83	0.79
1:A:89:PRO:HB2	1:A:204:THR:CG2	2.13	0.79
13:M:286:ILE:HD13	13:M:293:ILE:HG22	1.64	0.79
13:M:325:ASP:OD1	13:M:328:LEU:HB2	1.81	0.79
2:B:1165:ILE:CG2	4:D:17:LYS:HA	2.12	0.79
13:M:248:LEU:HD23	13:M:291:ILE:CD1	2.12	0.79
6:F:132:LEU:HD22	7:G:61:ILE:CD1	2.13	0.79
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.64	0.79
2:B:451:LYS:CE	13:M:138:ASP:CG	2.50	0.79
2:B:451:LYS:NZ	13:M:138:ASP:OD1	2.15	0.79
13:M:286:ILE:HG21	13:M:293:ILE:HG22	1.65	0.79
1:A:228:PHE:HZ	4:D:12:ARG:CZ	1.95	0.79
2:B:451:LYS:HE3	13:M:138:ASP:CG	2.04	0.79
23:W:535:VAL:O	23:W:539:ILE:CB	2.31	0.78
1:A:55:ASP:HA	1:A:58:LEU:HB2	1.63	0.78
2:B:900:ALA:HB3	12:L:61:THR:HG23	1.64	0.78
13:M:277:ILE:O	13:M:280:VAL:HG22	1.83	0.78
3:C:147:LEU:HB3	3:C:151:GLN:HB2	1.66	0.78
13:M:296:ALA:O	13:M:300:GLN:HG3	1.83	0.78
13:M:310:LYS:CD	13:M:342:VAL:HG22	2.13	0.78
13:M:248:LEU:HD21	13:M:286:ILE:CD1	2.14	0.77
13:M:315:ILE:HG23	13:M:316:LEU:HD12	1.64	0.77
2:B:108:VAL:HG13	13:M:240:PRO:HB2	1.64	0.77
2:B:451:LYS:NZ	13:M:138:ASP:CG	2.37	0.77
1:A:95:PHE:O	1:A:96:ILE:C	2.13	0.77
13:M:287:LEU:HD13	13:M:340:PRO:HG3	1.65	0.77
6:F:99:LEU:HD22	7:G:64:THR:O	1.83	0.77
13:M:330:ALA:HB1	13:M:334:VAL:O	1.84	0.77
2:B:1189:ILE:HG21	7:G:41:LYS:HB2	1.65	0.77
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.65	0.77
2:B:1166:CYS:HA	4:D:15:LEU:HA	1.65	0.77
13:M:269:ILE:HG21	13:M:277:ILE:CD1	2.14	0.77
13:M:249:PRO:HD3	13:M:291:ILE:HD11	1.66	0.76
13:M:311:SER:CA	13:M:314:LYS:HE2	2.13	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.67	0.76
1:A:1433:MET:CE	2:B:1145:SER:OG	2.33	0.76
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.66	0.76
20:T:47:DA:N7	20:T:48:DT:O4	2.19	0.76
6:F:132:LEU:CD2	7:G:61:ILE:CD1	2.62	0.76
2:B:1215:ARG:CG	4:D:15:LEU:HD13	2.14	0.76
2:B:1217:TYR:HB2	4:D:13:ARG:CZ	2.16	0.76
2:B:449:ASN:ND2	13:M:135:MET:HG3	1.99	0.75
13:M:320:ARG:NE	13:M:336:LEU:HB3	2.00	0.75
1:A:22:PHE:HB2	2:B:1211:ASN:CG	2.06	0.75
2:B:1184:GLY:O	4:D:17:LYS:CD	2.34	0.75
20:T:48:DT:H2'	20:T:49:DA:C8	2.21	0.75
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.66	0.75
1:A:497:THR:HG22	2:B:1146:PHE:HD1	1.52	0.75
17:Q:356:TRP:C	17:Q:392:ALA:HA	2.03	0.75
1:A:1390:ASN:O	1:A:1399:ARG:CD	2.34	0.75
2:B:902:GLY:O	12:L:65:VAL:CG1	2.36	0.74
13:M:286:ILE:HD13	13:M:293:ILE:CB	2.16	0.74
1:A:419:LYS:HG2	13:M:48:CYS:HA	1.68	0.74
13:M:272:LYS:CE	20:T:53:DA:P	2.76	0.74
1:A:418:SER:HA	13:M:48:CYS:C	2.07	0.74
1:A:420:ARG:NH1	24:X:174:ALA:CA	2.50	0.74
13:M:248:LEU:HA	13:M:291:ILE:HD11	1.69	0.74
1:A:836:TYR:CZ	1:A:1403:GLU:OE2	2.41	0.74
1:A:89:PRO:HG2	1:A:204:THR:CB	2.16	0.74
1:A:132:LYS:HZ2	1:A:1415:SER:CB	2.01	0.73
2:B:868:MET:HE3	13:M:182:ARG:HG2	0.76	0.73
13:M:249:PRO:CD	13:M:291:ILE:HD11	2.18	0.73
13:M:293:ILE:HD11	13:M:297:LYS:HB2	1.67	0.73
1:A:418:SER:CA	13:M:49:GLY:HA3	2.17	0.73
2:B:792:MET:HE2	20:T:21:DT:OP1	1.88	0.73
13:M:290:GLN:NE2	13:M:291:ILE:HG23	2.03	0.73
13:M:321:ASP:OD1	13:M:336:LEU:HD13	1.89	0.73
1:A:16:GLU:HB2	4:D:13:ARG:NH2	2.03	0.73
2:B:1217:TYR:CE2	4:D:13:ARG:NH1	2.47	0.73
13:M:275:ILE:CD1	13:M:302:LEU:HB3	2.19	0.73
13:M:290:GLN:CD	13:M:291:ILE:HG23	2.08	0.73
1:A:227:VAL:HG13	4:D:14:ARG:HH21	1.50	0.73
1:A:419:LYS:NZ	13:M:27:CYS:SG	2.62	0.72
1:A:228:PHE:HE2	4:D:12:ARG:HH12	1.35	0.72
2:B:1125:ASP:OD2	13:M:39:SER:O	2.07	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:O	1:A:52:GLY:N	2.23	0.72
13:M:233:ALA:HB1	13:M:237:THR:HG21	1.70	0.72
2:B:868:MET:O	13:M:182:ARG:NH2	2.21	0.72
1:A:91:PHE:HB2	1:A:96:ILE:HD11	1.72	0.72
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.72	0.72
1:A:91:PHE:HB3	1:A:96:ILE:CG1	2.18	0.72
13:M:335:SER:O	13:M:339:LEU:HD12	1.89	0.72
1:A:227:VAL:HG11	4:D:14:ARG:HB3	1.70	0.72
2:B:952:VAL:O	12:L:58:LYS:HB2	1.88	0.72
1:A:317:LYS:O	2:B:471:LYS:HE3	1.89	0.72
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.71	0.72
13:M:275:ILE:HD12	13:M:304:VAL:CG2	2.20	0.72
2:B:1198:TYR:CE2	2:B:1201:LYS:HE3	2.25	0.72
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.71	0.72
19:S:23:ARG:O	19:S:27:VAL:N	2.23	0.72
13:M:287:LEU:CD1	13:M:340:PRO:HG3	2.20	0.72
1:A:35:ILE:HA	1:A:52:GLY:O	1.89	0.71
4:D:123:LEU:HD11	4:D:146:GLN:HG2	1.72	0.71
13:M:274:PRO:CG	15:O:188:GLU:CD	2.57	0.71
13:M:286:ILE:HD13	13:M:293:ILE:HB	1.72	0.71
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.72	0.71
4:D:134:THR:HG23	4:D:136:GLY:H	1.56	0.71
13:M:342:VAL:HG13	13:M:343:GLU:N	2.06	0.71
2:B:429:PHE:HA	2:B:432:MET:HE2	1.73	0.71
1:A:418:SER:HA	13:M:48:CYS:O	1.90	0.70
2:B:563:MET:HE2	2:B:580:VAL:HB	1.72	0.70
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.72	0.70
2:B:1184:GLY:C	4:D:17:LYS:HD3	2.11	0.70
1:A:418:SER:HA	13:M:49:GLY:HA3	1.72	0.70
3:C:66:ARG:NH2	10:J:3:VAL:O	2.23	0.70
1:A:831:THR:HG23	20:T:15:DA:C5	2.27	0.70
20:T:46:DT:H2"	20:T:47:DA:O5'	1.91	0.70
1:A:346:ASP:OD1	2:B:1106:ARG:NE	2.21	0.70
1:A:417:TYR:CE2	13:M:37:ARG:CD	2.75	0.70
17:Q:355:THR:O	17:Q:392:ALA:CA	2.39	0.70
13:M:242:PHE:CD1	13:M:301:THR:HG22	2.24	0.69
2:B:1133:MET:SD	20:T:16:DT:H4'	2.32	0.69
5:E:185:ALA:HA	5:E:190:LEU:HD12	1.74	0.69
1:A:420:ARG:NH2	24:X:173:ALA:HA	2.07	0.69
13:M:286:ILE:CD1	13:M:293:ILE:HB	2.22	0.69
1:A:53:LEU:CD2	1:A:54:ASN:H	2.06	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:THR:HA	1:A:143:LYS:HE2	1.75	0.69
1:A:227:VAL:CG1	4:D:14:ARG:NE	2.36	0.69
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.74	0.69
1:A:831:THR:CG2	20:T:15:DA:C5	2.75	0.69
2:B:792:MET:HE2	20:T:21:DT:P	2.33	0.69
4:D:12:ARG:HD3	4:D:14:ARG:HG2	1.74	0.69
13:M:243:CYS:SG	13:M:253:THR:HG22	2.32	0.69
13:M:274:PRO:HG3	15:O:188:GLU:OE1	1.92	0.69
1:A:344:ARG:HA	2:B:1128:LEU:O	1.93	0.69
2:B:868:MET:O	13:M:182:ARG:CZ	2.40	0.69
17:Q:356:TRP:N	17:Q:392:ALA:HA	2.02	0.69
1:A:16:GLU:OE1	4:D:13:ARG:NH2	2.26	0.68
1:A:412:ARG:HB3	13:M:51:VAL:CG1	2.23	0.68
13:M:334:VAL:HA	13:M:338:ASN:HD21	1.58	0.68
1:A:320:ARG:NH2	13:M:81:GLU:HG3	2.08	0.68
13:M:294:THR:H	13:M:297:LYS:HG3	1.57	0.68
13:M:235:ASN:HD22	13:M:260:ALA:HB3	1.58	0.68
13:M:261:LYS:HG3	13:M:262:LYS:N	2.09	0.68
13:M:283:TYR:O	13:M:287:LEU:HG	1.93	0.68
2:B:868:MET:HE2	13:M:182:ARG:CG	2.20	0.68
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.74	0.68
13:M:334:VAL:HA	13:M:338:ASN:ND2	2.09	0.68
17:Q:355:THR:O	17:Q:392:ALA:HB1	1.94	0.68
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.76	0.68
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.75	0.68
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.75	0.68
1:A:419:LYS:HE3	13:M:47:LEU:C	2.15	0.67
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.59	0.67
13:M:306:GLU:HA	13:M:309:ILE:HG12	1.76	0.67
2:B:1217:TYR:HD2	4:D:13:ARG:CZ	1.93	0.67
13:M:324:VAL:CG2	13:M:328:LEU:HD22	2.24	0.67
1:A:420:ARG:HH22	24:X:173:ALA:HA	1.59	0.67
17:Q:358:GLY:HA2	17:Q:391:THR:CB	2.22	0.67
20:T:47:DA:C8	20:T:48:DT:O4	2.47	0.67
13:M:269:ILE:HG21	13:M:277:ILE:HD11	1.76	0.67
2:B:868:MET:CE	13:M:182:ARG:CD	2.73	0.67
1:A:420:ARG:CZ	24:X:174:ALA:N	2.57	0.67
1:A:496:GLU:OE1	7:G:64:THR:HA	1.94	0.67
13:M:269:ILE:HD11	13:M:316:LEU:CD1	2.23	0.67
13:M:70:ASP:HB3	13:M:78:ARG:HD2	1.75	0.67
1:A:420:ARG:CZ	24:X:174:ALA:H	2.06	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:48:DT:H2'	20:T:49:DA:N7	2.08	0.67
13:M:284:LEU:CD1	13:M:339:LEU:HD22	2.24	0.66
2:B:1215:ARG:CD	4:D:15:LEU:CD1	2.05	0.66
4:D:8:PHE:HD2	7:G:6:ASP:HB2	1.61	0.66
1:A:388:LEU:O	1:A:392:VAL:HG23	1.96	0.66
1:A:871:ASP:HB3	5:E:204:THR:HG23	1.76	0.66
13:M:242:PHE:O	13:M:246:LEU:HG	1.96	0.66
21:U:86:PHE:O	21:U:90:LEU:N	2.28	0.66
1:A:347:PHE:HE1	1:A:375:THR:HG22	1.60	0.66
13:M:290:GLN:HB3	13:M:331:ASN:ND2	2.11	0.66
1:A:1442:ASP:HB2	6:F:137:TYR:HE1	1.61	0.66
13:M:293:ILE:HG12	13:M:297:LYS:HD3	1.78	0.66
2:B:1165:ILE:HB	4:D:17:LYS:HB3	1.78	0.66
3:C:259:LEU:HD22	11:K:91:CYS:HB3	1.75	0.66
1:A:419:LYS:HZ2	13:M:48:CYS:CB	2.08	0.65
13:M:283:TYR:CE2	13:M:287:LEU:HD11	2.31	0.65
1:A:46:THR:HG22	1:A:47:ARG:H	1.61	0.65
1:A:316:GLN:O	1:A:318:SER:N	2.30	0.65
13:M:243:CYS:CB	13:M:253:THR:HG22	2.26	0.65
1:A:311:GLN:HG3	1:A:312:PRO:HD2	1.77	0.65
2:B:296:GLU:O	2:B:300:HIS:HD2	1.80	0.65
13:M:272:LYS:HB3	13:M:276:THR:HG21	1.77	0.65
13:M:269:ILE:CG1	13:M:315:ILE:HG21	2.25	0.65
2:B:868:MET:HE1	13:M:182:ARG:HG2	1.64	0.65
14:N:24:DT:H2"	14:N:25:DA:C5'	2.17	0.65
1:A:15:LYS:NZ	2:B:1220:ARG:HE	1.93	0.65
2:B:872:GLU:HG2	2:B:916:THR:HG22	1.78	0.65
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.26	0.65
17:Q:409:ASP:HA	17:Q:411:LYS:O	1.97	0.65
6:F:103:MET:HE3	7:G:65:ASP:HB2	1.77	0.65
13:M:311:SER:O	13:M:314:LYS:HD3	1.97	0.65
1:A:57:ARG:O	1:A:68:GLN:HG2	1.96	0.65
2:B:857:ARG:NH1	2:B:945:GLU:OE2	2.29	0.65
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.79	0.65
3:C:56:THR:HG21	3:C:145:CYS:SG	2.37	0.65
13:M:269:ILE:HD12	13:M:277:ILE:HD12	1.79	0.65
13:M:275:ILE:HD13	13:M:275:ILE:O	1.97	0.65
1:A:832:ALA:HB2	20:T:15:DA:C8	2.32	0.65
4:D:51:ASN:ND2	4:D:54:GLU:OE1	2.30	0.64
13:M:255:SER:OG	13:M:328:LEU:HD13	1.96	0.64
1:A:204:THR:HG22	1:A:235:ILE:HG21	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:286:ILE:HG12	13:M:292:PRO:HA	1.78	0.64
2:B:868:MET:HE2	13:M:182:ARG:CD	2.27	0.64
2:B:68:THR:HG22	2:B:91:SER:HA	1.80	0.64
13:M:269:ILE:CD1	13:M:277:ILE:HD12	2.28	0.64
2:B:917:PRO:HA	2:B:934:LYS:HB3	1.80	0.64
1:A:416:ARG:NH2	13:M:40:GLU:HG2	2.13	0.64
19:S:125:PHE:HA	19:S:155:ILE:O	1.98	0.64
13:M:275:ILE:HD12	13:M:304:VAL:HG21	1.80	0.64
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.79	0.63
2:B:806:THR:HG22	2:B:808:ALA:H	1.63	0.63
6:F:99:LEU:HD23	7:G:66:GLY:N	2.13	0.63
13:M:235:ASN:ND2	13:M:260:ALA:HB3	2.13	0.63
21:U:143:GLU:O	21:U:146:GLU:N	2.31	0.63
1:A:447:GLN:NE2	20:T:17:DG:H4'	2.13	0.63
12:L:28:LYS:HB2	12:L:39:SER:HA	1.80	0.63
23:W:534:ASN:O	23:W:538:ASP:N	2.30	0.63
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.81	0.63
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.81	0.63
1:A:417:TYR:HE2	13:M:37:ARG:HG3	1.64	0.63
2:B:1185:CYS:HA	4:D:17:LYS:HB2	1.81	0.63
13:M:242:PHE:CG	13:M:302:LEU:HG	2.34	0.63
13:M:288:LEU:O	13:M:334:VAL:HG23	1.98	0.63
13:M:335:SER:H	13:M:338:ASN:ND2	1.96	0.63
1:A:1433:MET:HE2	2:B:1145:SER:OG	1.97	0.63
3:C:10:ILE:HD12	11:K:108:GLU:HB3	1.81	0.63
2:B:841:MET:HB3	2:B:846:ILE:HD11	1.81	0.62
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.79	0.62
13:M:313:TYR:HD2	13:M:343:GLU:N	1.97	0.62
2:B:1184:GLY:O	4:D:17:LYS:CE	2.48	0.62
13:M:291:ILE:O	13:M:291:ILE:HG13	1.99	0.62
18:R:60:ASP:CB	18:R:213:ALA:HA	2.29	0.62
13:M:287:LEU:O	13:M:334:VAL:HG21	2.00	0.62
13:M:319:HIS:O	13:M:323:LEU:HG	2.00	0.62
20:T:49:DA:H2'	20:T:50:DT:H5'	1.80	0.62
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.82	0.62
1:A:89:PRO:CB	1:A:204:THR:HB	2.29	0.62
20:T:21:DT:H2"	20:T:22:DT:H5'	1.81	0.62
1:A:5:GLN:HG3	2:B:1175:LEU:HD11	1.82	0.62
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.80	0.62
1:A:420:ARG:CZ	24:X:174:ALA:HB2	2.28	0.62
2:B:1215:ARG:HD3	4:D:15:LEU:HD13	0.62	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:271:GLY:O	20:T:52:DC:H4'	1.99	0.62
1:A:11:LEU:CD1	2:B:1195:HIS:CD2	2.82	0.62
13:M:269:ILE:CG2	13:M:272:LYS:HB2	2.30	0.62
13:M:304:VAL:HG12	13:M:305:THR:N	2.15	0.62
13:M:310:LYS:HD3	13:M:342:VAL:HG22	1.82	0.61
17:Q:394:ASN:CB	17:Q:395:LYS:HA	2.30	0.61
1:A:344:ARG:CZ	2:B:1120:GLU:CG	2.74	0.61
1:A:22:PHE:N	2:B:1211:ASN:O	2.32	0.61
2:B:486:TYR:HB3	2:B:1096:ARG:CZ	2.31	0.61
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.82	0.61
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.83	0.61
13:M:279:VAL:HG13	13:M:309:ILE:HG22	1.78	0.61
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.83	0.61
13:M:256:ALA:HA	13:M:285:ASN:HD22	1.65	0.61
13:M:266:ILE:HD11	13:M:268:GLU:HB2	1.80	0.61
13:M:294:THR:N	13:M:297:LYS:HG3	2.16	0.61
1:A:420:ARG:HH22	24:X:173:ALA:CA	2.14	0.61
1:A:1390:ASN:O	1:A:1399:ARG:HG2	2.01	0.61
4:D:12:ARG:NH2	4:D:13:ARG:O	2.34	0.61
13:M:294:THR:H	13:M:297:LYS:CG	2.13	0.61
1:A:91:PHE:CB	1:A:96:ILE:HD11	2.30	0.61
2:B:249:ARG:HH12	2:B:418:LYS:HD2	1.66	0.61
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.82	0.61
3:C:11:ARG:HH21	3:C:229:TYR:HD2	1.48	0.61
1:A:66:LYS:HE2	1:A:68:GLN:H	1.65	0.61
13:M:324:VAL:HG22	13:M:325:ASP:N	2.15	0.61
1:A:419:LYS:NZ	13:M:48:CYS:CB	2.52	0.61
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.83	0.61
13:M:262:LYS:O	13:M:266:ILE:HG12	2.01	0.61
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.83	0.60
1:A:72:GLU:HB3	1:A:76:GLU:HB3	1.83	0.60
1:A:132:LYS:NZ	1:A:1415:SER:CB	2.64	0.60
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.81	0.60
13:M:280:VAL:HG12	13:M:309:ILE:O	2.01	0.60
1:A:448:PRO:O	1:A:449:SER:HB2	2.01	0.60
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.82	0.60
13:M:293:ILE:HD13	13:M:297:LYS:CG	2.29	0.60
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.83	0.60
2:B:1185:CYS:N	4:D:17:LYS:HD3	2.16	0.60
2:B:1215:ARG:CD	4:D:15:LEU:CB	2.65	0.60
2:B:205:ILE:HD11	2:B:461:LEU:HD13	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:PRO:HB2	1:A:204:THR:HG21	1.83	0.60
13:M:293:ILE:HD11	13:M:297:LYS:CB	2.31	0.60
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.83	0.60
4:D:52:LEU:O	4:D:54:GLU:N	2.34	0.60
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.82	0.60
13:M:336:LEU:HA	13:M:339:LEU:HD13	1.83	0.60
2:B:911:ILE:HD11	2:B:941:LEU:HD12	1.82	0.60
5:E:202:SER:HB3	5:E:205:SER:H	1.66	0.60
13:M:324:VAL:HG23	13:M:328:LEU:HD22	1.83	0.60
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.36	0.60
17:Q:105:ALA:HB3	18:R:90:GLN:O	2.01	0.60
2:B:976:ILE:O	2:B:990:ILE:HB	2.02	0.60
1:A:419:LYS:HE3	13:M:48:CYS:N	2.17	0.59
13:M:255:SER:HB3	13:M:285:ASN:OD1	2.01	0.59
