



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 04:33 PM UTC

PDB ID : 5FYW / pdb_00005fyw
EMDB ID : EMD-3378
Title : Transcription initiation complex structures elucidate DNA opening (OC)
Authors : Plaschka, C.; Hantsche, M.; Dienemann, C.; Burzinski, C.; Plitzko, J.; Cramer, P.
Deposited on : 2016-03-10
Resolution : 4.35 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

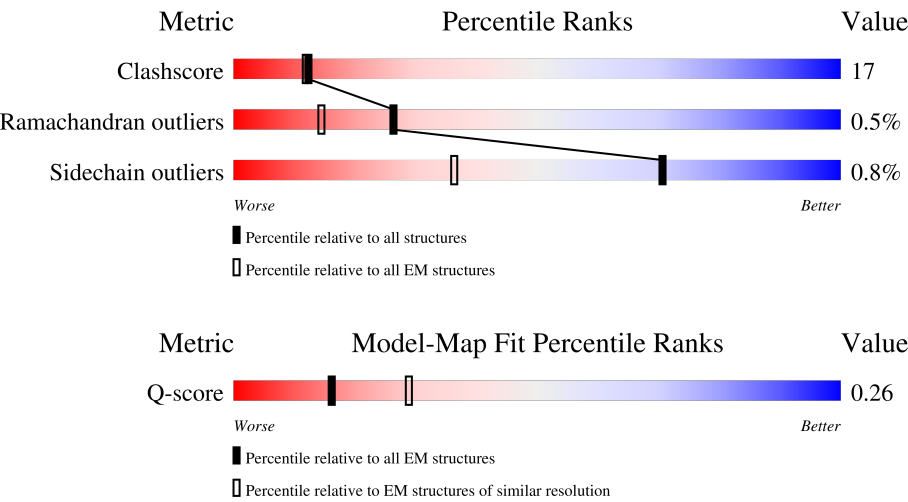
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.35 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3796 (3.85 - 4.85)

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

Mol	Chain	Length	Quality of chain
1	A	1733	14% 57% 24% 19%
2	B	1224	14% 61% 33% 5%
3	C	318	50% 32% 18%
4	D	221	57% 44% 26% 29%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	345	
14	N	72	
15	O	240	
16	Q	735	
17	R	400	
18	T	72	
19	U	286	
20	V	122	
21	W	482	
22	X	328	

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 41710 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
1	A	1398	Total	C	N	O	S	0	0
			10997	6931	1927	2078	61		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1157	Total	C	N	O	S	0	0
			9203	5822	1613	1713	55		

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	262	Total	C	N	O	S	0	0
			2061	1299	343	406	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	157	Total	C	N	O	S	0	0
			1253	779	220	252	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1744	1107	308	318	11		

- 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	83	Total	C	N	O	S	0	0
			670	428	114	125	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	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			944	581	172	181	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	112	Total	C	N	O	S	0	0
			904	580	154	168	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	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	231	Total	C	N	O	S	0	0
			1785	1145	299	326	15		

- Molecule 14 is a DNA chain called NONTEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	47	Total	C	N	O	P	0	0
			919	461	178	234	46		

- 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		

- Molecule 16 is a protein called TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	148	Total	C	N	O	S	0	0
			1144	733	195	212	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	199	Total	C	N	O	S	0	0
			1347	838	247	255	7		

- Molecule 18 is a DNA chain called NONTEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	47	Total	C	N	O	P	0	0
			909	458	172	233	46		

- Molecule 19 is a protein called TRANSCRIPTION INITIATION FACTOR IIA LARGE SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	92	Total	C	N	O	S	0	0
			757	474	130	150	3		

- Molecule 20 is a protein called TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT

2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	100	Total	C	N	O	S	0	0
			782	492	130	156	4		

- Molecule 21 is a protein called TRANSCRIPTION INITIATION FACTOR IIE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	168	Total	C	N	O		0	0
			835	499	168	168			

- Molecule 22 is a protein called TRANSCRIPTION INITIATION FACTOR IIE SUBUNIT BETA.

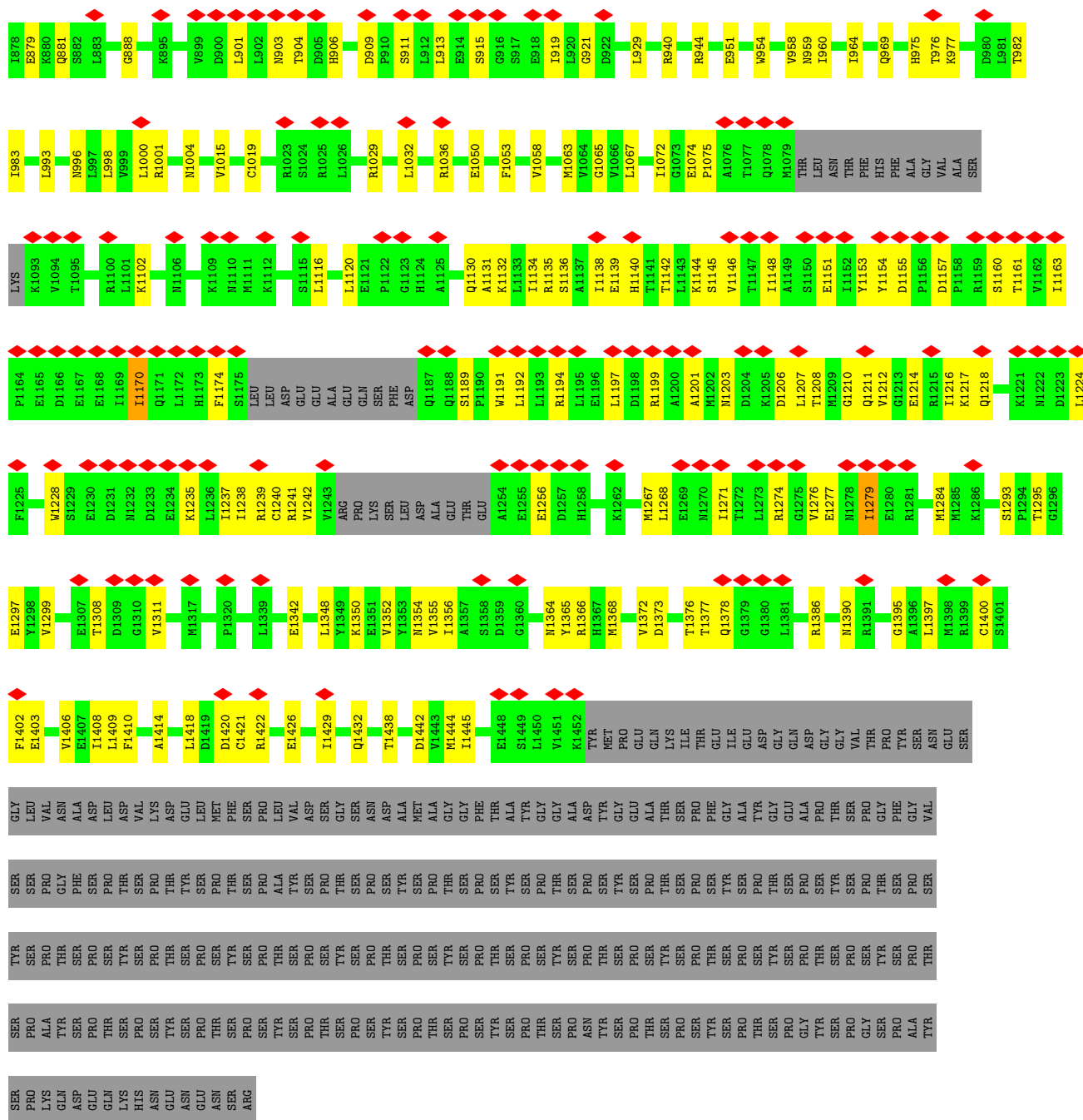
Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	143	Total	C	N	O		0	0
			710	424	143	143			

- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn).

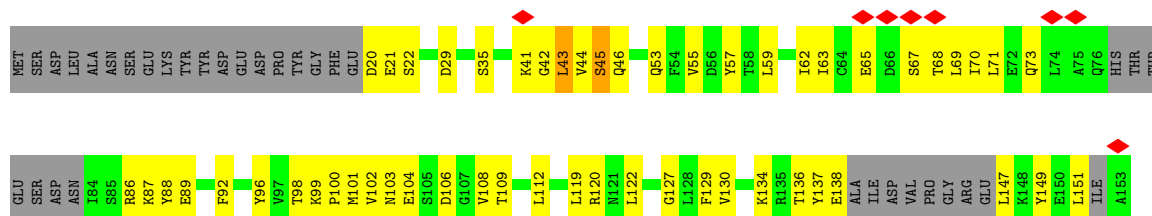
Mol	Chain	Residues	Atoms		AltConf
23	A	2	Total	Zn	0
			2	2	
23	B	1	Total	Zn	0
			1	1	
23	C	1	Total	Zn	0
			1	1	
23	I	2	Total	Zn	0
			2	2	
23	J	1	Total	Zn	0
			1	1	
23	L	1	Total	Zn	0
			1	1	
23	M	1	Total	Zn	0
			1	1	
23	W	1	Total	Zn	0
			1	1	