19:S:17:ILE:O	19:S:21:GLY:N	2.34	0.59
1:A:418:SER:HA	13:M:49:GLY:CA	2.32	0.59
1:A:629:LEU:O	1:A:633:VAL:HG23	2.02	0.59
1:A:839:ARG:NH2	1:A:1401:SER:O	2.35	0.59
1:A:1063:MET:SD	1:A:1436:ILE:HB	2.41	0.59
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.34	0.59
2:B:363:HIS:O	2:B:364:ILE:HB	2.02	0.59
2:B:1184:GLY:O	4:D:17:LYS:HE2	2.02	0.59
3:C:184:ASN:HD21	3:C:189:THR:H	1.50	0.59
5:E:4:GLU:HB3	5:E:7:ARG:NE	2.16	0.59
12:L:61:THR:HG21	12:L:63:ARG:HG2	1.84	0.59
1:A:1387:HIS:O	1:A:1391:ARG:HG2	2.02	0.59
12:L:47:ARG:HH21	12:L:54:ARG:HH21	1.50	0.59
20:T:48:DT:C2'	20:T:49:DA:C8	2.86	0.59
1:A:53:LEU:HD23	1:A:54:ASN:N	2.15	0.59
8:H:82:PRO:C	8:H:84:ALA:H	2.05	0.59
20:T:47:DA:H2'	20:T:48:DT:C5	2.38	0.59
21:U:129:VAL:O	21:U:133:SER:N	2.36	0.59
1:A:22:PHE:CB	2:B:1211:ASN:OD1	2.50	0.59
1:A:412:ARG:HB3	13:M:51:VAL:HG11	1.83	0.59
1:A:857:ARG:HD3	1:A:861:GLY:O	2.03	0.59
2:B:950:ASP:HB3	2:B:967:ARG:HG2	1.84	0.59
13:M:197:HIS:H	13:M:198:VAL:HA	1.67	0.59
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.85	0.59
13:M:248:LEU:HD23	13:M:291:ILE:HD12	1.85	0.59
1:A:420:ARG:HH22	24:X:173:ALA:C	2.05	0.58
6:F:132:LEU:CD2	7:G:61:ILE:HD12	2.24	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:47:PHE:HB3	8:H:95:TYR:CD2	2.38	0.58
1:A:483:ASP:HB2	2:B:987:LYS:HE3	1.84	0.58
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.84	0.58
14:N:22:DT:C2'	14:N:23:DA:H5'	2.33	0.58
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.86	0.58
13:M:320:ARG:HE	13:M:336:LEU:CB	2.13	0.58
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.85	0.58
1:A:588:LEU:HD23	1:A:607:ILE:HD12	1.86	0.58
1:A:836:TYR:CE1	1:A:1403:GLU:OE2	2.57	0.58
7:G:1:MET:CE	7:G:80:LYS:H	2.02	0.58
4:D:148:LEU:O	4:D:152:SER:OG	2.17	0.58
1:A:68:GLN:O	1:A:70:CYS:N	2.31	0.58
1:A:831:THR:CG2	20:T:15:DA:C6	2.87	0.58
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.84	0.58
2:B:1217:TYR:CE1	4:D:13:ARG:CB	2.86	0.58
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.36	0.58
2:B:451:LYS:HE3	13:M:138:ASP:OD2	1.99	0.58
4:D:67:ARG:HH21	4:D:129:LEU:HD13	1.68	0.58
1:A:228:PHE:CZ	4:D:12:ARG:NH2	2.71	0.57
1:A:417:TYR:CZ	13:M:37:ARG:CD	2.85	0.57
4:D:23:ASN:N	4:D:23:ASN:OD1	2.36	0.57
2:B:810:GLU:HA	2:B:815:ARG:HH12	1.69	0.57
4:D:8:PHE:CZ	4:D:37:GLN:HB2	2.40	0.57
14:N:61:DC:H2'	14:N:62:DA:C8	2.40	0.57
1:A:95:PHE:C	1:A:97:ALA:N	2.54	0.57
1:A:93:VAL:HA	1:A:96:ILE:HD12	1.86	0.57
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.85	0.57
1:A:344:ARG:CD	2:B:1118:PRO:O	2.47	0.57
13:M:269:ILE:HG23	13:M:272:LYS:CG	2.33	0.57
13:M:310:LYS:HE3	13:M:342:VAL:CG2	2.32	0.57
13:M:329:ILE:HG23	13:M:329:ILE:O	2.05	0.57
13:M:334:VAL:CA	13:M:338:ASN:HD21	2.17	0.57
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.87	0.57
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.87	0.57
6:F:105:ALA:HB2	7:G:15:PRO:CB	2.34	0.57
13:M:334:VAL:HA	13:M:338:ASN:OD1	2.05	0.57
4:D:52:LEU:HB3	4:D:148:LEU:HD23	1.85	0.56
13:M:288:LEU:CG	13:M:339:LEU:HD21	2.30	0.56
20:T:50:DT:H2"	20:T:51:DA:H5'	1.87	0.56
1:A:1390:ASN:O	1:A:1399:ARG:HD3	2.04	0.56
13:M:284:LEU:HD11	13:M:339:LEU:HD22	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:140:LEU:CB	21:U:141:LYS:HA	2.35	0.56
2:B:65:GLU:OE1	2:B:247:GLY:HA2	2.04	0.56
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.87	0.56
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.87	0.56
6:F:99:LEU:CD2	7:G:65:ASP:C	2.73	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
13:M:290:GLN:O	13:M:292:PRO:HD3	2.05	0.56
1:A:228:PHE:CZ	4:D:12:ARG:CZ	2.78	0.56
13:M:324:VAL:HG21	13:M:328:LEU:CD2	2.36	0.56
11:K:57:LEU:HB2	11:K:76:GLN:HG2	1.88	0.56
13:M:237:THR:HG23	13:M:238:TYR:N	2.21	0.56
2:B:868:MET:HE3	13:M:182:ARG:CD	2.35	0.56
13:M:248:LEU:HD23	13:M:291:ILE:HD11	1.85	0.56
17:Q:355:THR:O	17:Q:392:ALA:CB	2.53	0.56
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.70	0.56
1:A:419:LYS:CB	13:M:47:LEU:O	2.48	0.56
13:M:276:THR:O	13:M:280:VAL:HG13	2.06	0.56
1:A:74:MET:O	2:B:1116:ARG:NH2	2.39	0.56
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.88	0.56
1:A:417:TYR:HE2	13:M:37:ARG:CG	2.18	0.56
1:A:418:SER:CA	13:M:48:CYS:O	2.53	0.56
13:M:242:PHE:CD2	13:M:302:LEU:HG	2.41	0.56
13:M:242:PHE:CZ	13:M:302:LEU:HA	2.40	0.56
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.88	0.56
2:B:868:MET:HE2	13:M:182:ARG:NE	2.20	0.56
2:B:54:PHE:HA	2:B:58:THR:HB	1.88	0.56
13:M:305:THR:CG2	13:M:308:THR:HG23	2.36	0.56
2:B:792:MET:CE	20:T:21:DT:P	2.94	0.55
13:M:266:ILE:HD12	13:M:268:GLU:HB2	1.88	0.55
13:M:295:ALA:HA	13:M:298:VAL:HG12	1.87	0.55
1:A:5:GLN:HG3	2:B:1175:LEU:CD1	2.35	0.55
1:A:416:ARG:HH22	13:M:40:GLU:HG2	1.71	0.55
2:B:1217:TYR:HB2	4:D:13:ARG:NH2	2.21	0.55
23:W:234:GLU:HA	23:W:237:GLY:H	1.71	0.55
1:A:67:CYS:SG	1:A:77:CYS:SG	3.04	0.55
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.87	0.55
2:B:1124:ARG:HD3	13:M:61:SER:HB3	1.87	0.55
4:D:188:ALA:HB2	4:D:208:GLU:HG3	1.87	0.55
23:W:653:THR:O	23:W:657:ALA:N	2.39	0.55
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:89:GLU:O	6:F:93:ILE:HD12	2.06	0.55
1:A:257:ARG:HH11	1:A:257:ARG:HB2	1.71	0.55
1:A:608:ILE:HD12	1:A:613:ILE:HD13	1.89	0.55
1:A:1015:VAL:HG13	1:A:1019:CYS:SG	2.47	0.55
3:C:260:LEU:HD13	25:Y:14:PRO:CB	2.37	0.55
13:M:273:SER:HB2	13:M:274:PRO:HD2	1.86	0.55
13:M:279:VAL:HB	13:M:302:LEU:CD2	2.27	0.55
1:A:18:GLN:HG2	1:A:1418:LEU:HD13	1.89	0.55
1:A:228:PHE:HZ	4:D:12:ARG:NH2	2.03	0.55
13:M:284:LEU:HD12	13:M:339:LEU:HD22	1.88	0.55
1:A:344:ARG:CA	2:B:1128:LEU:O	2.55	0.55
6:F:100:GLN:NE2	7:G:66:GLY:O	2.37	0.55
6:F:109:VAL:HG23	6:F:127:GLU:OE1	2.07	0.55
10:J:1:MET:HB2	10:J:56:LEU:HB2	1.89	0.55
13:M:272:LYS:HE3	20:T:53:DA:OP1	2.06	0.55
13:M:304:VAL:HG12	13:M:305:THR:H	1.72	0.55
1:A:10:PRO:HG2	2:B:1192:TYR:HA	1.89	0.55
1:A:497:THR:HG23	2:B:1146:PHE:HA	1.89	0.55
2:B:343:ILE:O	2:B:344:LYS:HB2	2.07	0.55
2:B:486:TYR:HB3	2:B:1096:ARG:NH2	2.22	0.55
13:M:279:VAL:HA	13:M:302:LEU:HD22	1.88	0.55
13:M:294:THR:H	13:M:297:LYS:CD	2.20	0.55
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.89	0.55
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.88	0.55
1:A:228:PHE:CZ	4:D:14:ARG:HA	2.42	0.54
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.88	0.54
6:F:105:ALA:HB2	7:G:15:PRO:HB3	1.89	0.54
23:W:312:ILE:HA	23:W:315:SER:CB	2.36	0.54
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.90	0.54
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.40	0.54
2:B:1100:ASP:OD2	11:K:1:MET:HB3	2.08	0.54
15:O:169:PRO:HG2	15:O:240:MET:SD	2.47	0.54
2:B:405:ARG:NH2	2:B:629:ASP:OD2	2.40	0.54
17:Q:394:ASN:CB	17:Q:395:LYS:CA	2.86	0.54
4:D:35:LEU:HA	4:D:47:LEU:HB2	1.90	0.54
13:M:269:ILE:HG22	13:M:269:ILE:O	2.06	0.54
1:A:418:SER:CB	13:M:48:CYS:O	2.55	0.54
2:B:451:LYS:NZ	13:M:138:ASP:OD2	2.40	0.54
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.90	0.54
1:A:42:ASP:OD1	1:A:46:THR:N	2.41	0.54
2:B:338:GLY:CA	2:B:339:THR:HB	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:118:LEU:O	6:F:122:MET:HG3	2.06	0.54
13:M:58:ASP:O	13:M:62:GLU:HB2	2.08	0.54
13:M:268:GLU:HG2	13:M:316:LEU:HA	1.89	0.54
13:M:272:LYS:HD2	20:T:52:DC:H3'	1.89	0.54
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.90	0.54
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.88	0.54
13:M:75:ASP:HB3	13:M:78:ARG:HB3	1.89	0.54
13:M:243:CYS:HB3	13:M:253:THR:HG22	1.89	0.54
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.89	0.54
2:B:451:LYS:HZ2	13:M:138:ASP:CG	2.09	0.54
13:M:254:THR:CG2	13:M:258:TYR:HE2	2.19	0.54
1:A:33:ALA:HA	1:A:57:ARG:HD3	1.89	0.54
1:A:338:GLY:HA2	2:B:1129:ARG:NH2	2.23	0.54
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.72	0.54
1:A:1397:LEU:HB3	1:A:1429:ILE:HD12	1.90	0.54
1:A:1399:ARG:HB3	1:A:1408:ILE:HD13	1.89	0.54
7:G:153:GLN:O	7:G:155:SER:N	2.41	0.54
13:M:315:ILE:HG22	13:M:316:LEU:HD12	1.88	0.54
5:E:19:VAL:O	5:E:23:VAL:HG23	2.09	0.54
10:J:24:LEU:O	10:J:30:LEU:HB2	2.08	0.54
1:A:34:LYS:H	1:A:57:ARG:HH11	1.55	0.53
1:A:179:LEU:HD13	1:A:297:GLN:HG3	1.91	0.53
1:A:204:THR:HG22	1:A:235:ILE:CG2	2.37	0.53
1:A:320:ARG:HG2	1:A:321:PRO:HD2	1.89	0.53
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.73	0.53
1:A:658:LEU:HD23	1:A:659:HIS:NE2	2.23	0.53
3:C:73:GLN:O	3:C:129:ILE:HA	2.08	0.53
6:F:103:MET:HE1	7:G:65:ASP:HB2	1.89	0.53
13:M:236:LEU:HD23	13:M:237:THR:N	2.23	0.53
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.90	0.53
13:M:289:PHE:HA	13:M:331:ASN:OD1	2.07	0.53
1:A:345:VAL:N	2:B:1128:LEU:O	2.39	0.53
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.08	0.53
13:M:186:ALA:HB1	13:M:237:THR:HG1	1.69	0.53
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.42	0.53
13:M:286:ILE:HG23	13:M:287:LEU:N	2.24	0.53
1:A:228:PHE:CE1	4:D:15:LEU:HB3	2.44	0.53
1:A:22:PHE:HB3	2:B:1211:ASN:OD1	2.09	0.53
6:F:132:LEU:CD2	7:G:61:ILE:HD11	2.39	0.53
13:M:249:PRO:HD2	13:M:291:ILE:HD11	1.91	0.53
13:M:269:ILE:HG12	13:M:315:ILE:CG2	2.31	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:298:VAL:HG13	13:M:299:GLY:N	2.24	0.53
1:A:23:SER:HB2	1:A:233:TRP:CE2	2.44	0.53
1:A:320:ARG:HH22	13:M:81:GLU:HG3	1.74	0.53
1:A:412:ARG:CB	13:M:51:VAL:HG11	2.38	0.53
1:A:1116:LEU:H	1:A:1308:THR:HB	1.73	0.53
1:A:1390:ASN:O	1:A:1399:ARG:CG	2.57	0.53
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.90	0.53
2:B:174:LEU:HD11	2:B:204:ILE:HG13	1.91	0.53
2:B:295:GLY:HA2	2:B:298:LEU:HB2	1.91	0.53
3:C:164:ALA:HA	3:C:167:HIS:O	2.09	0.53
13:M:294:THR:H	13:M:297:LYS:HD2	1.74	0.53
1:A:253:ASN:O	1:A:255:SER:N	2.38	0.53
2:B:438:GLU:HG3	2:B:440:HIS:HB2	1.91	0.53
17:Q:356:TRP:CB	17:Q:391:THR:C	2.74	0.53
1:A:12:ARG:NH1	2:B:1218:THR:OG1	2.43	0.52
1:A:340:LEU:HD21	2:B:1199:ALA:HB3	1.91	0.52
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.89	0.52
2:B:249:ARG:HH12	2:B:418:LYS:CD	2.22	0.52
13:M:312:GLY:O	13:M:316:LEU:HD13	2.09	0.52
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.74	0.52
1:A:91:PHE:HD2	1:A:179:LEU:O	1.92	0.52
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.44	0.52
2:B:510:LYS:HB2	2:B:513:GLN:OE1	2.08	0.52
2:B:815:ARG:HG3	2:B:815:ARG:HH11	1.72	0.52
13:M:317:TYR:HE1	13:M:339:LEU:HB2	1.73	0.52
1:A:982:THR:HB	1:A:985:ASP:H	1.73	0.52
1:A:1108:ALA:HA	14:N:63:DC:OP1	2.09	0.52
2:B:291:ILE:HD12	2:B:291:ILE:H	1.74	0.52
15:O:69:ASN:HB2	20:T:48:DT:C4'	2.40	0.52
13:M:310:LYS:HE3	13:M:342:VAL:O	2.09	0.52
2:B:792:MET:CE	20:T:21:DT:OP1	2.57	0.52
7:G:15:PRO:HD3	7:G:67:SER:HA	1.92	0.52
1:A:831:THR:HG23	20:T:15:DA:C4	2.45	0.52
2:B:1122:ARG:HB2	20:T:19:DT:OP1	2.10	0.52
15:O:69:ASN:CB	20:T:48:DT:O4'	2.54	0.52
1:A:78:PRO:C	2:B:1201:LYS:HZ3	2.10	0.52
2:B:449:ASN:HD22	13:M:135:MET:HG3	1.72	0.52
13:M:266:ILE:HG13	13:M:268:GLU:H	1.75	0.52
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.92	0.52
1:A:494:SER:HB3	1:A:497:THR:OG1	2.10	0.52
2:B:90:ILE:HD11	2:B:134:LYS:HE2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ALA:HB2	1:A:57:ARG:HB2	1.90	0.52
1:A:228:PHE:HZ	4:D:14:ARG:HA	1.74	0.52
1:A:1431:GLY:HA3	2:B:1197:PRO:HD3	1.91	0.52
4:D:198:LEU:O	4:D:200:ASN:N	2.44	0.52
1:A:418:SER:OG	13:M:48:CYS:O	2.25	0.51
1:A:832:ALA:HB2	20:T:15:DA:H8	1.74	0.51
1:A:870:GLU:HB2	5:E:204:THR:CG2	2.40	0.51
3:C:52:GLU:HA	12:L:64:LEU:HD22	1.91	0.51
5:E:156:LEU:HD11	5:E:197:LYS:HB2	1.90	0.51
1:A:940:ARG:HB3	1:A:941:LYS:HE2	1.92	0.51
1:A:1095:THR:HG23	1:A:1113:THR:HG23	1.92	0.51
6:F:73:ALA:HB2	6:F:143:PHE:CZ	2.45	0.51
10:J:48:ARG:HE	10:J:49:MET:CE	2.20	0.51
13:M:157:CYS:HB3	13:M:210:MET:HE2	1.93	0.51
13:M:271:GLY:HA3	20:T:52:DC:H5"	1.92	0.51
14:N:22:DT:H2"	14:N:23:DA:H5'	1.93	0.51
1:A:412:ARG:CB	13:M:51:VAL:CG1	2.88	0.51
1:A:646:PHE:O	1:A:650:GLN:HG2	2.10	0.51
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.93	0.51
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.40	0.51
13:M:246:LEU:CD1	13:M:282:ILE:HG21	2.40	0.51
13:M:249:PRO:HD3	13:M:291:ILE:CD1	2.39	0.51
13:M:269:ILE:CG2	13:M:272:LYS:HG2	2.35	0.51
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.92	0.51
6:F:99:LEU:HD21	7:G:65:ASP:C	2.31	0.51
6:F:134:ILE:HG22	6:F:136:ARG:HG3	1.91	0.51
11:K:5:ASP:HB3	11:K:7:PHE:CE2	2.45	0.51
13:M:334:VAL:O	13:M:334:VAL:HG23	2.10	0.51
13:M:342:VAL:CG1	13:M:343:GLU:N	2.74	0.51
1:A:472:LEU:O	1:A:475:THR:HB	2.10	0.51
2:B:1217:TYR:CZ	4:D:13:ARG:HB2	2.45	0.51
26:Z:28:THR:HA	26:Z:29:THR:C	2.31	0.51
1:A:1444:MET:HB2	6:F:133:VAL:HG12	1.92	0.51
2:B:471:LYS:HG2	13:M:95:ARG:NH2	2.26	0.51
7:G:1:MET:SD	7:G:2:PHE:N	2.62	0.51
5:E:64:PRO:HB2	5:E:69:ILE:HD11	1.93	0.51
23:W:653:THR:O	23:W:656:ASN:N	2.44	0.51
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.93	0.51
13:M:320:ARG:HG3	13:M:321:ASP:N	2.26	0.51
13:M:334:VAL:HA	13:M:338:ASN:CG	2.30	0.51
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:15:ALA:O	5:E:19:VAL:HG23	2.10	0.51
1:A:412:ARG:HB3	13:M:51:VAL:HG12	1.92	0.51
1:A:67:CYS:O	1:A:70:CYS:HB3	2.11	0.50
2:B:530:GLY:O	2:B:532:ALA:N	2.44	0.50
2:B:1201:LYS:HD3	2:B:1205:GLN:OE1	2.11	0.50
13:M:283:TYR:CE2	13:M:287:LEU:CD1	2.94	0.50
1:A:417:TYR:HE2	13:M:37:ARG:CD	2.22	0.50
2:B:70:ILE:HG22	2:B:89:GLU:HG2	1.93	0.50
8:H:89:LEU:C	8:H:91:ASP:H	2.14	0.50
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.45	0.50
13:M:333:VAL:HG12	13:M:333:VAL:O	2.11	0.50
14:N:23:DA:N6	20:T:51:DA:N6	2.60	0.50
20:T:19:DT:H2'	20:T:20:DA:C8	2.46	0.50
2:B:60:GLN:OE1	2:B:95:ILE:HG22	2.12	0.50
2:B:373:ARG:HG2	2:B:566:LEU:HD23	1.92	0.50
13:M:306:GLU:O	13:M:309:ILE:HG12	2.12	0.50
20:T:51:DA:H2"	20:T:52:DC:C5	2.47	0.50
1:A:55:ASP:HA	1:A:58:LEU:H	1.76	0.50
1:A:343:LYS:HB2	2:B:1117:GLN:OE1	2.11	0.50
13:M:237:THR:CG2	13:M:238:TYR:CD2	2.95	0.50
1:A:714:PHE:O	1:A:718:VAL:HG23	2.12	0.50
1:A:919:ILE:HG12	1:A:983:ILE:HD13	1.94	0.50
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.94	0.50
2:B:806:THR:HB	2:B:809:MET:HG3	1.94	0.50
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.77	0.50
13:M:254:THR:CG2	13:M:258:TYR:CE2	2.94	0.50
13:M:263:CYS:HA	13:M:266:ILE:HG12	1.94	0.50
1:A:228:PHE:HE1	4:D:15:LEU:HB3	1.77	0.50
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.52	0.50
2:B:1072:MET:HB3	2:B:1081:LEU:HD12	1.94	0.50
14:N:26:DT:H4'	15:O:158:GLN:O	2.12	0.50
15:O:71:VAL:HG21	20:T:47:DA:H2	1.77	0.50
4:D:118:THR:HG21	4:D:121:LYS:HE3	1.94	0.50
1:A:12:ARG:O	2:B:1194:ILE:HG22	2.12	0.49
1:A:245:PRO:O	2:B:1114:LEU:HD12	2.12	0.49
2:B:211:VAL:HG13	2:B:495:LEU:HD23	1.93	0.49
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.93	0.49
2:B:792:MET:HE2	20:T:20:DA:O3'	2.12	0.49
3:C:85:ASP:CG	25:Y:146:THR:CB	2.72	0.49
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.93	0.49
13:M:307:GLY:O	13:M:310:LYS:HB3	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:THR:HG21	1:A:259:GLU:OE2	2.12	0.49
1:A:275:SER:OG	13:M:117:ASN:OD1	2.24	0.49
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.93	0.49
2:B:948:ILE:HD13	12:L:67:PHE:HE2	1.77	0.49
14:N:26:DT:H1'	15:O:159:ASN:HB2	1.93	0.49
1:A:1095:THR:HG21	1:A:1112:LYS:HB2	1.93	0.49
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.12	0.49
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.11	0.49
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.94	0.49
13:M:262:LYS:O	13:M:266:ILE:HG23	2.13	0.49
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.94	0.49
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	1.94	0.49
4:D:173:HIS:CG	4:D:174:PRO:HD2	2.47	0.49
1:A:497:THR:CG2	2:B:1146:PHE:HD1	2.23	0.49
6:F:99:LEU:HD21	7:G:64:THR:C	2.33	0.49
13:M:249:PRO:HG2	13:M:252:VAL:HG23	1.94	0.49
13:M:283:TYR:CE1	13:M:287:LEU:HD11	2.47	0.49
15:O:171:ARG:HG3	15:O:239:LYS:HD3	1.95	0.49
25:Y:48:ASN:O	25:Y:49:LEU:C	2.51	0.49
1:A:89:PRO:HB2	1:A:204:THR:HB	1.93	0.49
1:A:418:SER:N	13:M:49:GLY:HA3	2.28	0.49
1:A:1444:MET:CE	6:F:135:ARG:HB2	2.39	0.49
2:B:338:GLY:HA2	2:B:339:THR:HB	1.93	0.49
13:M:196:ILE:HG13	13:M:197:HIS:HB3	1.92	0.49
13:M:234:GLN:HB2	13:M:236:LEU:HD22	1.91	0.49
19:S:165:THR:CB	19:S:168:LYS:H	2.26	0.49
1:A:411:ASP:CG	13:M:50:LEU:HD11	2.33	0.49
1:A:1193:LEU:HB2	1:A:1260:LEU:CD2	2.42	0.49
1:A:1004:ASN:CG	5:E:167:ARG:HD2	2.33	0.49
2:B:35:SER:HA	2:B:811:TYR:HE1	1.77	0.49
2:B:249:ARG:NH1	2:B:418:LYS:CD	2.76	0.49
1:A:216:VAL:O	1:A:220:THR:HB	2.12	0.49
2:B:574:SER:HB3	2:B:591:ARG:HE	1.77	0.49
2:B:693:ILE:HG21	2:B:701:ILE:HD13	1.95	0.49
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.93	0.49
13:M:237:THR:HG23	13:M:238:TYR:CD2	2.48	0.49
1:A:228:PHE:HE2	4:D:12:ARG:NH1	1.99	0.49
1:A:1402:PHE:CE1	1:A:1403:GLU:HG3	2.48	0.49
2:B:451:LYS:HZ2	13:M:147:LYS:HZ3	1.61	0.49
13:M:276:THR:HA	13:M:279:VAL:HG12	1.94	0.49
1:A:418:SER:HA	13:M:49:GLY:N	2.27	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.95	0.48
4:D:118:THR:O	4:D:120:GLU:N	2.42	0.48
6:F:100:GLN:HE22	7:G:61:ILE:HG21	1.77	0.48
1:A:22:PHE:CB	2:B:1211:ASN:CG	2.78	0.48
2:B:62:ILE:HG21	2:B:417:PHE:HD2	1.78	0.48
8:H:80:ARG:HG2	11:K:57:LEU:HD22	1.95	0.48
13:M:294:THR:OG1	13:M:297:LYS:HG2	2.13	0.48
1:A:260:ASP:OD1	1:A:328:ARG:NH2	2.42	0.48
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.96	0.48
2:B:449:ASN:HD21	13:M:135:MET:HG3	1.75	0.48
2:B:705:MET:H	2:B:710:LEU:HD12	1.79	0.48
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.93	0.48
8:H:40:LEU:HD13	8:H:123:MET:HG3	1.96	0.48
15:O:68:GLN:O	20:T:48:DT:H4’	2.12	0.48
1:A:11:LEU:HA	2:B:1193:GLN:HG2	1.95	0.48
2:B:640:VAL:HG22	2:B:651:LEU:HG	1.95	0.48
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.94	0.48
13:M:286:ILE:HG13	13:M:291:ILE:O	2.13	0.48
1:A:261:ASP:HB3	1:A:322:VAL:HG13	1.95	0.48
2:B:441:ASP:O	2:B:443:ASN:N	2.47	0.48
2:B:1113:VAL:HG22	13:M:57:VAL:HG11	1.96	0.48
6:F:100:GLN:NE2	7:G:61:ILE:HG21	2.29	0.48
13:M:246:LEU:HD22	13:M:293:ILE:HG13	1.96	0.48
13:M:293:ILE:HD11	13:M:297:LYS:C	2.34	0.48
19:S:23:ARG:H	19:S:26:ASN:CB	2.27	0.48
1:A:1116:LEU:HG	1:A:1327:ILE:HD11	1.95	0.48
2:B:451:LYS:NZ	13:M:147:LYS:NZ	2.61	0.48
12:L:50:ASP:HA	13:M:250:MET:HE1	1.95	0.48
13:M:250:MET:HG3	13:M:251:GLN:N	2.27	0.48
2:B:486:TYR:HB3	2:B:1096:ARG:NE	2.28	0.48
2:B:773:MET:CE	2:B:985:GLY:HA2	2.40	0.48
4:D:130:LEU:O	4:D:134:THR:HG22	2.13	0.48
4:D:168:LYS:HD2	4:D:168:LYS:HA	1.53	0.48
13:M:72:ASN:ND2	13:M:74:ASP:OD2	2.47	0.48
13:M:234:GLN:HB2	13:M:236:LEU:HD21	1.91	0.48
1:A:71:GLN:O	1:A:73:GLY:N	2.47	0.48
1:A:257:ARG:HB2	1:A:257:ARG:NH1	2.29	0.48
2:B:122:LEU:HD22	2:B:958:GLN:HG2	1.96	0.48
2:B:345:LYS:HA	2:B:348:ARG:HD2	1.96	0.48
2:B:542:MET:HG3	2:B:747:MET:HB3	1.96	0.48
2:B:840:ILE:HG21	2:B:994:TYR:HD2	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:259:THR:HG23	13:M:323:LEU:CB	2.30	0.48
13:M:280:VAL:O	13:M:283:TYR:HB3	2.14	0.48
1:A:832:ALA:CB	20:T:15:DA:C8	2.97	0.48
12:L:27:LEU:HD13	12:L:37:LYS:HG2	1.95	0.48
15:O:171:ARG:HD3	15:O:238:ARG:O	2.14	0.48
1:A:929:LEU:HD21	1:A:983:ILE:HG21	1.96	0.48
2:B:473:MET:SD	13:M:72:ASN:OD1	2.72	0.48
5:E:176:PRO:O	5:E:212:ARG:HA	2.14	0.48
13:M:285:ASN:O	13:M:288:LEU:HB2	2.14	0.48
1:A:275:SER:O	1:A:279:LEU:HD12	2.14	0.47
1:A:1450:LEU:HD21	7:G:18:PHE:O	2.15	0.47
2:B:219:ALA:HB2	2:B:405:ARG:HG2	1.95	0.47
8:H:115:TYR:CE1	8:H:124:ARG:HG3	2.49	0.47
13:M:136:LEU:HD21	13:M:196:ILE:HG22	1.96	0.47
1:A:89:PRO:HB2	1:A:204:THR:CB	2.44	0.47
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.95	0.47
1:A:448:PRO:O	1:A:449:SER:CB	2.63	0.47
1:A:1172:LEU:C	1:A:1174:PHE:H	2.16	0.47
2:B:951:GLN:OE1	12:L:57:LEU:CD2	2.62	0.47
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.95	0.47
15:O:170:ILE:HD13	15:O:234:LEU:HD22	1.96	0.47
1:A:67:CYS:C	1:A:68:GLN:HG3	2.34	0.47
1:A:285:PRO:O	1:A:287:HIS:N	2.46	0.47
1:A:419:LYS:HE3	13:M:48:CYS:CA	2.44	0.47
1:A:831:THR:HG23	20:T:15:DA:C6	2.49	0.47
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.95	0.47
1:A:1445:ILE:HG13	7:G:61:ILE:CG1	2.45	0.47
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.95	0.47
7:G:118:ASP:OD1	7:G:118:ASP:N	2.42	0.47
13:M:196:ILE:HA	13:M:197:HIS:HA	1.65	0.47
1:A:280:GLU:HG2	1:A:289:ILE:HD13	1.96	0.47
3:C:58:LEU:HD21	10:J:57:ILE:HD12	1.97	0.47
4:D:8:PHE:CD2	7:G:6:ASP:HB2	2.45	0.47
12:L:68:GLU:HB2	12:L:70:ARG:HD2	1.96	0.47
13:M:271:GLY:O	20:T:52:DC:C4'	2.62	0.47
13:M:289:PHE:CG	13:M:290:GLN:N	2.82	0.47
13:M:311:SER:HA	13:M:314:LYS:CD	2.44	0.47
14:N:24:DT:H3'	14:N:24:DT:H6	1.79	0.47
16:P:7:A:H2'	16:P:8:U:O4'	2.14	0.47
8:H:23:VAL:HG11	8:H:121:LEU:HD22	1.95	0.47
11:K:63:VAL:HG12	11:K:71:PHE:HB3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:289:PHE:CD2	13:M:290:GLN:N	2.82	0.47
1:A:475:THR:HG21	2:B:836:GLU:OE2	2.14	0.47
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.96	0.47
4:D:138:ASN:ND2	7:G:35:GLU:HG2	2.30	0.47
6:F:99:LEU:HD23	7:G:65:ASP:C	2.33	0.47
6:F:132:LEU:HD21	7:G:61:ILE:CD1	2.45	0.47
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.95	0.47
13:M:255:SER:HG	13:M:328:LEU:HD13	1.80	0.47
13:M:306:GLU:CA	13:M:309:ILE:HG12	2.43	0.47
2:B:193:LYS:NZ	12:L:32:ALA:O	2.48	0.47
13:M:293:ILE:HD13	13:M:294:THR:N	2.29	0.47
20:T:50:DT:H3'	20:T:50:DT:H6	1.79	0.47
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.69	0.47
1:A:568:PRO:HG2	8:H:46:LEU:HD12	1.95	0.47
1:A:832:ALA:HA	20:T:15:DA:C1'	2.45	0.47
2:B:901:PRO:HG2	12:L:60:ARG:HA	1.97	0.47
3:C:100:THR:HG22	3:C:119:VAL:HG22	1.97	0.47
13:M:293:ILE:CD1	13:M:297:LYS:CG	2.93	0.47
20:T:49:DA:C2'	20:T:50:DT:C5'	2.86	0.47
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.50	0.47
1:A:956:LEU:HD21	1:A:1017:LEU:HG	1.96	0.47
9:I:102:VAL:HG22	9:I:109:ILE:HG12	1.98	0.47
24:X:237:GLN:O	24:X:243:ASN:HA	2.15	0.47
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.45	0.46
2:B:662:MET:HA	2:B:665:GLU:HB2	1.97	0.46
2:B:849:GLY:HA2	2:B:852:ARG:CD	2.39	0.46
4:D:7:THR:OG1	4:D:8:PHE:N	2.48	0.46
7:G:138:THR:HG22	7:G:139:ILE:H	1.80	0.46
9:I:106:CYS:SG	9:I:108:HIS:HB3	2.55	0.46
20:T:19:DT:H2'	20:T:20:DA:H8	1.80	0.46
1:A:228:PHE:CE1	4:D:14:ARG:C	2.88	0.46
1:A:709:THR:HG22	1:A:711:ARG:H	1.80	0.46
1:A:738:LYS:HA	8:H:19:ARG:HH12	1.79	0.46
4:D:40:HIS:CE1	7:G:73:LYS:HB3	2.51	0.46
13:M:298:VAL:CG2	13:M:302:LEU:HD13	2.36	0.46
14:N:22:DT:H2'	14:N:23:DA:H5'	1.96	0.46
1:A:91:PHE:CD2	1:A:179:LEU:O	2.68	0.46
1:A:95:PHE:O	1:A:97:ALA:N	2.49	0.46
1:A:132:LYS:NZ	1:A:1415:SER:HB3	2.30	0.46
6:F:99:LEU:CD2	7:G:66:GLY:N	2.78	0.46
7:G:127:PRO:HD2	7:G:138:THR:HG21	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:237:THR:CG2	13:M:238:TYR:CE2	2.98	0.46
1:A:7:SER:HG	2:B:1161:HIS:CE1	2.22	0.46
1:A:34:LYS:N	1:A:57:ARG:HH11	2.13	0.46
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.96	0.46
7:G:1:MET:CE	7:G:2:PHE:H	2.27	0.46
13:M:272:LYS:HB2	13:M:277:ILE:HD11	1.98	0.46
13:M:305:THR:HG22	13:M:308:THR:OG1	2.15	0.46
17:Q:394:ASN:H	17:Q:395:LYS:HA	1.79	0.46
20:T:47:DA:C8	20:T:48:DT:C4	3.02	0.46
6:F:105:ALA:HB2	7:G:15:PRO:HB2	1.97	0.46
1:A:56:PRO:O	1:A:57:ARG:HG3	2.16	0.46
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.97	0.46
1:A:228:PHE:CE1	4:D:14:ARG:O	2.68	0.46
1:A:579:SER:HA	1:A:582:ILE:HG13	1.97	0.46
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.15	0.46
2:B:108:VAL:HG13	13:M:240:PRO:CB	2.42	0.46
2:B:756:ILE:O	2:B:759:PRO:HD3	2.15	0.46
3:C:18:VAL:HG12	3:C:20:PHE:HD1	1.81	0.46
8:H:30:SER:HB3	8:H:36:CYS:HB3	1.98	0.46
13:M:85:PRO:HA	13:M:89:GLY:O	2.15	0.46
13:M:193:GLN:HG2	13:M:198:VAL:HG12	1.96	0.46
13:M:276:THR:O	13:M:279:VAL:HG12	2.15	0.46
1:A:58:LEU:HD22	1:A:80:HIS:O	2.16	0.46
1:A:1074:GLU:O	1:A:1077:THR:HB	2.16	0.46
3:C:34:ARG:HA	3:C:37:MET:HE2	1.98	0.46
7:G:13:LEU:HA	7:G:13:LEU:HD23	1.64	0.46
1:A:227:VAL:HG13	4:D:16:LYS:HE3	1.98	0.46
2:B:291:ILE:HD12	2:B:291:ILE:N	2.30	0.46
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.80	0.46
3:C:165:LYS:O	11:K:6:ARG:NH1	2.46	0.46
5:E:65:THR:O	5:E:69:ILE:HD12	2.16	0.46
1:A:565:ILE:O	1:A:570:PRO:HA	2.16	0.46
1:A:923:LEU:O	1:A:927:VAL:HG23	2.16	0.46
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.46	0.46
2:B:471:LYS:HE3	13:M:95:ARG:HE	1.80	0.46
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.96	0.46
13:M:242:PHE:CD1	13:M:302:LEU:HA	2.50	0.46
24:X:83:LYS:O	24:X:84:PRO:C	2.55	0.46
2:B:468:GLU:HG2	2:B:469:GLN:HB2	1.99	0.45
13:M:258:TYR:O	13:M:261:LYS:HG2	2.17	0.45
13:M:293:ILE:CD1	13:M:298:VAL:N	2.79	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:24:DT:H2'	14:N:25:DA:C8	2.51	0.45
15:O:239:LYS:O	15:O:240:MET:HG3	2.16	0.45
1:A:11:LEU:HD13	2:B:1195:HIS:NE2	2.31	0.45
1:A:399:HIS:O	1:A:401:GLY:N	2.48	0.45
9:I:72:ASP:O	9:I:81:ARG:HG2	2.16	0.45
25:Y:4:SER:HA	25:Y:155:LEU:O	2.16	0.45
2:B:64:CYS:HA	2:B:67:SER:HB3	1.98	0.45
2:B:365:THR:HG21	2:B:370:PHE:CG	2.51	0.45
4:D:39:ASN:ND2	4:D:43:GLU:OE2	2.49	0.45
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.99	0.45
7:G:119:LEU:HD21	7:G:137:ILE:HD12	1.97	0.45
13:M:282:ILE:O	13:M:286:ILE:HG22	2.16	0.45
1:A:420:ARG:CZ	24:X:174:ALA:CB	2.91	0.45
2:B:1185:CYS:CA	4:D:17:LYS:HB2	2.41	0.45
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.97	0.45
5:E:167:ARG:HD3	5:E:167:ARG:HA	1.78	0.45
7:G:9:LEU:HD22	7:G:34:VAL:HG23	1.98	0.45
13:M:313:TYR:CD2	13:M:343:GLU:N	2.81	0.45
13:M:331:ASN:O	13:M:334:VAL:HG22	2.16	0.45
1:A:883:LEU:HD23	1:A:1021:LEU:HB2	1.97	0.45
1:A:1393:ASN:ND2	1:A:1393:ASN:H	2.15	0.45
2:B:86:ARG:HG2	2:B:138:GLU:HG3	1.98	0.45
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.97	0.45
5:E:90:VAL:HG23	5:E:123:LEU:HD11	1.98	0.45
13:M:254:THR:HG22	13:M:258:TYR:CD2	2.51	0.45
13:M:286:ILE:HD11	13:M:293:ILE:HB	1.98	0.45
15:O:94:TYR:CZ	15:O:96:PRO:HG3	2.52	0.45
13:M:279:VAL:HG21	13:M:309:ILE:HG21	1.99	0.45
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.98	0.45
1:A:497:THR:HG22	2:B:1146:PHE:CD1	2.41	0.45
2:B:89:GLU:HB2	2:B:135:ARG:HB2	1.99	0.45
2:B:900:ALA:CB	12:L:61:THR:HG23	2.42	0.45
13:M:248:LEU:HD13	13:M:252:VAL:CG1	2.37	0.45
13:M:269:ILE:CD1	13:M:277:ILE:CD1	2.94	0.45
17:Q:108:LYS:CB	18:R:86:ASN:CB	2.95	0.45
1:A:832:ALA:CB	20:T:15:DA:H8	2.29	0.45
2:B:394:ASP:OD2	9:I:91:ARG:HD2	2.17	0.45
2:B:803:LEU:HG	10:J:52:THR:HG21	1.98	0.45
13:M:238:TYR:HB3	13:M:242:PHE:HE2	1.75	0.45
13:M:280:VAL:HG11	13:M:312:GLY:HA3	1.98	0.45
14:N:23:DA:N6	20:T:51:DA:H61	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:47:DA:C5	20:T:48:DT:O4	2.70	0.45
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.97	0.45
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.99	0.45
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.81	0.45
6:F:100:GLN:CG	7:G:66:GLY:CA	2.84	0.45
13:M:27:CYS:SG	13:M:48:CYS:HB3	2.57	0.45
13:M:269:ILE:CG2	13:M:272:LYS:CG	2.94	0.45
13:M:289:PHE:CE2	13:M:290:GLN:HG3	2.52	0.45
14:N:25:DA:C8	14:N:25:DA:O5'	2.70	0.45
20:T:55:DA:H2"	20:T:56:DG:C8	2.52	0.45
1:A:180:LYS:CE	1:A:294:SER:HB3	2.46	0.45
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.52	0.45
13:M:193:GLN:HG2	13:M:198:VAL:CG1	2.47	0.45
13:M:289:PHE:CD2	13:M:290:GLN:HG3	2.52	0.45
13:M:295:ALA:HB3	13:M:306:GLU:HG3	1.96	0.45
14:N:17:DC:H2"	14:N:18:DT:H71	1.98	0.45
1:A:91:PHE:CB	1:A:96:ILE:CG1	2.90	0.44
1:A:151:ASP:HA	1:A:163:SER:HA	1.99	0.44
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.97	0.44
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.99	0.44
9:I:83:ASN:HA	9:I:104:LEU:HG	1.98	0.44
13:M:279:VAL:HG23	13:M:302:LEU:HD13	1.98	0.44
1:A:42:ASP:O	1:A:44:THR:N	2.50	0.44
1:A:589:GLN:HG2	1:A:606:LEU:HD13	1.99	0.44
1:A:743:VAL:O	1:A:747:VAL:HG23	2.17	0.44
7:G:89:GLY:HA3	7:G:103:VAL:HG22	2.00	0.44
13:M:236:LEU:HD23	13:M:237:THR:H	1.82	0.44