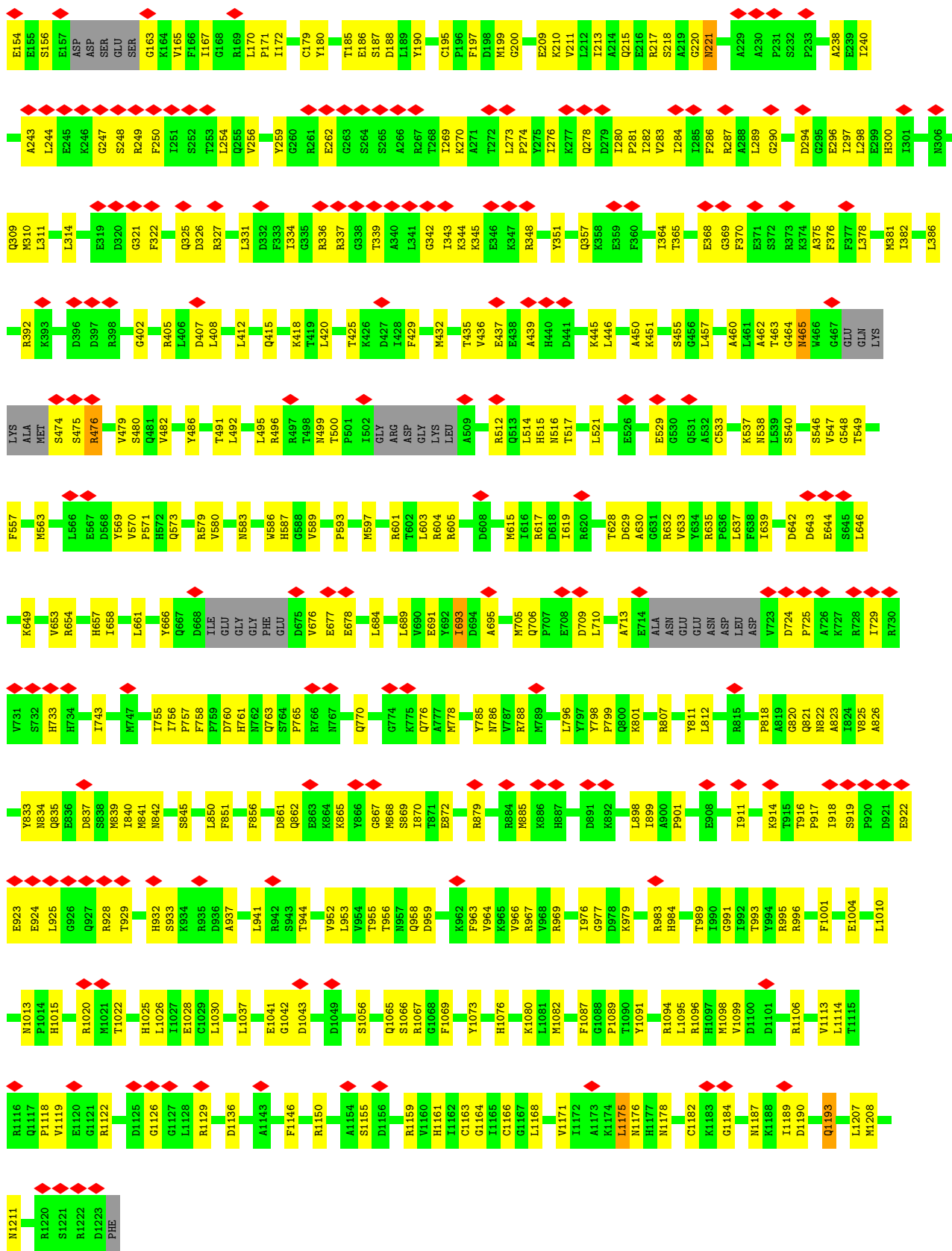
- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

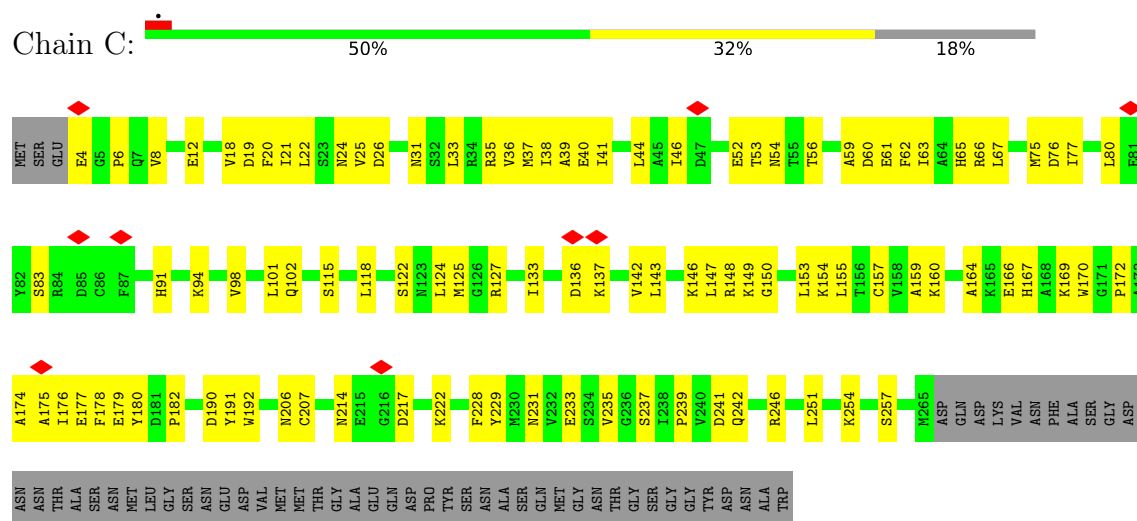


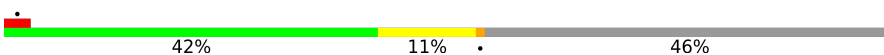
• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2





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

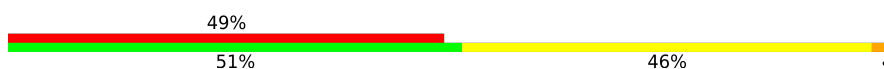


Chain F: 

MET SER ASP TYR GLU ARG ALA PHE ASN ASP GLU ASN PHE ASP PHE VAL HIS PHE SER ASP GLU THR TYR GLU LYS PRO GLN PHE LYS ASP GLY THR ILE VAL THR GLY ASN PRO ASP PHE GLN

HIS GLU GLN ILE ARG ARG LYS THR LEU LYS GLU K72 T82 P83 Y84 R90 A91 R92 I93 L94 L99 S102 A105 F108 V109 D110 L111 E112 V133 I134 R135 R136 Y137 D140 F143 S147 E150 D154 LEU

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

Chain G: 

M1 F2 F3 I4 K5 D6 L7 M10 H14 P15 F17 F18 R21 R22 K23 Q24 Y25 L26 L31 E32 E33 Y34 E35 C36 S37 C38 K41 F42 C43 V44 I45 L46 C47 V48 L49 D50 D52 Y51 D52 N53 I54 D55 Q57 R58 G59 R60 T61 L62 P63 T64 D65 G66 F70

V74 V77 V78 V79 R80 F81 F82 R83 G84 E85 V86 V87 D88 Y92 S93 C94 S95 G96 H97 F99 E100 Q102 V103 G104 P105 M106 K107 V108 F109 C110 T111 K112 H113 L114 M115 P116 Q117 D118 L119 T120 F121 N122 A123 G124 S125 N126 P127 Y130 Q131 S132 E134 D135 V136

I137 T138 I139 K140 S141 I142 I143 R144 V145 K146 I147 E148 C149 I151 S152 Q153 V154 S155 S156 I157 H158 A159 I160 G161 S162 I163 K164 E165 D166 Y167 L168 G169 A170 I171

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

Chain H: 

MET S2 T3 L5 F6 D7 R8 F10 S13 K22 C24 R25 T26 E27 S30 D34 Q35 C36 D41 T42 N43 V44 L46 T56 A60 S61 N64 L65 G66 THR PRO ALA ASN ASP SER A75 T76 R77 Q83 A84 G85 D86 S88 L89

A90 D91 Y93 Y95 V96 R97 Y98 T100 A101 Y102 K103 F104 E105 E106 V107 K109 D110 L111 I112 Y115 S117 F118 G119 G120 R124 L122 L125 E126 Y129 R130 N131 M133 K136 Q137 E138 N139 L142 L143 I144 R145 T146

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

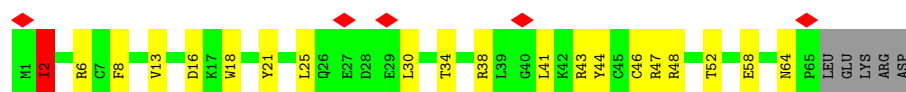
Chain I: 

MET T2 T3 F4 R5 F6 C7 R8 D9 M13 L14 R17 E18 D19 K20 E21 N22 N23 R24 L25 L26 F27 E28 T31 C32 S33 Y34 V35 E36 E37 A38 G39 S40 P41 L42 V43 Y44 R45 H46 E47 L48 I49 T50 N51 I52 G53 E54 T55 A56 G57 V58 V59 Q60 D61 T62 G63 S64

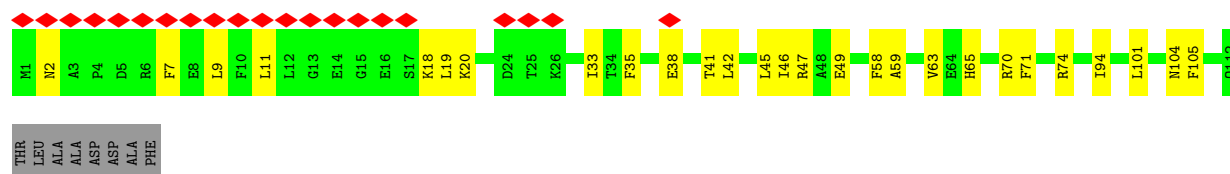
D65 P66 T67 R70 S71 E74 K77 C78 H79 S80 E82 N83 V84 Q87 S88 Q89 R91 R92 K93 D94 T95 F100 F101 V102 C103 L104 S105 C106 S107 H108 I109 S112 D113 Q114 K115 N116 K117 ARG THR GLN PHE SER

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

Chain J: 



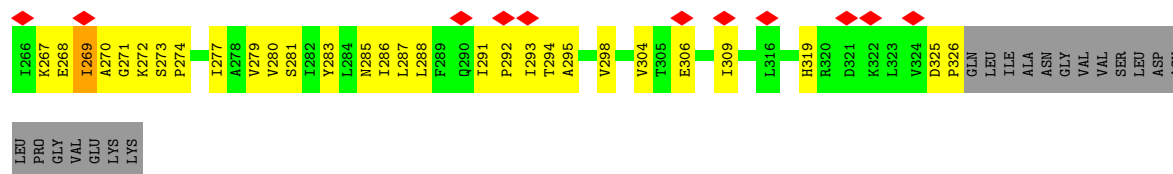
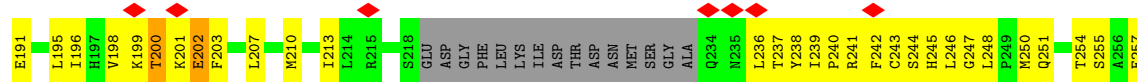
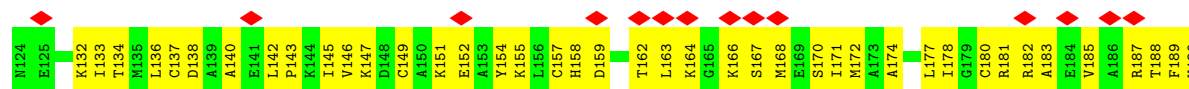
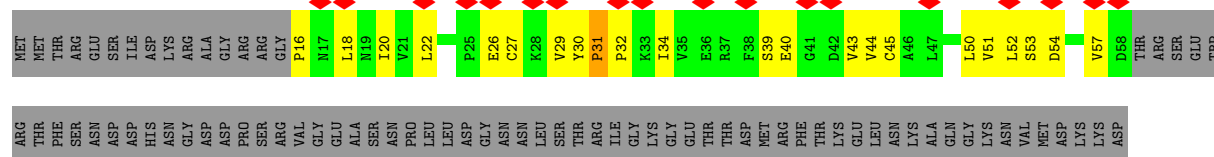
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11