1:A:228:PHE:HE1	4:D:14:ARG:C	2.20	0.44
1:A:1154:TYR:CE1	9:I:18:GLU:HG3	2.53	0.44
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.99	0.44
2:B:542:MET:HE3	2:B:636:PRO:HG2	1.99	0.44
9:I:50:THR:HG22	9:I:52:ILE:H	1.81	0.44
17:Q:394:ASN:N	17:Q:395:LYS:HA	2.29	0.44
1:A:337:ARG:NH1	2:B:1132:GLU:OE1	2.49	0.44
1:A:1356:ILE:HG21	1:A:1363:VAL:HG23	1.99	0.44
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.99	0.44
13:M:293:ILE:CD1	13:M:297:LYS:CB	2.94	0.44
20:T:52:DC:H1'	20:T:53:DA:H5'	2.00	0.44
1:A:11:LEU:CD1	2:B:1195:HIS:NE2	2.80	0.44
1:A:66:LYS:CE	1:A:68:GLN:H	2.31	0.44
2:B:901:PRO:O	12:L:60:ARG:HA	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:55:THR:HB	3:C:151:GLN:HA	1.99	0.44
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.99	0.44
1:A:70:CYS:O	1:A:72:GLU:HG2	2.17	0.44
1:A:1148:ILE:HA	9:I:49:ILE:HD12	2.00	0.44
1:A:1436:ILE:O	2:B:1144:ALA:HB2	2.17	0.44
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.53	0.44
2:B:102:VAL:HG23	2:B:112:LEU:HD22	2.00	0.44
2:B:1158:PHE:HE2	2:B:1160:VAL:HG13	1.83	0.44
13:M:313:TYR:HH	13:M:317:TYR:HD1	1.65	0.44
13:M:316:LEU:HD12	13:M:316:LEU:N	2.33	0.44
19:S:195:GLN:O	19:S:199:GLY:N	2.50	0.44
20:T:44:DA:H2'	20:T:45:DT:H71	1.99	0.44
1:A:22:PHE:HB2	2:B:1211:ASN:O	2.18	0.44
1:A:449:SER:HA	1:A:454:SER:HB3	1.99	0.44
2:B:69:LEU:HD22	2:B:425:THR:HG23	2.00	0.44
2:B:125:SER:HA	2:B:171:PRO:HA	2.00	0.44
14:N:27:DA:H2'	14:N:28:DA:C8	2.52	0.44
20:T:49:DA:H2'	20:T:50:DT:C5'	2.48	0.44
1:A:548:ASN:HD21	11:K:47:ARG:HH21	1.65	0.44
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	2.00	0.44
3:C:11:ARG:HE	3:C:21:ILE:HD11	1.83	0.44
4:D:11:ARG:HD3	4:D:12:ARG:N	2.33	0.44
6:F:92:ARG:HH21	7:G:63:PRO:HG3	1.83	0.44
11:K:65:HIS:HE1	11:K:67:PHE:CG	2.35	0.44
13:M:269:ILE:CG2	13:M:272:LYS:CB	2.95	0.44
1:A:33:ALA:HB1	1:A:56:PRO:HB2	2.00	0.44
2:B:104:GLU:CD	12:L:54:ARG:NE	2.71	0.44
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.46	0.44
7:G:165:GLU:HG2	7:G:168:LEU:HD12	1.99	0.44
1:A:514:PRO:HG2	1:A:1067:LEU:HD11	1.99	0.43
2:B:935:ARG:H	2:B:935:ARG:HD2	1.83	0.43
4:D:23:ASN:HA	4:D:28:GLN:O	2.18	0.43
4:D:172:LEU:HB3	4:D:176:GLU:OE1	2.18	0.43
13:M:24:CYS:HA	13:M:25:PRO:HD3	1.87	0.43
14:N:29:DT:OP1	15:O:120:LYS:HG3	2.18	0.43
1:A:358:ASN:HB2	11:K:65:HIS:HD2	1.84	0.43
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.53	0.43
1:A:869:GLY:O	5:E:204:THR:HG21	2.18	0.43
2:B:521:LEU:HD22	2:B:633:VAL:HG12	2.01	0.43
8:H:4:THR:HA	8:H:60:ALA:HB2	2.00	0.43
8:H:105:GLU:HB3	8:H:113:ALA:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:62:GLU:O	13:M:65:THR:OG1	2.30	0.43
1:A:58:LEU:HB3	1:A:59:GLY:H	1.25	0.43
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.18	0.43
2:B:955:THR:HG22	2:B:956:THR:N	2.34	0.43
2:B:980:PHE:CD1	2:B:1094:ARG:HA	2.54	0.43
13:M:272:LYS:NZ	20:T:53:DA:P	2.91	0.43
20:T:48:DT:H2'	20:T:49:DA:C5	2.54	0.43
1:A:446:ARG:HB2	1:A:487:MET:SD	2.57	0.43
8:H:123:MET:HE1	8:H:142:LEU:HD11	2.00	0.43
13:M:269:ILE:HD13	13:M:277:ILE:CD1	2.48	0.43
1:A:91:PHE:HB3	1:A:96:ILE:CD1	2.48	0.43
1:A:187:LYS:HE3	1:A:198:GLU:HB2	1.99	0.43
1:A:449:SER:HA	1:A:454:SER:CB	2.49	0.43
1:A:875:ALA:HB2	1:A:1366:ARG:CD	2.48	0.43
1:A:1025:ARG:O	1:A:1035:TYR:HE2	2.01	0.43
1:A:1151:GLU:HG2	9:I:45:ARG:HG3	1.98	0.43
2:B:831:SER:HG	2:B:994:TYR:HE2	1.62	0.43
2:B:1165:ILE:HG21	4:D:17:LYS:CA	2.24	0.43
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.82	0.43
13:M:263:CYS:CA	13:M:266:ILE:HG12	2.49	0.43
13:M:268:GLU:HG3	13:M:315:ILE:HG12	2.00	0.43
13:M:324:VAL:HG21	13:M:328:LEU:HD22	1.93	0.43
1:A:873:MET:HB3	1:A:878:ILE:HD11	2.01	0.43
1:A:1438:THR:HB	2:B:1142:GLY:O	2.19	0.43
2:B:915:THR:O	2:B:917:PRO:HD3	2.19	0.43
10:J:36:LEU:HD11	10:J:51:LEU:HB2	2.00	0.43
1:A:22:PHE:HD2	2:B:1211:ASN:HA	1.83	0.43
1:A:130:ASP:HB3	1:A:133:LYS:HB2	2.00	0.43
1:A:534:LEU:O	1:A:574:GLY:HA3	2.17	0.43
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.66	0.43
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.84	0.43
2:B:1143:ALA:HB1	2:B:1146:PHE:HB3	2.01	0.43
1:A:306:ASN:O	1:A:313:GLN:HG2	2.19	0.43
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	2.01	0.43
4:D:202:ILE:HD13	4:D:207:LEU:HB2	2.01	0.43
12:L:49:LYS:O	12:L:50:ASP:HB2	2.19	0.43
13:M:286:ILE:CG2	13:M:287:LEU:N	2.82	0.43
13:M:304:VAL:HG12	13:M:308:THR:OG1	2.19	0.43
1:A:91:PHE:CB	1:A:96:ILE:CD1	2.96	0.43
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.84	0.43
1:A:343:LYS:NZ	2:B:1156:ASP:HB2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:ARG:HB2	2:B:454:THR:HG23	2.01	0.43
2:B:617:ARG:HG3	2:B:624:LEU:HD12	2.00	0.43
8:H:15:VAL:HG22	8:H:26:ILE:HG13	2.00	0.43
15:O:69:ASN:HB2	20:T:48:DT:H5'	2.00	0.43
1:A:413:ILE:HD13	1:A:424:ILE:HD11	2.01	0.43
2:B:171:PRO:HG2	2:B:461:LEU:HD12	2.01	0.43
2:B:583:ASN:ND2	2:B:628:THR:HG22	2.12	0.43
2:B:841:MET:HG2	2:B:1010:LEU:HD12	2.01	0.43
7:G:1:MET:HE1	7:G:2:PHE:N	2.34	0.43
13:M:189:PHE:O	13:M:193:GLN:HG3	2.18	0.43
13:M:275:ILE:CG2	13:M:276:THR:N	2.82	0.43
2:B:766:ARG:NH2	2:B:1020:ARG:HD3	2.33	0.42
3:C:148:ARG:HG3	3:C:151:GLN:HG3	2.01	0.42
13:M:280:VAL:HG23	13:M:281:SER:N	2.33	0.42
1:A:332:LYS:O	1:A:333:GLU:HB2	2.19	0.42
1:A:709:THR:HB	1:A:712:GLU:H	1.83	0.42
1:A:774:ARG:HH21	1:A:797:LYS:HB2	1.83	0.42
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.01	0.42
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.84	0.42
13:M:335:SER:H	13:M:338:ASN:CG	2.23	0.42
24:X:163:PRO:HA	24:X:190:ILE:O	2.18	0.42
1:A:11:LEU:HA	2:B:1193:GLN:O	2.19	0.42
1:A:332:LYS:HA	1:A:337:ARG:CB	2.50	0.42
1:A:481:ASP:OD1	1:A:485:ASP:OD1	2.37	0.42
2:B:65:GLU:HG3	2:B:66:ASP:H	1.85	0.42
6:F:103:MET:O	7:G:14:HIS:CE1	2.72	0.42
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.99	0.42
13:M:236:LEU:HD23	13:M:236:LEU:N	2.34	0.42
14:N:31:DG:H2"	14:N:32:DT:C6	2.54	0.42
1:A:37:PHE:HA	1:A:38:PRO:HD3	1.93	0.42
1:A:332:LYS:HA	1:A:337:ARG:HB2	2.00	0.42
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.20	0.42
3:C:251:LEU:O	3:C:255:VAL:HG23	2.19	0.42
5:E:10:SER:O	5:E:14:ARG:HG3	2.19	0.42
6:F:92:ARG:NH2	7:G:63:PRO:HG3	2.35	0.42
13:M:248:LEU:CD2	13:M:286:ILE:CD1	2.93	0.42
13:M:339:LEU:HB3	13:M:340:PRO:CD	2.38	0.42
1:A:469:ARG:NH2	2:B:991:GLY:O	2.52	0.42
1:A:832:ALA:HA	20:T:15:DA:C8	2.54	0.42
1:A:1444:MET:HE1	6:F:135:ARG:NE	2.34	0.42
3:C:133:ILE:HG21	3:C:236:GLY:HA3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:12:ARG:CZ	4:D:14:ARG:HA	2.48	0.42
7:G:34:VAL:HG13	7:G:45:ILE:HG21	2.00	0.42
15:O:227:PHE:HA	15:O:230:ILE:HG22	2.02	0.42
2:B:226:PHE:HA	2:B:395:GLN:CG	2.49	0.42
2:B:273:LEU:HD12	2:B:280:ILE:HD12	2.01	0.42
2:B:951:GLN:OE1	12:L:57:LEU:HD22	2.18	0.42
8:H:38:LEU:HD13	8:H:125:LEU:HD13	2.02	0.42
8:H:125:LEU:HG	8:H:130:ARG:HH22	1.85	0.42
13:M:269:ILE:HD12	13:M:277:ILE:HG23	2.02	0.42
13:M:339:LEU:HD12	13:M:339:LEU:H	1.84	0.42
1:A:399:HIS:HB3	1:A:400:PRO:HD3	2.02	0.42
2:B:311:LEU:HB3	9:I:4:PHE:HE2	1.85	0.42
3:C:184:ASN:ND2	3:C:189:THR:O	2.52	0.42
5:E:181:ALA:HA	5:E:186:LEU:HD21	2.01	0.42
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.85	0.42
13:M:123:ASP:HA	13:M:126:VAL:HG23	2.02	0.42
14:N:25:DA:O5'	14:N:25:DA:H8	2.03	0.42
1:A:239:LEU:HD12	1:A:239:LEU:HA	1.77	0.42
1:A:420:ARG:HH11	24:X:174:ALA:HB2	1.68	0.42
1:A:729:ALA:HA	1:A:732:LEU:HD12	2.01	0.42
2:B:986:GLN:OE1	2:B:1016:ALA:HB1	2.20	0.42
2:B:1165:ILE:CG2	4:D:17:LYS:CA	2.93	0.42
6:F:82:THR:HG22	6:F:83:PRO:HD2	2.01	0.42
7:G:110:VAL:HG11	7:G:163:ILE:HG23	2.01	0.42
13:M:64:ARG:NH2	20:T:22:DT:O4	2.49	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
1:A:266:LEU:HD23	1:A:266:LEU:HA	1.92	0.42
1:A:541:ILE:HG21	1:A:549:MET:CE	2.49	0.42
2:B:279:ASP:OD1	2:B:279:ASP:N	2.53	0.42
2:B:383:ASN:O	2:B:387:LEU:HB2	2.19	0.42
4:D:8:PHE:CE1	4:D:37:GLN:HB2	2.55	0.42
17:Q:106:ILE:HA	17:Q:381:MET:O	2.20	0.42
1:A:262:LEU:HG	1:A:328:ARG:NH2	2.35	0.41
1:A:270:LEU:O	1:A:274:ILE:HG13	2.20	0.41
1:A:1094:VAL:HG22	1:A:1113:THR:HB	2.02	0.41
2:B:190:TYR:CE2	2:B:196:PRO:HG3	2.55	0.41
2:B:216:GLU:OE2	2:B:404:LYS:HD2	2.20	0.41
2:B:854:LEU:HD23	2:B:854:LEU:HA	1.86	0.41
2:B:856:PHE:CE2	2:B:969:ARG:HG3	2.55	0.41
4:D:32:GLU:O	7:G:5:LYS:NZ	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:185:CYS:SG	4:D:190:GLU:HG2	2.60	0.41
13:M:263:CYS:SG	13:M:316:LEU:CG	3.08	0.41
13:M:276:THR:CG2	13:M:277:ILE:N	2.82	0.41
1:A:11:LEU:HD21	2:B:1195:HIS:HD2	1.84	0.41
1:A:253:ASN:C	1:A:255:SER:H	2.22	0.41
2:B:315:LYS:N	2:B:316:PRO:HD2	2.36	0.41
13:M:174:ALA:O	13:M:178:ILE:HG12	2.20	0.41
13:M:298:VAL:CG1	13:M:299:GLY:N	2.82	0.41
2:B:789:MET:HG3	2:B:953:LEU:HD21	2.02	0.41
4:D:17:LYS:HD2	4:D:18:VAL:HG13	2.02	0.41
10:J:22:LEU:O	10:J:26:GLN:HG2	2.20	0.41
13:M:276:THR:HG23	13:M:277:ILE:N	2.35	0.41
17:Q:355:THR:C	17:Q:392:ALA:HB1	2.39	0.41
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.85	0.41
5:E:3:GLN:HB2	5:E:4:GLU:H	1.74	0.41
14:N:24:DT:C2'	14:N:25:DA:C5'	2.90	0.41
1:A:11:LEU:HD21	2:B:1195:HIS:CD2	2.55	0.41
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.02	0.41
2:B:211:VAL:CG1	2:B:495:LEU:HD23	2.51	0.41
2:B:955:THR:HG22	2:B:956:THR:H	1.85	0.41
13:M:283:TYR:HD2	13:M:313:TYR:CD1	2.38	0.41
21:U:93:THR:HA	23:W:257:ASP:O	2.19	0.41
1:A:78:PRO:C	2:B:1201:LYS:NZ	2.69	0.41
1:A:562:THR:O	1:A:576:GLN:NE2	2.53	0.41
2:B:848:ARG:HD2	10:J:8:PHE:O	2.20	0.41
3:C:148:ARG:N	3:C:151:GLN:HG3	2.22	0.41
11:K:12:LEU:HA	11:K:37:LYS:HG3	2.03	0.41
13:M:237:THR:CG2	13:M:238:TYR:N	2.83	0.41
20:T:51:DA:H2"	20:T:52:DC:C6	2.55	0.41
1:A:420:ARG:HH12	24:X:174:ALA:HA	1.79	0.41
2:B:509:ALA:O	2:B:511:PRO:HD3	2.20	0.41
2:B:871:THR:HG22	2:B:872:GLU:O	2.21	0.41
2:B:951:GLN:CD	12:L:57:LEU:HD22	2.41	0.41
4:D:57:LEU:HD12	4:D:160:VAL:HG21	2.03	0.41
5:E:156:LEU:HD23	5:E:160:GLU:HB3	2.03	0.41
9:I:111:THR:HG21	9:I:118:ARG:HD2	2.03	0.41
13:M:199:LYS:O	13:M:201:LYS:N	2.54	0.41
17:Q:100:GLU:HA	18:R:95:ILE:O	2.21	0.41
1:A:343:LYS:HA	2:B:1129:ARG:NH1	2.36	0.41
2:B:1111:MET:O	13:M:57:VAL:HG12	2.21	0.41
3:C:99:LEU:HB3	3:C:118:LEU:HD22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:99:LEU:HD12	3:C:118:LEU:HB3	2.02	0.41
13:M:279:VAL:HA	13:M:302:LEU:CD2	2.50	0.41
1:A:16:GLU:HB2	4:D:13:ARG:HH21	1.83	0.41
1:A:34:LYS:HG2	1:A:36:ARG:NH1	2.36	0.41
1:A:227:VAL:HG11	4:D:14:ARG:CD	2.48	0.41
1:A:567:LYS:HA	1:A:568:PRO:C	2.41	0.41
2:B:622:LYS:HE3	9:I:59:VAL:HG22	2.02	0.41
2:B:904:ARG:HG3	2:B:948:ILE:HG13	2.02	0.41
2:B:1166:CYS:O	2:B:1168:LEU:N	2.42	0.41
7:G:14:HIS:CD2	7:G:15:PRO:HD2	2.56	0.41
14:N:21:DG:C2'	14:N:22:DT:H5'	2.51	0.41
1:A:10:PRO:HG2	2:B:1192:TYR:HD1	1.85	0.41
1:A:369:SER:HB3	11:K:2:ASN:OD1	2.21	0.41
1:A:1196:GLU:HA	1:A:1236:LEU:O	2.21	0.41
2:B:642:ASP:HA	2:B:649:LYS:HA	2.02	0.41
8:H:104:PHE:CE1	8:H:136:LYS:HG3	2.57	0.41
13:M:142:LEU:HD12	13:M:142:LEU:HA	1.89	0.41
13:M:293:ILE:CD1	13:M:297:LYS:HB2	2.43	0.41
14:N:26:DT:C1'	15:O:159:ASN:HB2	2.51	0.41
15:O:169:PRO:HB2	15:O:239:LYS:HB2	2.03	0.41
1:A:133:LYS:HE3	1:A:1391:ARG:HH12	1.85	0.40
1:A:1404:GLU:HB3	1:A:1408:ILE:HG13	2.02	0.40
2:B:46:GLN:H	2:B:46:GLN:HG3	1.38	0.40
2:B:610:ASN:HB3	2:B:613:VAL:HG23	2.03	0.40
1:A:354:SER:O	1:A:469:ARG:HA	2.21	0.40
1:A:982:THR:H	1:A:985:ASP:HB2	1.86	0.40
2:B:1166:CYS:CA	4:D:15:LEU:HD12	2.50	0.40
2:B:1169:MET:HE2	2:B:1204:PHE:HB2	2.04	0.40
4:D:54:GLU:OE1	4:D:164:ILE:HD11	2.21	0.40
7:G:62:LEU:HA	7:G:63:PRO:HD3	1.81	0.40
11:K:39:ASP:OD1	11:K:41:THR:HB	2.21	0.40
13:M:254:THR:O	13:M:258:TYR:CD2	2.75	0.40
1:A:974:ASP:C	1:A:976:THR:H	2.25	0.40
2:B:341:LEU:HD11	2:B:343:ILE:HB	2.02	0.40
2:B:681:TRP:HA	2:B:684:LEU:HD12	2.03	0.40
2:B:1119:VAL:HG23	2:B:1126:GLY:HA2	2.03	0.40
4:D:12:ARG:NH1	4:D:14:ARG:HA	2.36	0.40
4:D:63:LEU:HD23	4:D:63:LEU:HA	1.88	0.40
7:G:168:LEU:HD23	7:G:168:LEU:HA	1.92	0.40
9:I:8:ARG:O	9:I:9:ASP:CB	2.69	0.40
10:J:28:ASP:C	10:J:30:LEU:H	2.24	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:43:ARG:O	10:J:47:ARG:HG3	2.21	0.40
13:M:254:THR:HG22	13:M:258:TYR:CE2	2.55	0.40
13:M:282:ILE:HD12	13:M:302:LEU:HD21	2.03	0.40
1:A:7:SER:HB2	2:B:1175:LEU:HD22	2.03	0.40
1:A:255:SER:HB3	13:M:86:LEU:HD12	2.02	0.40
1:A:626:ASN:O	1:A:631:HIS:ND1	2.53	0.40
1:A:1141:THR:HG23	1:A:1205:LYS:HD3	2.04	0.40
2:B:577:ALA:HB1	2:B:589:VAL:HB	2.03	0.40
2:B:979:LYS:HD3	2:B:1095:LEU:HD13	2.04	0.40
3:C:69:LEU:HD23	10:J:6:ARG:HB2	2.04	0.40
6:F:89:GLU:C	6:F:93:ILE:HD12	2.42	0.40
12:L:27:LEU:HD22	12:L:37:LYS:HE3	2.02	0.40
12:L:38:LEU:HD21	12:L:48:CYS:HA	2.02	0.40
13:M:242:PHE:CE1	13:M:301:THR:O	2.74	0.40
23:W:261:TYR:HA	23:W:264:PRO:CB	2.51	0.40
25:Y:71:LEU:O	25:Y:77:ALA:HA	2.22	0.40
1:A:420:ARG:HE	1:A:420:ARG:HB3	1.80	0.40
1:A:441:PRO:HD2	1:A:498:ARG:CZ	2.51	0.40
1:A:450:LEU:H	1:A:450:LEU:HG	1.71	0.40
1:A:497:THR:CG2	2:B:1146:PHE:CD1	3.02	0.40
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.52	0.40
2:B:758:PHE:CE1	2:B:1044:ALA:HA	2.56	0.40
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.36	0.40
3:C:62:PHE:O	3:C:66:ARG:HG3	2.22	0.40
13:M:137:CYS:SG	13:M:147:LYS:HG2	2.62	0.40
13:M:269:ILE:CG1	13:M:316:LEU:HD11	2.50	0.40
13:M:283:TYR:O	13:M:286:ILE:HG22	2.22	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%)	157 (90%)	12 (7%)	5 (3%)	4 29
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%)	152 (90%)	15 (9%)	2 (1%)	13 50
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
19	S	133/295 (45%)	122 (92%)	9 (7%)	2 (2%)	10 46
21	U	154/222 (69%)	148 (96%)	5 (3%)	1 (1%)	25 66
22	V	95/115 (83%)	94 (99%)	1 (1%)	0	100 100
23	W	403/687 (59%)	382 (95%)	18 (4%)	3 (1%)	22 63
24	X	226/307 (74%)	210 (93%)	13 (6%)	3 (1%)	12 48
25	Y	199/209 (95%)	180 (90%)	17 (8%)	2 (1%)	15 55
26	Z	83/120 (69%)	82 (99%)	1 (1%)	0	100 100
All	All	5907/8111 (73%)	5340 (90%)	425 (7%)	142 (2%)	9 33