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

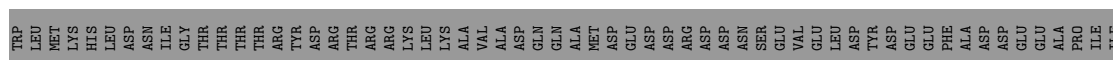


• Molecule 13: TRANSCRIPTION INITIATION FACTOR IIB



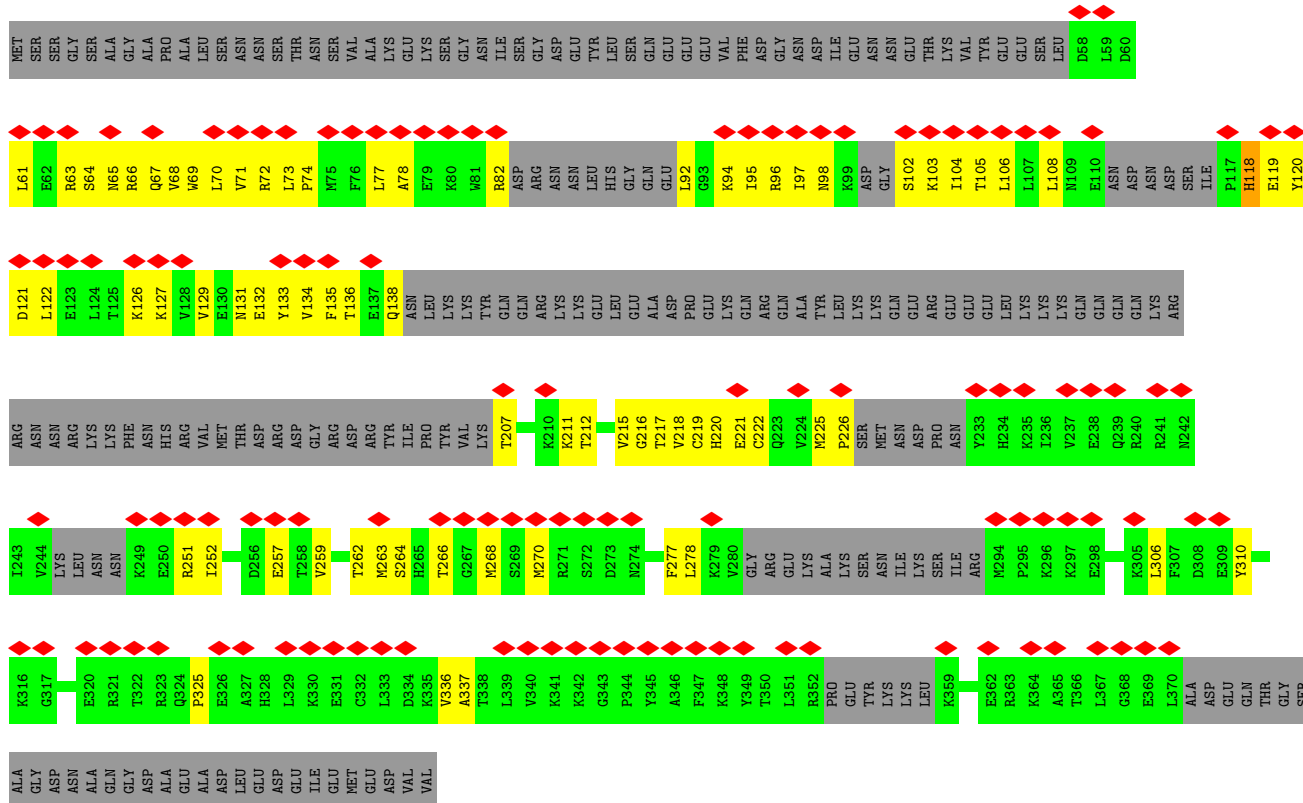
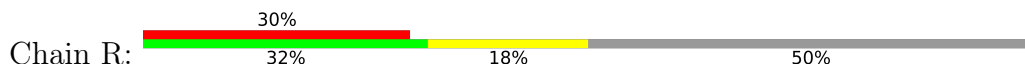
• Molecule 14: NONTEMPLATE DNA



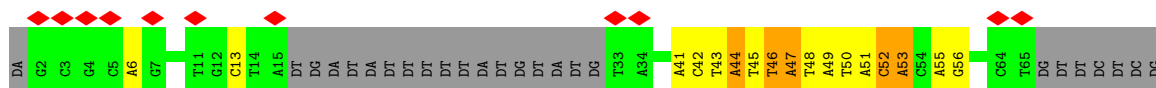
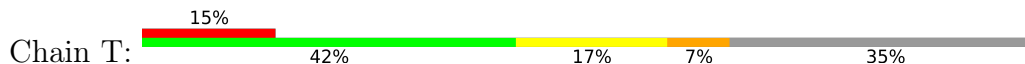


ARG	LEU	HIS	GLU	ASN	LYS	GLY	ASP
LYS	ASN	LYS	LEU	ASN	LYS	GLY	ASP
VAL	SER	GLU	ALA	ASN	GLU	ALA	ASN
GLY	THR	PRO	THR	THR	THR	ALA	GLN
ASN	VAL	LEU	LEU	ARG	LEU	TVR	GLU
ASP	ALA	LEU	ASN	SER	SER	ASN	ASN
HIS	GLU	ARG	VAL	VAL	LYS	ASN	LYS
MET	ARG	VAL	VAL	CYS	ASN	ILE	ARG
GLU	GLU	LYS	THR	THR	VAL	PRO	ILE
LEU	GLU	LYS	THR	ILE	ILE	TYR	LYS
LYS	THR	ILE	THR	ILE	ILE	LEU	GLU
LYS	PRO	ASN	LYS	ASN	ASN	GLU	GLN
GLU	ALA	ASN	ASN	ASN	ASN	ILE	ARG
	PRO	CYS	ASN	ASN	ASN	ASN	ILE
	THR	VAL	VAL	VAL	PRO	PRO	LYS
	ILE	ILE	ILE	ILE	TYR	TYR	LYS
	THR	THR	THR	LEU	SER	SER	GLU
	LYS	LYS	GLY	LYS	GLY	GLN	LEU
	GLY	ASN	ASP	ASN	ASN	GLN	GLN
	ILE	ILE	ILE	ASN	ILE	ASN	MET
	ALA	GLU	GLU	LYS	GLY	ALA	ALA
	ILE	LEU	LEU	LEU	LYS	ASN	GLY
	GLY	LYS	GLU	GLY	GLU	LEU	LEU
	ASP	SER	ASP	SER	ASN	ASN	ARG
	GLY	PHE	GLY	PHE	GLU	GLU	ASP
	LYS	LYS	LYS	PRO	SER	GLU	ASN
	VAL	GLY	VAL	GLY	PRO	ASP	GLU
	ASN	ASN	GLY	GLY	VAL	GLU	GLU
	ILE	GLU	ILE	GLU	LYS	LYS	PRO
	LYS	THR	LYS	TRP	LYS	LYS	ALA
	PHE	GLU	GLU	ASN	GLY	GLY	ALA
	GLY	PRO	GLY	GLN	GLU	ASN	GLU
	LYS	THR	ASP	THR	ASP	SER	GLU
	THR	LYS	THR	THR	THR	GLY	GLY
	ARG	ALA	ALA	ALA	LEU	LEU	PHE
	ARG	VAL	VAL	VAL	SER	SER	GLY
	LYS	ASP	LYS	ASP	LYS	LYS	GLY
	TYR	SER	TYR	SER	SER	GLU	GLU
	PRO	PRO	PRO	SER	LYS	LYS	ASN
	GLY	ASN	GLY	ASN	ARG	ARG	ASP
	ALA	ASN	ALA	ASN	LYS	ILE	GLY
	GLY	ASN	GLY	ASN	LYS	GLN	ARG
	ASN	ALA	ASN	SER	ASN	LYS	ILE
	LYS	LYS	LYS	ASN	LYS	LYS	LYS
	LEU	LEU	LEU	THR	ALA	ALA	LYS
	PHE	THR	VAL	VAL	THR	LYS	ALA
	ALA	ILE	VAL	VAL	ASN	GLN	ALA
	ILE	LYS	LYS	LYS	LEU	GLN	GLN
	THR	GLY	GLY	GLY	LEU	LYS	LYS
	CYS	GLY	GLY	GLY	THR	HIS	THR

● Molecule 17: TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT BETA

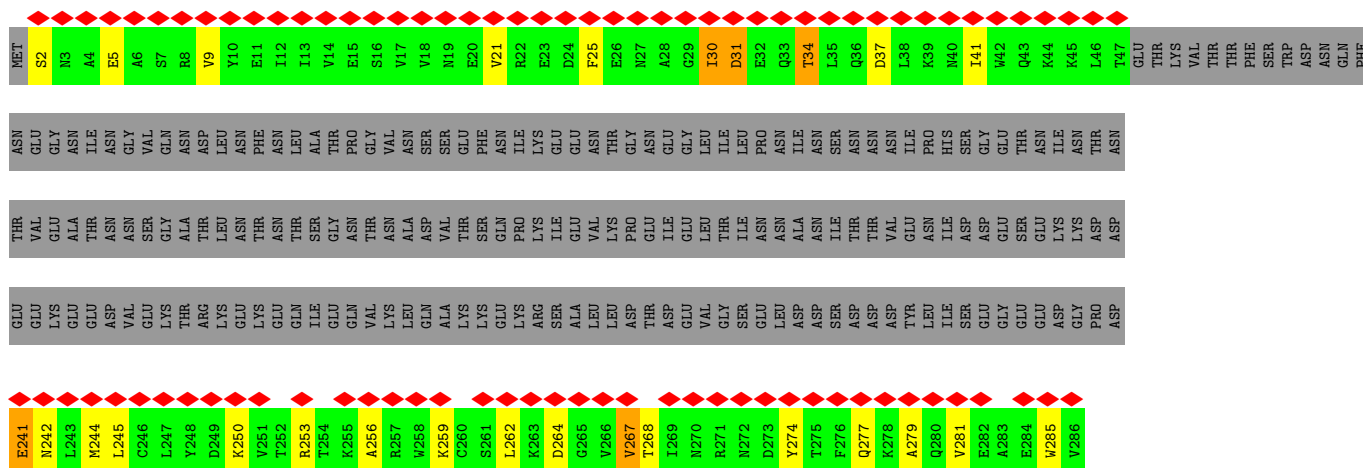


- Molecule 18: NONTEMPLATE DNA

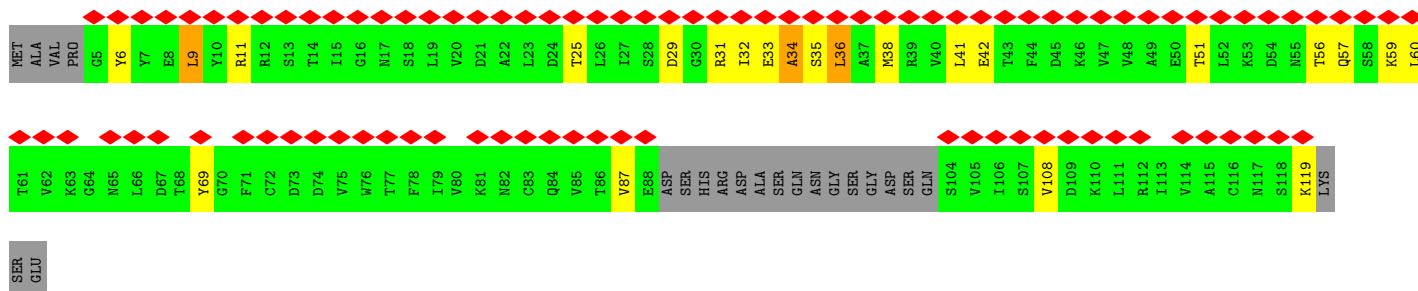
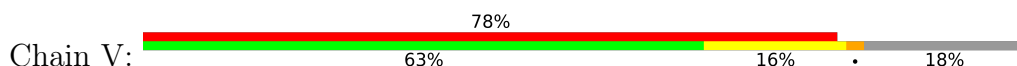


● Molecule 19: TRANSCRIPTION INITIATION FACTOR IIA LARGE SUBUNIT

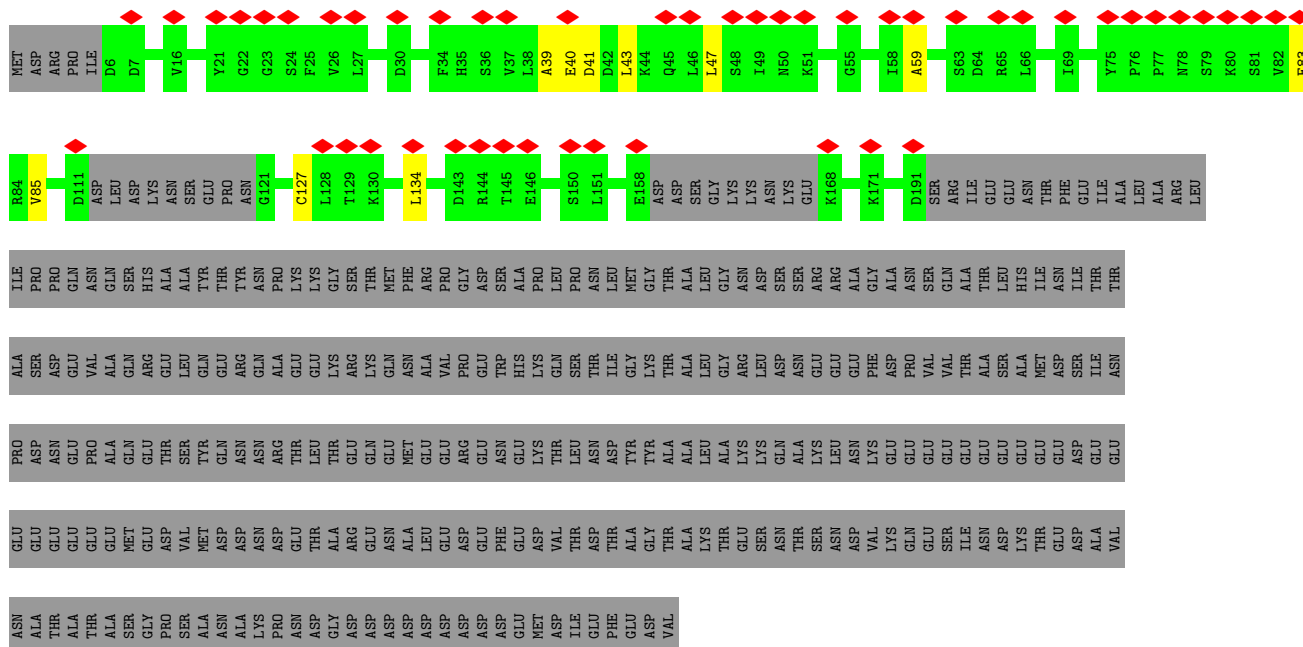




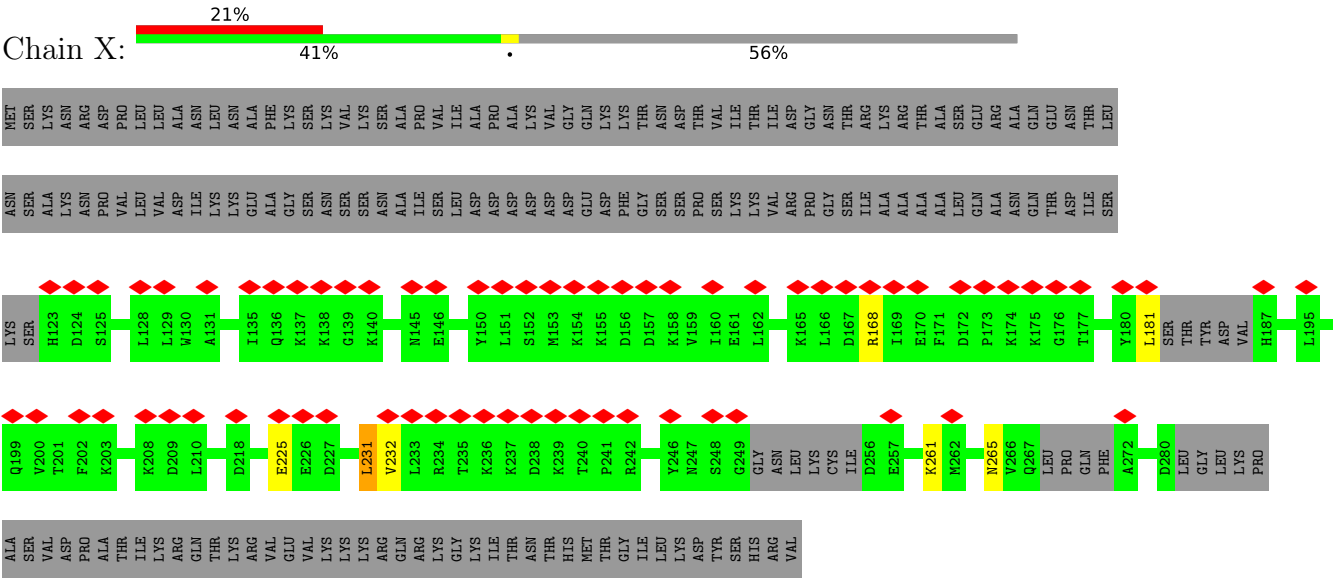
• Molecule 20: TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 2



• Molecule 21: TRANSCRIPTION INITIATION FACTOR IIE SUBUNIT ALPHA



● Molecule 22: TRANSCRIPTION INITIATION FACTOR IIE SUBUNIT BETA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11231	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	33	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	4200	Depositor
Magnification	37037	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.039	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0325	Depositor
Map size ($\text{\AA}$)	405.0, 405.0, 405.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.45	6/11192 (0.1%)	0.59	7/15128 (0.0%)
2	B	0.49	6/9381 (0.1%)	0.65	11/12650 (0.1%)
3	C	0.52	2/2099 (0.1%)	0.60	4/2845 (0.1%)
4	D	0.32	0/1262	0.79	3/1693 (0.2%)
5	E	0.36	1/1780 (0.1%)	0.53	0/2395
6	F	0.40	0/682	0.50	0/922
7	G	0.31	0/1368	0.67	1/1844 (0.1%)
8	H	0.76	2/1107 (0.2%)	1.22	6/1499 (0.4%)
9	I	0.43	1/962 (0.1%)	0.52	2/1295 (0.2%)
10	J	0.45	0/541	0.58	0/727
11	K	0.39	0/922	0.53	0/1244
12	L	0.36	0/360	0.70	0/478
13	M	0.39	0/1809	0.68	0/2435
14	N	0.54	0/1036	1.10	4/1530 (0.3%)
15	O	0.72	0/1443	1.10	7/1942 (0.4%)
16	Q	0.59	0/1168	0.90	1/1579 (0.1%)
17	R	0.46	1/1354 (0.1%)	0.81	5/1832 (0.3%)
18	T	0.66	2/1023 (0.2%)	1.18	9/1507 (0.6%)
19	U	0.47	0/766	0.89	1/1032 (0.1%)
20	V	0.43	0/789	0.90	3/1066 (0.3%)
21	W	0.29	0/832	0.57	1/1157 (0.1%)
22	X	0.25	0/706	0.58	0/979
All	All	0.48	21/42582 (0.0%)	0.72	65/57779 (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
2	B	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	2
10	J	0	1
13	M	0	1
All	All	0	5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	131	ASN	C-N	-21.23	1.03	1.33
18	T	47	DA	C1'-N9	-6.80	1.32	1.46
18	T	53	DA	P-O5'	-6.10	1.48	1.60
9	I	46	HIS	ND1-CE1	5.38	1.38	1.32
2	B	932	HIS	ND1-CE1	5.38	1.38	1.32
2	B	657	HIS	CD2-NE2	-5.32	1.31	1.37
1	A	1140	HIS	ND1-CE1	5.29	1.37	1.32
3	C	91	HIS	ND1-CE1	5.27	1.37	1.32
3	C	65	HIS	CD2-NE2	-5.18	1.32	1.37
1	A	169	ASN	CG-OD1	5.16	1.33	1.23
2	B	657	HIS	ND1-CE1	5.15	1.37	1.32
1	A	83	HIS	ND1-CE1	5.14	1.37	1.32
8	H	83	GLN	CD-OE1	5.14	1.33	1.23
5	E	104	ASN	CG-OD1	5.14	1.33	1.23
2	B	538	ASN	CG-ND2	-5.13	1.22	1.33
1	A	109	HIS	ND1-CE1	5.06	1.37	1.32
2	B	1161	HIS	CD2-NE2	-5.06	1.32	1.37
1	A	1140	HIS	CD2-NE2	-5.05	1.32	1.37
17	R	118	HIS	ND1-CE1	5.04	1.37	1.32
1	A	83	HIS	CD2-NE2	-5.01	1.32	1.37
2	B	1193	GLN	CD-NE2	-5.01	1.22	1.33