All (142) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	5	THR
7	G	154	VAL
7	G	155	SER
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
19	S	166	ILE
24	X	79	THR
1	A	40	THR
1	A	44	THR
1	A	51	GLY
1	A	52	GLY
1	A	57	ARG
1	A	66	LYS
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	199	ASN
5	E	36	GLU
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
25	Y	161	GLY
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
2	B	1157	ALA
2	B	1167	GLY
4	D	52	LEU
5	E	45	LYS
5	E	48	ASP
8	H	18	GLY
12	L	59	ALA
18	R	115	SER
21	U	143	GLU
23	W	317	SER
25	Y	159	GLU
1	A	69	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
23	W	547	GLY
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	119	ARG
8	H	60	ALA
8	H	128	ASN
10	J	2	ILE
1	A	35	ILE
1	A	155	GLU
1	A	885	THR
3	C	214	ASN
13	M	164	LYS
13	M	271	GLY
19	S	165	THR
24	X	196	LYS
1	A	196	GLU
1	A	1388	GLY
1	A	1437	GLY
5	E	90	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	364	ILE
1	A	192	GLY
2	B	1121	GLY
1	A	448	PRO
2	B	1214	PRO
4	D	18	VAL
8	H	59	ILE
24	X	84	PRO
23	W	541	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1240/1520 (82%)	1066 (86%)	174 (14%)	3 17
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%)	140 (88%)	20 (12%)	4 19
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%)	136 (90%)	16 (10%)	7 24
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
15	O	152/153 (99%)	140 (92%)	12 (8%)	12 35
All	All	3853/4461 (86%)	3378 (88%)	475 (12%)	8 19