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	131	ASN	CA-C-N	20.61	160.91	121.54
8	H	131	ASN	C-N-CA	20.61	160.91	121.54
8	H	131	ASN	N-CA-C	20.60	154.67	110.80
8	H	131	ASN	O-C-N	-18.98	97.34	122.59
17	R	336	VAL	CB-CA-C	-12.62	90.60	111.29
18	T	6	DA	O3'-P-O5'	-11.49	86.76	104.00
2	B	1176	ASN	N-CA-C	-8.63	102.51	113.72
18	T	52	DC	N1-C1'-C2'	7.76	125.14	113.50
17	R	337	ALA	N-CA-C	7.45	120.61	110.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	131	ASN	N-CA-CB	-7.35	98.07	110.49
7	G	159	ALA	N-CA-C	7.35	119.33	108.60
2	B	43	LEU	N-CA-C	7.21	119.22	111.36
2	B	932	HIS	CB-CG-CD2	-7.09	121.99	131.20
20	V	36	LEU	N-CA-C	-6.99	103.74	111.36
2	B	45	SER	N-CA-C	6.91	118.82	111.28
1	A	83	HIS	CB-CG-CD2	-6.91	122.22	131.20
2	B	42	GLY	N-CA-C	-6.85	104.05	112.68
15	O	95	ASN	CA-C-N	6.83	128.38	119.84
15	O	95	ASN	C-N-CA	6.83	128.38	119.84
2	B	1161	HIS	CB-CG-CD2	-6.75	122.42	131.20
18	T	47	DA	C4'-C3'-O3'	-6.67	100.00	110.00
3	C	91	HIS	CB-CG-CD2	-6.65	122.56	131.20
2	B	657	HIS	CB-CG-CD2	-6.63	122.58	131.20
18	T	44	DA	C2'-C3'-O3'	-6.55	101.67	111.50
1	A	109	HIS	CB-CG-CD2	-6.54	122.70	131.20
18	T	52	DC	C4'-C3'-O3'	-6.54	100.20	110.00
1	A	525	GLN	CB-CA-C	-6.53	109.05	116.63
9	I	46	HIS	CB-CG-CD2	-6.53	122.71	131.20
20	V	34	ALA	N-CA-C	-6.47	102.17	110.19
14	N	22	DT	C2'-C3'-O3'	-6.44	101.84	111.50
1	A	1140	HIS	CB-CG-CD2	-6.43	122.84	131.20
8	H	131	ASN	CB-CA-C	-6.42	97.65	110.42
17	R	118	HIS	CB-CG-CD2	-6.41	122.87	131.20
18	T	53	DA	P-O5'-C5'	6.38	129.56	120.00
3	C	65	HIS	CB-CG-CD2	-6.35	122.95	131.20
16	Q	335	LEU	N-CA-C	6.34	119.44	110.50
14	N	65	DA	C5'-C4'-C3'	-6.17	105.64	114.90
18	T	46	DT	C5'-C4'-C3'	-6.09	105.76	114.90
2	B	932	HIS	CB-CG-ND1	6.06	131.79	122.70
18	T	52	DC	C2'-C3'-O3'	-5.95	102.58	111.50
2	B	1161	HIS	CB-CG-ND1	5.81	131.42	122.70
1	A	83	HIS	CB-CG-ND1	5.79	131.39	122.70
15	O	186	GLU	CA-C-N	5.75	127.03	119.84
15	O	186	GLU	C-N-CA	5.75	127.03	119.84
2	B	657	HIS	CB-CG-ND1	5.74	131.30	122.70
18	T	47	DA	C5'-C4'-C3'	-5.70	106.36	114.90
2	B	218	SER	CB-CA-C	-5.68	100.58	109.84
3	C	91	HIS	CB-CG-ND1	5.66	131.19	122.70
9	I	46	HIS	CB-CG-ND1	5.66	131.18	122.70
1	A	109	HIS	CB-CG-ND1	5.65	131.18	122.70
15	O	147	GLY	N-CA-C	5.63	122.89	114.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	R	118	HIS	CB-CG-ND1	5.54	131.01	122.70
15	O	180	GLY	N-CA-C	5.52	119.57	112.83
20	V	31	ARG	N-CA-C	-5.40	104.30	112.99
14	N	68	DG	P-O3'-C3'	5.39	128.29	120.20
1	A	1140	HIS	CB-CG-ND1	5.39	130.79	122.70
3	C	65	HIS	CB-CG-ND1	5.36	130.74	122.70
17	R	336	VAL	N-CA-C	-5.33	98.24	109.34
15	O	82	LEU	N-CA-C	5.27	117.77	111.71
21	W	83	GLU	N-CA-C	-5.12	99.44	108.20
14	N	62	DA	C2'-C3'-O3'	5.11	119.17	111.50
19	U	34	THR	N-CA-C	-5.05	105.48	111.69
4	D	24	ALA	CA-C-N	-5.04	115.84	122.85
4	D	24	ALA	C-N-CA	-5.04	115.84	122.85
4	D	26	THR	N-CA-C	-5.04	106.38	112.88

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1175	LEU	Peptide
8	H	131	ASN	Peptide,Mainchain
10	J	2	ILE	Peptide
13	M	292	PRO	Peptide

5.2 Too-close contacts

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	10997	0	11082	299	0
2	B	9203	0	9203	385	0
3	C	2061	0	2029	75	0
4	D	1253	0	1273	63	0
5	E	1744	0	1772	33	0
6	F	670	0	690	16	0
7	G	1340	0	1356	97	0
8	H	1089	0	1061	45	0
9	I	944	0	899	30	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	532	0	543	22	0
11	K	904	0	911	20	0
12	L	358	0	380	23	0
13	M	1785	0	1891	180	0
14	N	919	0	533	33	0
15	O	1416	0	1493	69	0
16	Q	1144	0	1034	102	0
17	R	1347	0	1130	92	0
18	T	909	0	533	65	0
19	U	757	0	747	21	0
20	V	782	0	790	16	0
21	W	835	0	349	13	0
22	X	710	0	287	4	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	C	1	0	0	0	0
23	I	2	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
23	M	1	0	0	0	0
23	W	1	0	0	0	0
24	A	1	0	0	0	0
All	All	41710	0	39986	1391	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 17.

All (1391) 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:865:LYS:CE	13:M:145:ILE:HD11	1.46	1.44
2:B:405:ARG:NH1	2:B:632:ARG:HG2	1.23	1.40
2:B:868:MET:HB2	13:M:149:CYS:SG	1.64	1.35
13:M:267:LYS:HE3	15:O:208:VAL:CG1	1.59	1.31
13:M:272:LYS:HB3	18:T:53:DA:P	1.71	1.29
12:L:47:ARG:NH1	13:M:250:MET:HE1	1.45	1.27
13:M:272:LYS:HB3	18:T:53:DA:OP1	1.37	1.24
13:M:267:LYS:CE	15:O:208:VAL:CG1	2.16	1.24
13:M:272:LYS:HE2	18:T:52:DC:OP1	1.37	1.22
2:B:199:MET:CE	2:B:491:THR:HG22	1.69	1.21
2:B:865:LYS:HE2	13:M:145:ILE:CD1	1.70	1.19

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:405:ARG:NH1	2:B:632:ARG:CG	2.04	1.17
15:O:91:ASN:OD1	20:V:69:TYR:CZ	1.98	1.16
13:M:267:LYS:HE3	15:O:208:VAL:HG13	1.25	1.12
13:M:272:LYS:CB	18:T:53:DA:OP1	1.98	1.12
13:M:267:LYS:NZ	15:O:169:PRO:HB3	1.64	1.12
13:M:198:VAL:O	13:M:202:GLU:OE1	1.68	1.11
13:M:270:ALA:HB2	15:O:208:VAL:HG11	1.26	1.10
2:B:865:LYS:CE	13:M:145:ILE:CD1	2.27	1.09
14:N:24:DT:H2''	14:N:25:DA:H5'	1.25	1.09
2:B:865:LYS:HE2	13:M:145:ILE:HD11	1.09	1.08
2:B:199:MET:HE1	2:B:491:THR:HG22	1.22	1.07
15:O:191:PRO:CB	18:T:52:DC:H5''	1.83	1.07
2:B:199:MET:CE	2:B:491:THR:CG2	2.32	1.07
13:M:269:ILE:HG23	13:M:272:LYS:HE3	1.33	1.06
14:N:21:DG:H2''	14:N:22:DT:H5'	1.10	1.05
4:D:29:LEU:HD22	7:G:82:PHE:CZ	1.93	1.04
2:B:199:MET:HE3	2:B:491:THR:CG2	1.88	1.04
18:T:42:DC:H2''	18:T:43:DT:C5	1.93	1.04
2:B:868:MET:CB	13:M:149:CYS:SG	2.46	1.04
19:U:2:SER:N	19:U:274:TYR:HH	1.56	1.03
2:B:70:ILE:HD11	16:Q:333:LYS:HB2	1.42	1.02
15:O:91:ASN:ND2	19:U:285:TRP:CZ2	2.28	1.01
2:B:325:GLN:HB3	16:Q:401:TYR:OH	1.59	1.01
4:D:29:LEU:HD22	7:G:82:PHE:CE2	1.96	1.00
14:N:21:DG:C2'	14:N:22:DT:H5'	1.92	0.99
14:N:29:DT:H2''	14:N:30:DA:C8	1.97	0.99
2:B:475:SER:O	2:B:476:ARG:HG3	1.61	0.99
2:B:865:LYS:HE3	13:M:145:ILE:HD11	1.41	0.99
13:M:274:PRO:HD2	15:O:188:GLU:CG	1.92	0.98
7:G:151:ILE:CD1	21:W:134:LEU:CB	2.43	0.97
2:B:44:VAL:HG11	2:B:495:LEU:HD13	1.47	0.96
12:L:47:ARG:NH1	13:M:250:MET:CE	2.27	0.96
2:B:199:MET:HE3	2:B:491:THR:HG21	1.48	0.95
14:N:22:DT:H2''	14:N:23:DA:H5'	1.47	0.95
16:Q:127:ILE:HG22	16:Q:129:PRO:HD3	1.47	0.95
22:X:225:GLU:HA	22:X:231:LEU:HA	1.49	0.95
13:M:269:ILE:CG2	13:M:272:LYS:HG3	1.96	0.95
2:B:44:VAL:HG11	2:B:495:LEU:CD1	1.98	0.94
2:B:249:ARG:NH1	2:B:415:GLN:O	1.89	0.94
7:G:79:PHE:HE2	7:G:81:PRO:HG3	1.31	0.94
2:B:405:ARG:HH12	2:B:632:ARG:HG2	1.17	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:21:DG:H2''	14:N:22:DT:C5'	1.97	0.94
1:A:70:CYS:SG	1:A:80:HIS:NE2	2.41	0.93
13:M:269:ILE:HG23	13:M:272:LYS:CE	1.99	0.92
7:G:79:PHE:CE2	7:G:81:PRO:HG3	2.05	0.92
15:O:191:PRO:HB3	18:T:52:DC:H5''	1.48	0.92
2:B:199:MET:HE1	2:B:491:THR:CG2	1.99	0.92
2:B:68:THR:HB	16:Q:335:LEU:CD1	2.00	0.92
12:L:47:ARG:HH11	13:M:250:MET:HE1	1.31	0.91
13:M:272:LYS:CE	18:T:52:DC:OP1	2.18	0.91
13:M:269:ILE:HG22	13:M:272:LYS:HG3	1.50	0.91
2:B:405:ARG:HH11	2:B:632:ARG:HG2	1.08	0.91
12:L:47:ARG:HH12	13:M:250:MET:CE	1.84	0.90
2:B:914:LYS:HB3	2:B:937:ALA:O	1.73	0.89
4:D:49:ALA:HA	7:G:3:PHE:CD1	2.09	0.88
13:M:270:ALA:HB1	15:O:208:VAL:HG21	1.53	0.88
18:T:43:DT:H2''	18:T:44:DA:C8	2.09	0.87
18:T:49:DA:C2'	18:T:50:DT:H5'	2.03	0.87
13:M:267:LYS:CE	15:O:208:VAL:HG11	2.03	0.87
13:M:267:LYS:HE3	15:O:208:VAL:HG11	1.52	0.87
2:B:868:MET:HB2	13:M:149:CYS:HG	1.34	0.87
14:N:22:DT:H2''	14:N:23:DA:C5'	2.04	0.87
13:M:274:PRO:HD2	15:O:188:GLU:HG3	1.55	0.86
17:R:98:ASN:HB3	17:R:103:LYS:O	1.75	0.86
1:A:326:ARG:HG3	1:A:1406:VAL:HG11	1.57	0.85
13:M:274:PRO:HD2	15:O:188:GLU:HG2	1.55	0.85
16:Q:336:ASP:OD1	16:Q:337:GLU:N	2.09	0.85
2:B:872:GLU:HG2	2:B:916:THR:HG22	1.57	0.85
2:B:405:ARG:HH11	2:B:632:ARG:CG	1.77	0.85
2:B:247:GLY:HA2	2:B:418:LYS:NZ	1.91	0.85
12:L:47:ARG:HH12	13:M:250:MET:HE1	1.32	0.85
2:B:1041:GLU:O	16:Q:22:ILE:CB	2.23	0.85
2:B:247:GLY:N	2:B:418:LYS:HZ1	1.75	0.84
16:Q:373:TYR:CD1	17:R:70:LEU:HD21	2.13	0.84
2:B:644:GLU:HG3	2:B:646:LEU:H	1.43	0.84
4:D:32:GLU:HG3	7:G:42:PHE:CE1	2.11	0.84
2:B:642:ASP:HB3	2:B:649:LYS:HZ2	1.42	0.83
13:M:267:LYS:HZ3	15:O:169:PRO:HB3	1.43	0.83
16:Q:141:ARG:HA	16:Q:350:TRP:HA	1.58	0.83
2:B:217:ARG:NH1	2:B:407:ASP:OD2	2.12	0.83
16:Q:366:GLU:HB3	16:Q:392:VAL:HG13	1.61	0.83
2:B:87:LYS:HB2	2:B:137:TYR:HB2	1.58	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:24:DT:C2'	14:N:25:DA:H5'	2.09	0.82
7:G:151:ILE:HD11	21:W:134:LEU:CB	2.08	0.82
13:M:267:LYS:CE	15:O:208:VAL:HG12	2.09	0.82
2:B:247:GLY:N	2:B:418:LYS:NZ	2.28	0.81
18:T:49:DA:H2''	18:T:50:DT:H5'	1.61	0.81
2:B:220:GLY:O	2:B:221:ASN:HB2	1.79	0.81
13:M:274:PRO:HG2	15:O:188:GLU:OE2	1.80	0.81
16:Q:104:ARG:HG2	17:R:92:LEU:HD22	1.62	0.81
17:R:138:GLN:HB2	17:R:211:LYS:HB3	1.64	0.80
2:B:68:THR:CB	16:Q:335:LEU:CD1	2.60	0.80
7:G:4:ILE:HG12	7:G:77:VAL:HG22	1.63	0.80
15:O:91:ASN:ND2	19:U:285:TRP:HZ2	1.77	0.80
2:B:757:PRO:HD3	2:B:983:ARG:HE	1.46	0.80
4:D:190:GLU:HA	7:G:167:TYR:CE2	2.16	0.80
15:O:91:ASN:OD1	20:V:69:TYR:CE2	2.35	0.79
2:B:365:THR:HG21	2:B:370:PHE:CD2	2.17	0.79
15:O:191:PRO:CB	18:T:52:DC:C5'	2.60	0.79
2:B:71:LEU:HD21	2:B:436:VAL:HG11	1.64	0.79
13:M:267:LYS:HE2	15:O:208:VAL:CG1	2.09	0.79
15:O:91:ASN:OD1	20:V:69:TYR:OH	2.01	0.79
18:T:52:DC:P	18:T:52:DC:H3'	2.23	0.78
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.65	0.78
2:B:53:GLN:OE1	2:B:547:VAL:HG22	1.84	0.78
8:H:129:TYR:O	8:H:133:ASN:ND2	2.17	0.78
17:R:129:VAL:HG11	17:R:221:GLU:HG2	1.66	0.77
13:M:268:GLU:OE1	13:M:319:HIS:NE2	2.12	0.77
8:H:89:LEU:HG	8:H:90:ALA:H	1.48	0.77
13:M:269:ILE:CG2	13:M:272:LYS:HE3	2.13	0.77
2:B:666:TYR:OH	16:Q:27:MET:HB3	1.84	0.77
9:I:82:GLU:HG2	9:I:104:LEU:HD12	1.65	0.77
2:B:868:MET:HE2	13:M:182:ARG:O	1.83	0.77
16:Q:121:PHE:HB2	17:R:131:ASN:HB3	1.67	0.77
1:A:451:HIS:CE1	1:A:1074:GLU:HG3	2.19	0.77
2:B:247:GLY:CA	2:B:418:LYS:NZ	2.48	0.77
2:B:68:THR:OG1	16:Q:335:LEU:HD12	1.85	0.77
17:R:73:LEU:HD12	17:R:74:PRO:HD2	1.65	0.76
1:A:1397:LEU:HB2	1:A:1426:GLU:HG2	1.68	0.76
3:C:149:LYS:HG3	3:C:150:GLY:H	1.51	0.76
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.67	0.75
16:Q:102:PRO:HA	17:R:94:LYS:HA	1.67	0.75
2:B:247:GLY:H	2:B:418:LYS:NZ	1.83	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:375:LEU:O	16:Q:386:MET:HA	1.87	0.75
18:T:48:DT:H2'	18:T:49:DA:C8	2.21	0.75
7:G:159:ALA:C	7:G:160:ILE:HD12	2.11	0.75
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.19	0.75
16:Q:376:LEU:HD23	16:Q:386:MET:HG2	1.68	0.75
2:B:369:GLY:HA3	16:Q:367:ALA:HB2	1.68	0.74
18:T:47:DA:N7	18:T:48:DT:O4	2.19	0.74
18:T:42:DC:H2''	18:T:43:DT:C6	2.23	0.74
1:A:379:VAL:HG22	1:A:431:LYS:HG2	1.69	0.74
7:G:160:ILE:HD12	7:G:160:ILE:N	2.02	0.73
2:B:345:LYS:HA	2:B:348:ARG:HG2	1.70	0.73