All (475) 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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	8	PHE
4	D	11	ARG
4	D	12	ARG
4	D	17	LYS
4	D	19	GLU
4	D	20	GLU
4	D	23	ASN
4	D	31	GLN
4	D	34	GLN
4	D	35	LEU
4	D	43	GLU
4	D	47	LEU
4	D	48	ILE
4	D	50	LEU
4	D	120	GLU
4	D	123	LEU
4	D	156	ASP
4	D	201	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	203	SER
4	D	204	ASP
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
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	1	MET
7	G	2	PHE
7	G	22	MET
7	G	56	ILE
7	G	60	ARG
7	G	62	LEU
7	G	90	THR
7	G	106	MET
7	G	111	THR
7	G	112	LYS
7	G	117	GLN
7	G	131	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	134	GLU
7	G	138	THR
7	G	139	ILE
7	G	165	GLU
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 (32) 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	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	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	51	ASN
5	E	3	GLN
8	H	35	GLN
8	H	83	GLN
9	I	83	ASN
9	I	89	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 (i)

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
20	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	36.29
1	B	351:TYR	C	352:ALA	N	3.28
1	A	234:MET	C	235:ILE	N	1.07
1	A	95:PHE	C	96:ILE	N	1.00

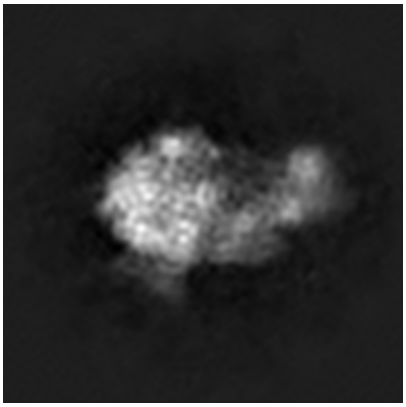
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2786. These allow visual inspection of the internal detail of the map and identification of artifacts.