2:B:287:ARG:NH2	2:B:294:ASP:OD1	2.20	0.73
18:T:52:DC:H1'	18:T:53:DA:H5'	1.69	0.73
4:D:56:ARG:NH1	4:D:122:GLU:OE2	2.21	0.73
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.69	0.73
13:M:238:TYR:HB3	13:M:242:PHE:HE2	1.54	0.73
17:R:120:TYR:HD1	17:R:226:PRO:HA	1.54	0.73
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.22	0.73
2:B:919:SER:HB2	2:B:922:GLU:HB2	1.72	0.72
1:A:362:ASP:OD2	1:A:459:ARG:NH1	2.21	0.72
12:L:32:ALA:HB2	12:L:55:ILE:HB	1.70	0.72
2:B:247:GLY:HA2	2:B:418:LYS:HZ3	1.53	0.72
13:M:236:LEU:HD11	13:M:257:GLU:HG3	1.72	0.72
16:Q:139:LEU:HB3	17:R:212:THR:HG21	1.71	0.72
1:A:1136:SER:O	1:A:1274:ARG:NH1	2.22	0.72
13:M:267:LYS:HZ2	15:O:239:LYS:HD2	1.55	0.72
5:E:56:LYS:NZ	5:E:84:ASP:OD2	2.22	0.72
5:E:116:ILE:HB	5:E:121:MET:HE2	1.72	0.72
13:M:157:CYS:HB2	13:M:163:LEU:HD11	1.72	0.72
13:M:270:ALA:CB	15:O:208:VAL:HG11	2.13	0.72
7:G:130:TYR:HB2	7:G:137:ILE:HB	1.72	0.72
1:A:405:VAL:HG23	1:A:415:LEU:HD11	1.71	0.71
13:M:166:LYS:HB3	13:M:170:SER:HB3	1.70	0.71
17:R:73:LEU:HD11	17:R:77:LEU:HD23	1.72	0.71
13:M:267:LYS:NZ	15:O:169:PRO:CB	2.51	0.71
13:M:274:PRO:CD	15:O:188:GLU:HG3	2.20	0.71
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.72	0.71
17:R:64:SER:HA	17:R:216:GLY:HA2	1.72	0.71
9:I:31:THR:O	16:Q:401:TYR:HB2	1.89	0.71
13:M:272:LYS:O	18:T:53:DA:OP1	2.08	0.71
17:R:104:ILE:HD11	17:R:122:LEU:HB3	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:GLY:O	2:B:221:ASN:CB	2.38	0.71
13:M:270:ALA:CB	15:O:208:VAL:HG21	2.20	0.71
1:A:61:ILE:HG22	1:A:62:ASP:H	1.55	0.71
2:B:475:SER:O	2:B:476:ARG:CG	2.38	0.71
4:D:54:GLU:HB2	4:D:160:VAL:HG11	1.73	0.71
13:M:267:LYS:NZ	15:O:239:LYS:HD2	2.06	0.71
1:A:881:GLN:NE2	1:A:959:ASN:HA	2.06	0.71
2:B:437:GLU:OE2	16:Q:330:ARG:O	2.09	0.71
1:A:107:CYS:SG	1:A:171:GLN:NE2	2.63	0.70
7:G:151:ILE:HG13	21:W:134:LEU:CB	2.21	0.70
4:D:24:ALA:HA	7:G:83:LYS:HB2	1.73	0.70
1:A:871:ASP:OD2	1:A:1366:ARG:NH2	2.24	0.70
2:B:73:GLN:HB3	2:B:86:ARG:HB3	1.73	0.70
2:B:549:THR:OG1	2:B:628:THR:OG1	2.09	0.70
2:B:984:HIS:NE2	2:B:1028:GLU:OE1	2.24	0.70
7:G:111:THR:HB	7:G:114:LEU:HD13	1.74	0.70
15:O:191:PRO:HB2	18:T:52:DC:H5''	1.68	0.70
2:B:1056:SER:OG	2:B:1067:ARG:NH1	2.24	0.70
18:T:46:DT:H2''	18:T:47:DA:O5'	1.91	0.70
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.73	0.70
7:G:79:PHE:CD2	7:G:81:PRO:HD3	2.26	0.70
17:R:67:GLN:HB3	17:R:219:CYS:HB2	1.73	0.70
2:B:1187:ASN:HD21	2:B:1190:ASP:HB3	1.56	0.69
1:A:441:PRO:HA	1:A:458:HIS:O	1.92	0.69
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.74	0.69
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.75	0.69
4:D:39:ASN:HD21	4:D:43:GLU:HB2	1.58	0.69
12:L:28:LYS:HA	12:L:39:SER:HA	1.74	0.69
1:A:598:LEU:HD21	8:H:124:ARG:HB2	1.73	0.69
1:A:1136:SER:HB3	1:A:1274:ARG:HH12	1.58	0.69
5:E:26:ARG:HH12	5:E:189:GLY:HA3	1.58	0.69
18:T:48:DT:H2'	18:T:49:DA:N7	2.08	0.69
1:A:626:ASN:O	1:A:631:HIS:ND1	2.23	0.69
2:B:463:THR:O	2:B:465:ASN:OD1	2.11	0.69
13:M:270:ALA:HB2	15:O:208:VAL:CG1	2.14	0.69
17:R:106:LEU:O	17:R:119:GLU:HA	1.93	0.68
2:B:593:PRO:HB2	2:B:617:ARG:HE	1.56	0.68
2:B:71:LEU:HD23	2:B:88:TYR:HD2	1.57	0.68
13:M:269:ILE:CG2	13:M:272:LYS:CG	2.72	0.68
1:A:477:PRO:HG3	1:A:521:MET:HE2	1.75	0.68
2:B:53:GLN:OE1	2:B:547:VAL:CG2	2.42	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:63:ARG:NH1	17:R:66:ARG:HH22	1.92	0.68
1:A:906:HIS:O	1:A:1029:ARG:NH2	2.27	0.68
4:D:66:ARG:NH2	7:G:47:CYS:SG	2.67	0.67
13:M:267:LYS:HG3	13:M:268:GLU:H	1.59	0.67
3:C:66:ARG:NH2	3:C:143:LEU:O	2.26	0.67
4:D:32:GLU:HG3	7:G:41:LYS:HE2	1.76	0.67
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.59	0.67
4:D:32:GLU:CG	7:G:41:LYS:HE2	2.24	0.67
4:D:190:GLU:HA	7:G:167:TYR:CD2	2.28	0.67
1:A:524:VAL:HG12	1:A:525:GLN:HG2	1.77	0.67
17:R:105:THR:HA	17:R:120:TYR:O	1.95	0.67
1:A:407:ARG:HH11	1:A:413:ILE:HD11	1.60	0.67
4:D:192:LYS:NZ	4:D:204:ASP:OD1	2.23	0.67
16:Q:101:PHE:N	17:R:95:ILE:O	2.24	0.67
2:B:369:GLY:HA3	16:Q:367:ALA:CB	2.25	0.67
16:Q:397:ALA:HB3	16:Q:400:LYS:HE3	1.76	0.67
18:T:51:DA:H2'	18:T:52:DC:C6	2.29	0.67
2:B:215:GLN:NE2	2:B:479:VAL:HG22	2.09	0.67
16:Q:135:LEU:HB2	16:Q:136:PRO:HA	1.77	0.67
1:A:888:GLY:O	1:A:940:ARG:NH2	2.27	0.66
13:M:136:LEU:HD13	13:M:196:ILE:HD11	1.78	0.66
18:T:47:DA:C8	18:T:48:DT:O4	2.48	0.66
9:I:78:CYS:SG	9:I:105:SER:OG	2.54	0.66
15:O:191:PRO:HG3	18:T:52:DC:C5'	2.24	0.66
1:A:115:LEU:O	1:A:164:ARG:NH1	2.29	0.66
13:M:286:ILE:HG13	13:M:291:ILE:HG13	1.77	0.66
2:B:309:GLN:OE1	2:B:392:ARG:NH2	2.28	0.66
2:B:629:ASP:OD1	2:B:630:ALA:N	2.29	0.66
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.77	0.66
8:H:8:ASP:OD1	8:H:9:ILE:N	2.29	0.66
1:A:362:ASP:O	1:A:458:HIS:ND1	2.28	0.66
2:B:92:PHE:HD2	2:B:130:VAL:HG11	1.61	0.66
3:C:22:LEU:HD11	11:K:101:LEU:HD11	1.77	0.66
2:B:68:THR:OG1	16:Q:335:LEU:CD1	2.44	0.65
13:M:272:LYS:HB3	18:T:52:DC:O3'	1.96	0.65
2:B:68:THR:HB	16:Q:335:LEU:HD11	1.76	0.65
16:Q:397:ALA:HB3	16:Q:400:LYS:CE	2.26	0.65
3:C:75:MET:O	3:C:246:ARG:NH2	2.23	0.65
2:B:247:GLY:CA	2:B:418:LYS:HZ3	2.06	0.65
3:C:54:ASN:ND2	3:C:60:ASP:OD1	2.29	0.65
13:M:272:LYS:HB2	18:T:53:DA:OP1	1.94	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:245:HIS:CD2	17:R:264:SER:HB2	2.32	0.65
14:N:31:DG:H3'	17:R:325:PRO:CB	2.26	0.65
7:G:151:ILE:CG1	21:W:134:LEU:CB	2.75	0.65
13:M:34:ILE:HG22	13:M:45:CYS:HA	1.79	0.65
4:D:32:GLU:HG3	7:G:42:PHE:CZ	2.30	0.65
13:M:22:LEU:HB3	13:M:52:LEU:HD23	1.77	0.65
16:Q:378:VAL:HG22	16:Q:384:PHE:HE1	1.61	0.65
19:U:30:ILE:HG23	19:U:31:ASP:H	1.60	0.65
1:A:821:ARG:HE	2:B:514:LEU:HB2	1.62	0.65
13:M:245:HIS:HA	17:R:264:SER:HB3	1.79	0.64
16:Q:373:TYR:HD1	17:R:70:LEU:HD21	1.59	0.64
1:A:198:GLU:OE2	1:A:200:ARG:NH2	2.27	0.64
2:B:835:GLN:HA	2:B:1013:ASN:HD22	1.62	0.64
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.30	0.64
2:B:959:ASP:HB2	13:M:143:PRO:HB2	1.79	0.64
3:C:166:GLU:OE2	12:L:70:ARG:NH2	2.30	0.64
1:A:881:GLN:HE21	1:A:959:ASN:HA	1.62	0.64
13:M:188:THR:HG22	13:M:190:LYS:H	1.63	0.64
2:B:44:VAL:CG1	2:B:495:LEU:HD13	2.26	0.64
14:N:30:DA:O5'	14:N:30:DA:H8	1.81	0.64
15:O:191:PRO:HG3	18:T:52:DC:H5'	1.79	0.64