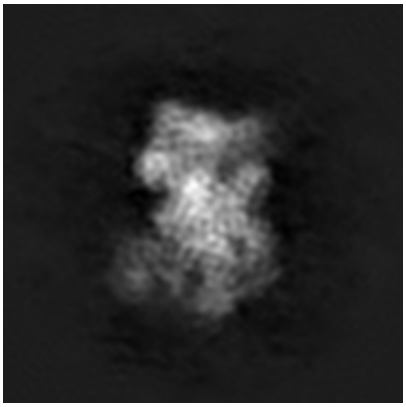
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

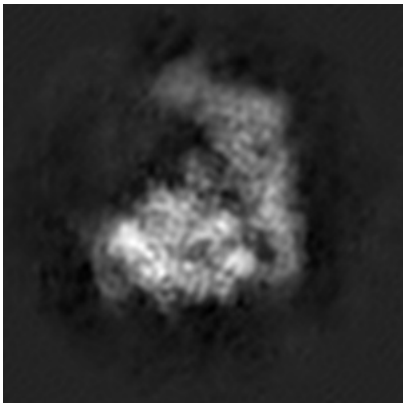
6.1.1 Primary map



X



Y

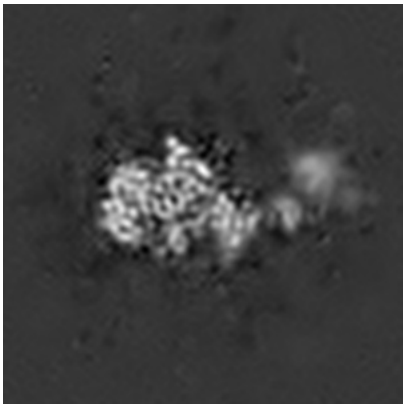


Z

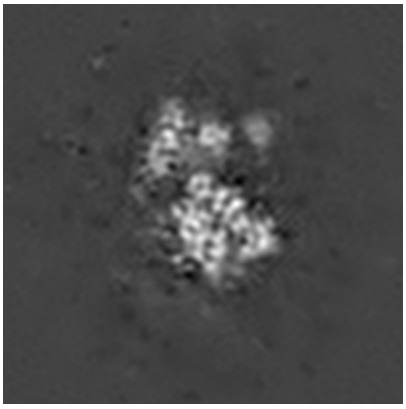
The images above show the map projected in three orthogonal directions.

6.2 Central slices

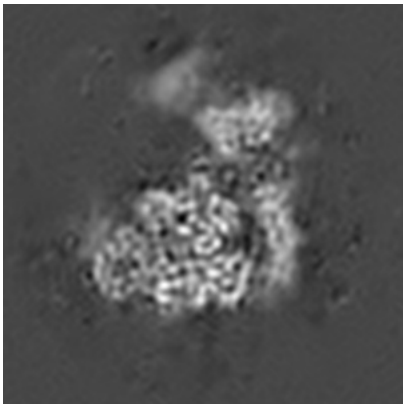
6.2.1 Primary map



X Index: 140



Y Index: 140

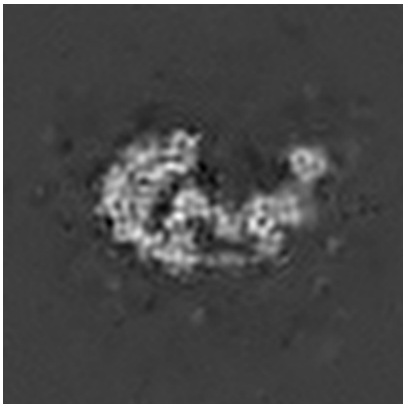


Z Index: 140

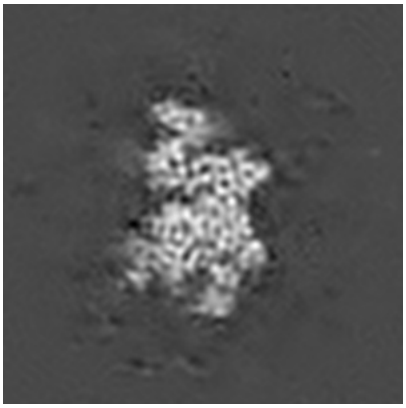
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

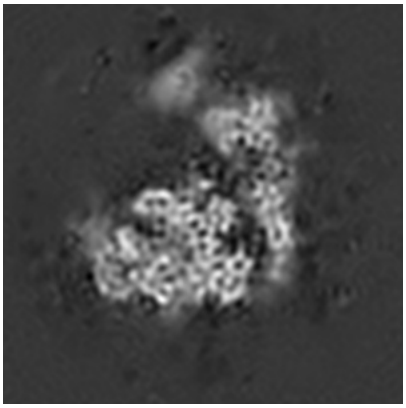
6.3.1 Primary map



X Index: 155



Y Index: 96

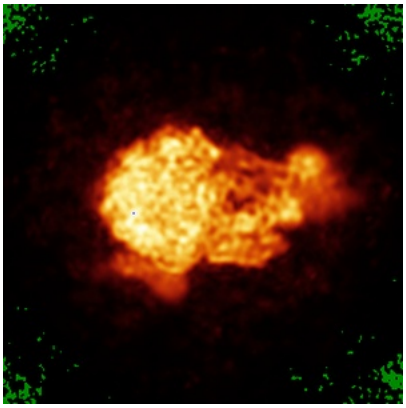


Z Index: 143

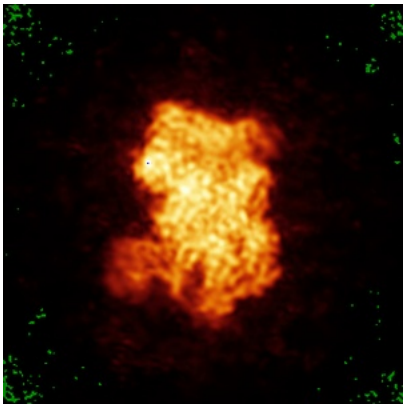
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

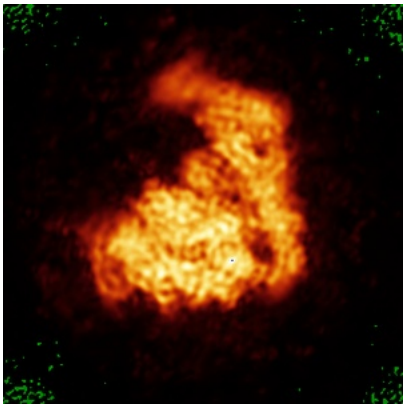
6.4.1 Primary map



X



Y

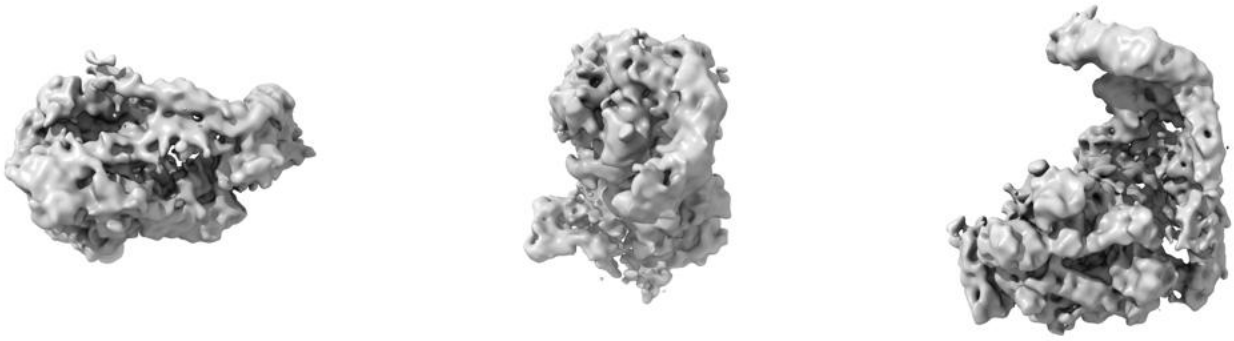


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0135. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

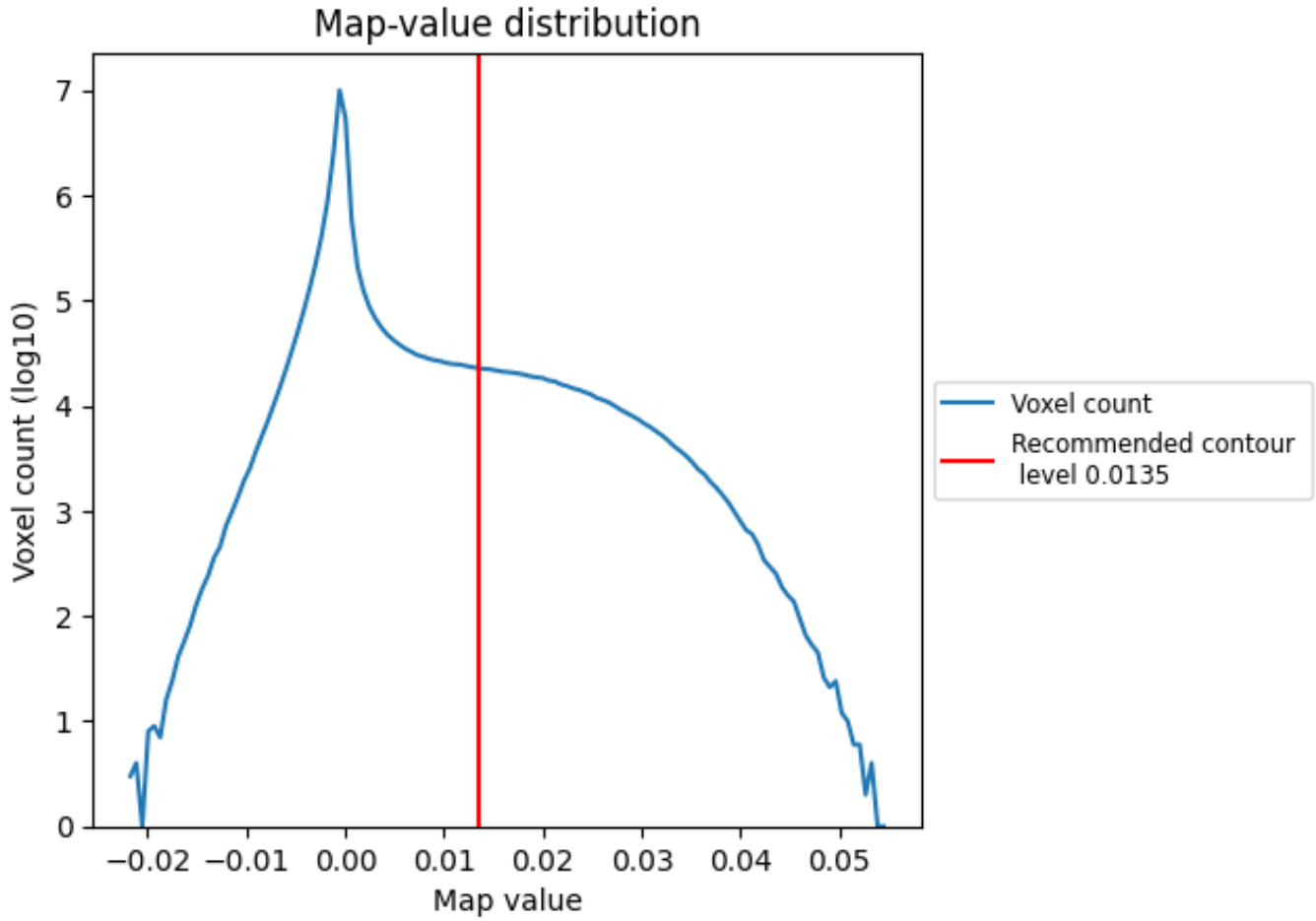
6.6 Mask visualisation (i)

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

7 Map analysis

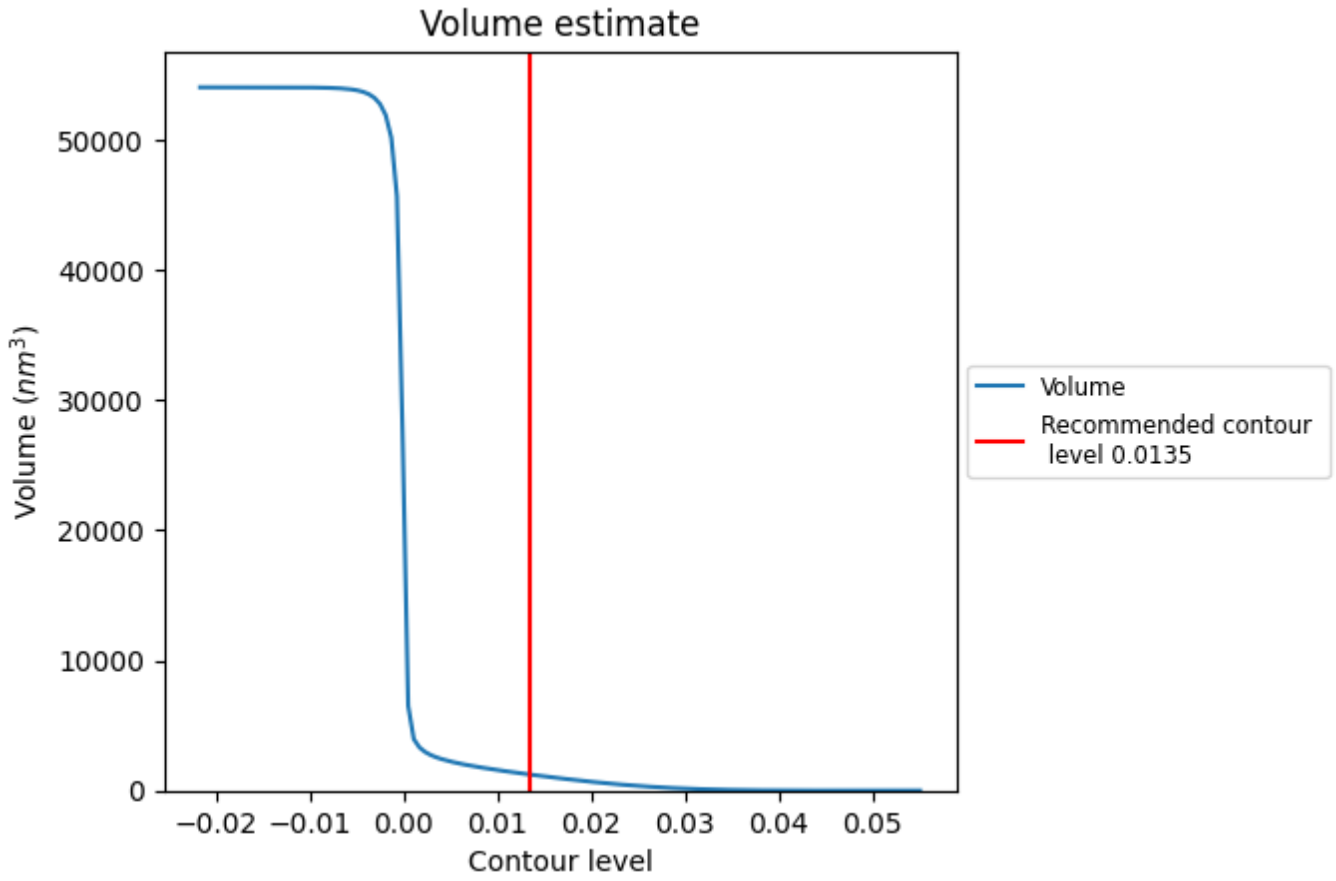
This section contains the results of statistical analysis of the map.

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.

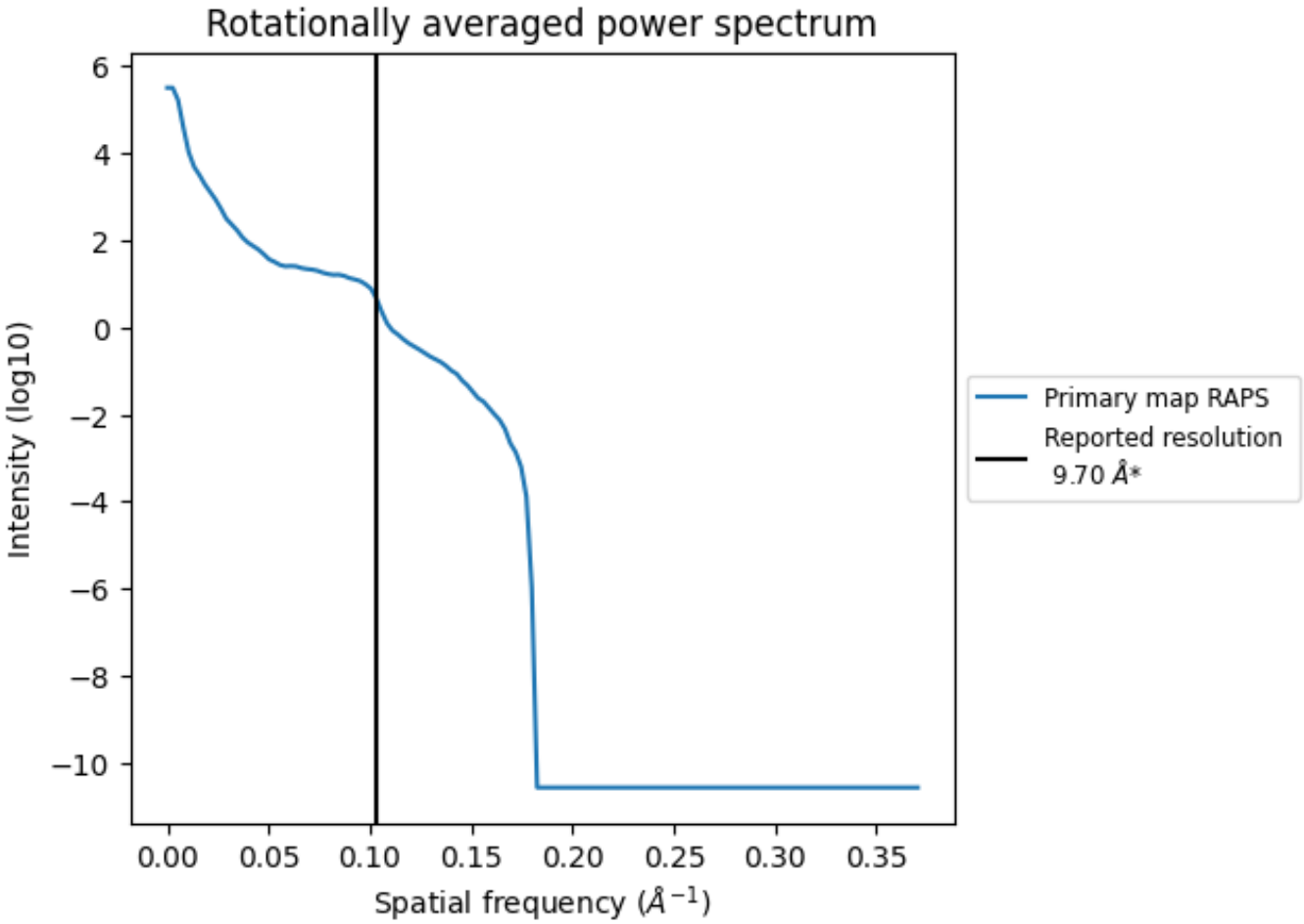
7.2 Volume estimate



The volume at the recommended contour level is 1227 nm^3; this corresponds to an approximate mass of 1108 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 0.103 Å^{-1}

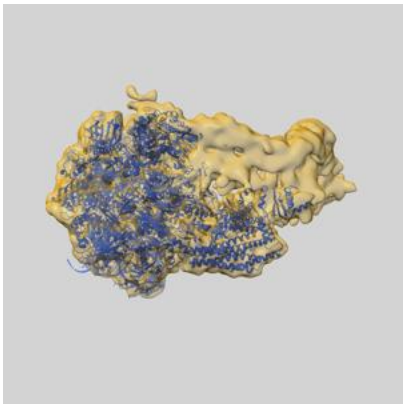
8 Fourier-Shell correlation

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

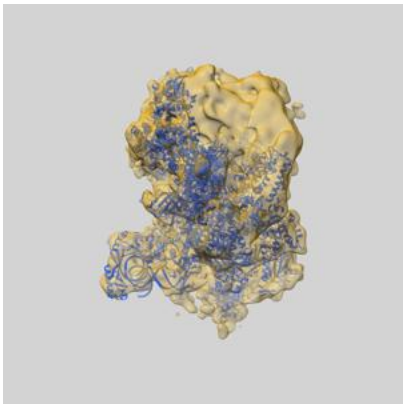
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2786 and PDB model 4V1O. Per-residue inclusion information can be found in section 3 on page 9.

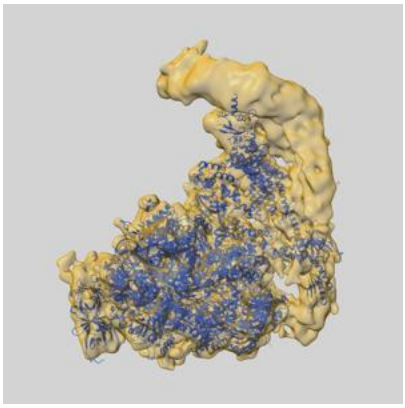
9.1 Map-model overlay



X



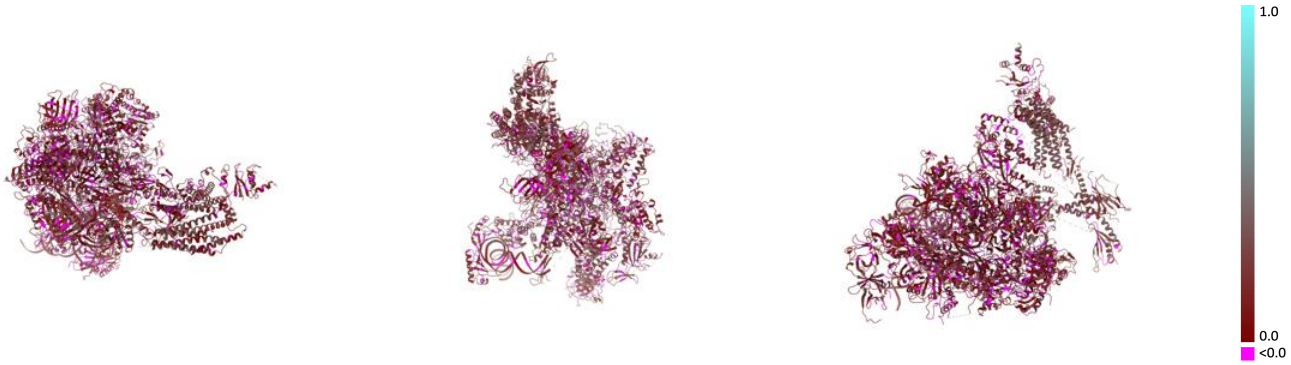
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0135 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

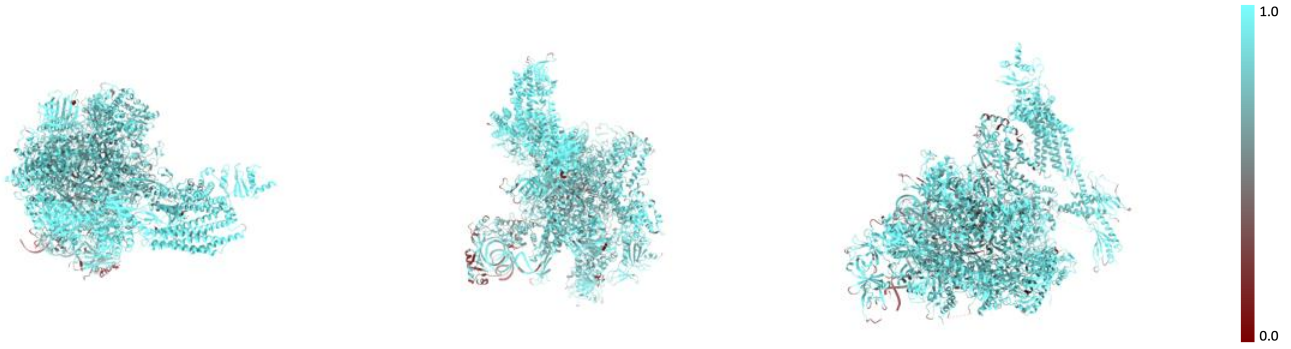
9.2 Q-score mapped to coordinate model



X Y Z

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

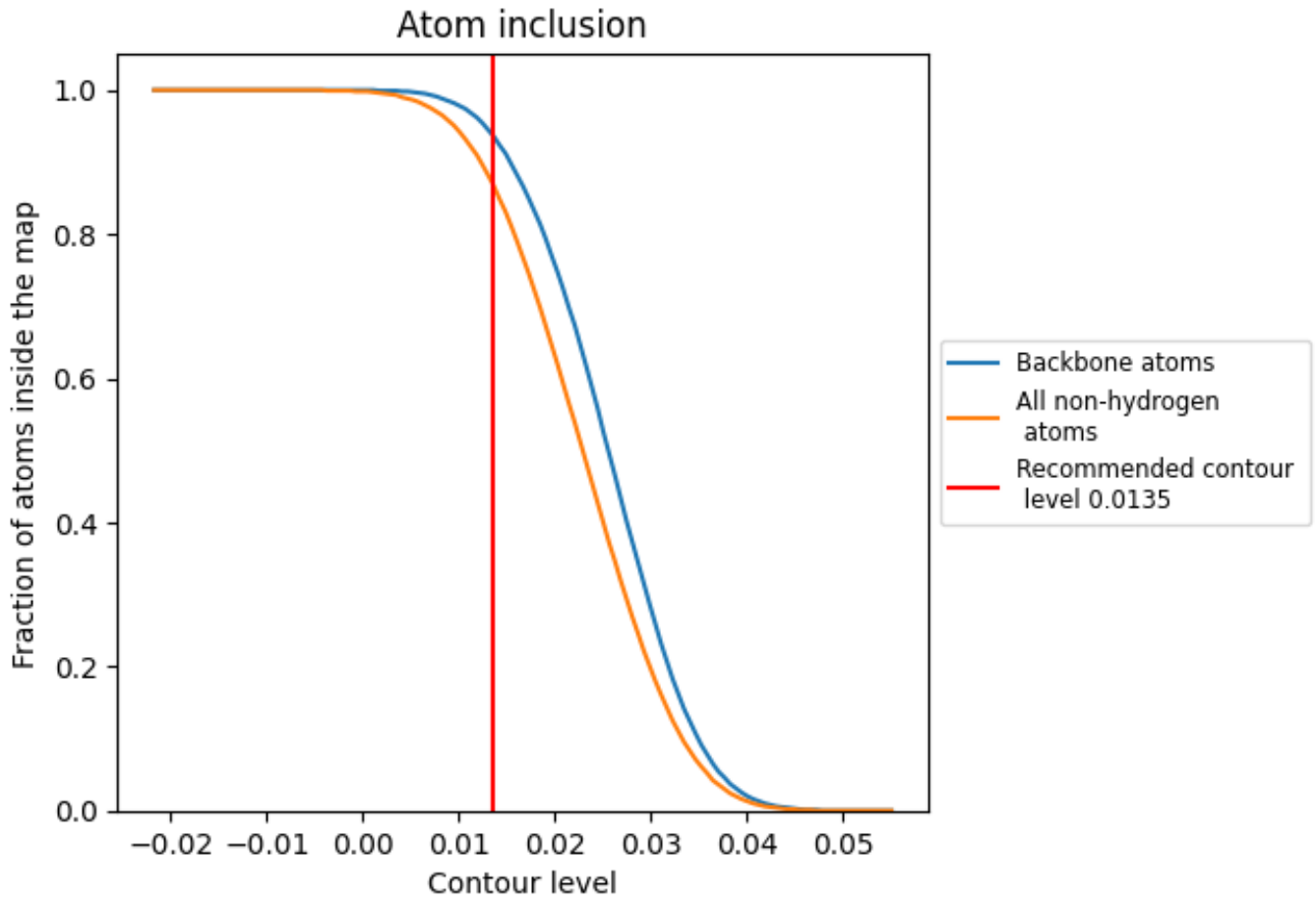
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0135).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 87% 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 (0.0135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8710	0.1160
A	0.8940	0.1140
B	0.8820	0.0970
C	0.9170	0.1140
D	0.7990	0.0810
E	0.9070	0.1100
F	0.8910	0.1220
G	0.8680	0.0910
H	0.9070	0.1220
I	0.9080	0.1040
J	0.9030	0.0950
K	0.8820	0.1240
L	0.8750	0.1000
M	0.6800	0.0870
N	0.7760	0.1280
O	0.5990	0.0670
P	0.4310	-0.0260
Q	0.8190	0.1300
R	0.8220	0.1360
S	0.9940	0.1600
T	0.7090	0.0970
U	0.9820	0.1990
V	0.9980	0.2100
W	0.9590	0.1880
X	0.9530	0.1730
Y	0.9660	0.1820
Z	0.9680	0.2060