1:A:134:ARG:NH1	1:A:221:SER:O	2.31	0.64
1:A:537:ARG:NH1	8:H:120:GLY:O	2.31	0.64
7:G:111:THR:HG22	7:G:113:HIS:H	1.61	0.64
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.80	0.64
8:H:110:ASP:O	8:H:129:TYR:N	2.30	0.64
2:B:798:TYR:O	2:B:821:GLN:NE2	2.20	0.63
7:G:1:MET:HE3	7:G:85:GLU:OE2	1.99	0.63
2:B:44:VAL:HG11	2:B:495:LEU:HD12	1.80	0.63
4:D:49:ALA:CB	7:G:3:PHE:CE1	2.82	0.63
9:I:9:ASP:OD2	16:Q:125:LYS:CE	2.47	0.63
3:C:75:MET:HE1	3:C:239:PRO:HG3	1.80	0.63
13:M:200:THR:O	13:M:203:PHE:HB3	1.97	0.63
16:Q:141:ARG:O	17:R:207:THR:OG1	2.13	0.63
1:A:326:ARG:HE	1:A:1406:VAL:HG21	1.62	0.63
1:A:806:ARG:HH22	2:B:729:ILE:HG13	1.63	0.63
18:T:49:DA:H2'	18:T:50:DT:H5'	1.79	0.63
5:E:76:GLY:N	5:E:106:GLN:OE1	2.31	0.63
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.80	0.63
2:B:278:GLN:HB2	2:B:337:ARG:HD2	1.79	0.63
17:R:98:ASN:HB3	17:R:103:LYS:HG3	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:44:DA:H2''	18:T:45:DT:O5'	1.99	0.63
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.81	0.62
9:I:58:VAL:HG21	9:I:109:ILE:HD11	1.80	0.62
1:A:1189:SER:N	1:A:1242:VAL:O	2.28	0.62
5:E:78:LEU:HD21	5:E:109:ILE:HD12	1.80	0.62
1:A:282:ASN:HA	21:W:59:ALA:CB	2.29	0.62
10:J:8:PHE:HB2	10:J:48:ARG:HH22	1.64	0.62
13:M:201:LYS:HA	14:N:23:DA:OP1	1.99	0.62
13:M:274:PRO:CD	15:O:188:GLU:CG	2.74	0.62
2:B:901:PRO:HG2	12:L:60:ARG:HA	1.80	0.62
3:C:146:LYS:NZ	10:J:58:GLU:OE2	2.24	0.62
13:M:267:LYS:CE	15:O:208:VAL:HG13	2.03	0.62
3:C:56:THR:HG22	3:C:147:LEU:HD21	1.81	0.62
5:E:55:ARG:HB2	5:E:84:ASP:OD1	1.99	0.62
1:A:352:VAL:HB	1:A:467:THR:HG22	1.81	0.62
2:B:41:LYS:O	2:B:45:SER:HB3	1.99	0.62
13:M:281:SER:O	13:M:285:ASN:ND2	2.31	0.62
7:G:151:ILE:HD12	21:W:134:LEU:CB	2.29	0.62
18:T:52:DC:H2''	18:T:53:DA:H5'	1.82	0.62
1:A:1146:VAL:HG12	1:A:1201:ALA:HB1	1.81	0.62
4:D:56:ARG:HA	4:D:148:LEU:HD13	1.81	0.62
18:T:42:DC:H2''	18:T:43:DT:C4	2.35	0.62
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.35	0.62
3:C:153:LEU:HD11	3:C:155:LEU:HD23	1.82	0.62
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.82	0.61
3:C:179:GLU:OE1	3:C:206:ASN:ND2	2.32	0.61
9:I:14:LEU:HB3	9:I:27:PHE:HB3	1.81	0.61
2:B:217:ARG:NH1	2:B:407:ASP:CG	2.58	0.61
3:C:254:LYS:HG2	11:K:42:LEU:HD12	1.82	0.61
7:G:1:MET:CE	7:G:85:GLU:OE2	2.49	0.61
15:O:170:ILE:O	15:O:239:LYS:HE2	2.00	0.61
1:A:587:HIS:CD2	1:A:969:GLN:HG3	2.35	0.61
2:B:870:ILE:HG23	2:B:917:PRO:HD2	1.83	0.61
1:A:335:ARG:NH2	2:B:1114:LEU:HD21	2.14	0.61
1:A:544:ASP:OD1	1:A:545:GLN:N	2.33	0.61
2:B:325:GLN:NE2	16:Q:401:TYR:OH	2.28	0.61
2:B:868:MET:HG2	13:M:182:ARG:HG3	1.83	0.61
4:D:32:GLU:CG	7:G:42:PHE:CE1	2.84	0.61
1:A:260:ASP:OD1	1:A:261:ASP:N	2.34	0.61
2:B:68:THR:CB	16:Q:335:LEU:HD12	2.30	0.61
2:B:865:LYS:NZ	13:M:145:ILE:CD1	2.63	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:865:LYS:HE2	13:M:145:ILE:HD12	1.76	0.61
16:Q:339:ALA:HB1	16:Q:343:ARG:HH12	1.65	0.61
19:U:37:ASP:O	19:U:41:ILE:HG13	2.01	0.61
1:A:929:LEU:HD11	1:A:983:ILE:HG21	1.83	0.60
13:M:43:VAL:HG12	13:M:53:SER:HB3	1.82	0.60
13:M:267:LYS:HD3	15:O:239:LYS:CD	2.31	0.60
2:B:119:LEU:HD22	2:B:953:LEU:HD21	1.82	0.60
2:B:199:MET:SD	2:B:492:LEU:HD23	2.42	0.60
21:W:39:ALA:HA	21:W:85:VAL:O	2.01	0.60
18:T:51:DA:C2'	18:T:52:DC:C6	2.83	0.60
1:A:261:ASP:HB3	1:A:322:VAL:HG13	1.83	0.60
13:M:242:PHE:HE1	17:R:270:MET:HE1	1.65	0.60
8:H:104:PHE:HZ	8:H:137:GLN:H	1.48	0.60
18:T:50:DT:H2''	18:T:51:DA:H5'	1.82	0.60
1:A:1199:ARG:O	1:A:1203:ASN:ND2	2.35	0.60
2:B:465:ASN:OD1	2:B:465:ASN:N	2.33	0.60
3:C:115:SER:HB3	3:C:142:VAL:HB	1.83	0.60
16:Q:378:VAL:HG22	16:Q:384:PHE:CE1	2.36	0.60
18:T:43:DT:C6	18:T:43:DT:P	2.94	0.60
19:U:31:ASP:HB3	19:U:34:THR:OG1	2.02	0.60
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.02	0.59
2:B:429:PHE:CZ	16:Q:332:LEU:HB2	2.37	0.59
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.82	0.59
1:A:993:LEU:HD11	1:A:1050:GLU:HB2	1.84	0.59
2:B:247:GLY:CA	2:B:418:LYS:HZ1	2.13	0.59
2:B:283:VAL:HG11	2:B:321:GLY:HA3	1.82	0.59
18:T:47:DA:H2'	18:T:48:DT:C5	2.38	0.59
2:B:326:ASP:OD1	2:B:327:ARG:N	2.35	0.59
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.83	0.59
7:G:138:THR:HG22	7:G:139:ILE:H	1.67	0.59
1:A:95:PHE:HE1	1:A:1414:ALA:HB2	1.67	0.59
1:A:568:PRO:HG2	8:H:46:LEU:HD23	1.84	0.59
3:C:124:LEU:O	3:C:127:ARG:HG2	2.01	0.59
21:W:39:ALA:O	21:W:41:ASP:N	2.28	0.59
1:A:345:VAL:HG12	2:B:1155:SER:HB2	1.84	0.59
1:A:1116:LEU:HB2	1:A:1308:THR:HB	1.84	0.59
2:B:186:GLU:HG2	2:B:190:TYR:HE2	1.67	0.59
2:B:62:ILE:O	2:B:65:GLU:HG2	2.01	0.59
2:B:71:LEU:HD12	16:Q:331:GLN:O	2.02	0.59
7:G:57:GLN:HG2	7:G:58:ARG:H	1.67	0.59
16:Q:373:TYR:OH	17:R:72:ARG:NH2	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:242:ASN:HA	19:U:268:THR:O	2.02	0.59
1:A:390:GLN:OE1	1:A:393:ARG:NH2	2.36	0.59
2:B:1042:GLY:HA2	16:Q:22:ILE:HA	1.83	0.59
15:O:191:PRO:CG	18:T:52:DC:C5'	2.80	0.59
7:G:148:GLU:H	7:G:161:GLY:HA2	1.67	0.59
12:L:33:GLU:HG3	12:L:34:CYS:N	2.18	0.59
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.84	0.58
2:B:1065:GLN:OE1	2:B:1066:SER:N	2.37	0.58
1:A:472:LEU:HD22	2:B:835:GLN:NE2	2.17	0.58
2:B:43:LEU:HD11	2:B:812:LEU:HD23	1.84	0.58
2:B:1037:LEU:O	10:J:47:ARG:NH2	2.36	0.58
16:Q:119:LEU:O	17:R:132:GLU:HA	2.03	0.58
5:E:58:MET:HE2	5:E:82:PHE:HE2	1.68	0.58
13:M:267:LYS:HE2	15:O:208:VAL:HG11	1.79	0.58
17:R:138:GLN:HB2	17:R:211:LYS:CB	2.31	0.58
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.38	0.58
4:D:54:GLU:HG2	4:D:58:VAL:HG23	1.84	0.58
4:D:57:LEU:O	4:D:61:GLU:N	2.32	0.58
4:D:153:ARG:NH1	4:D:183:LEU:O	2.37	0.58
18:T:50:DT:H2'	18:T:51:DA:C8	2.38	0.58
1:A:1206:ASP:O	1:A:1274:ARG:NH2	2.37	0.58
2:B:835:GLN:HA	2:B:1013:ASN:ND2	2.19	0.58
12:L:33:GLU:HG3	12:L:34:CYS:H	1.69	0.58
2:B:109:THR:HG21	17:R:263:MET:HG3	1.86	0.58
17:R:306:LEU:O	17:R:310:TYR:N	2.37	0.58
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.39	0.58
1:A:381:THR:HG23	1:A:383:TYR:H	1.69	0.58
16:Q:373:TYR:HD1	17:R:70:LEU:HD11	1.68	0.58
16:Q:373:TYR:CE1	17:R:70:LEU:HD21	2.38	0.58
1:A:42:ASP:OD1	1:A:43:GLU:N	2.37	0.58
8:H:7:ASP:OD1	8:H:8:ASP:N	2.37	0.58
1:A:1444:MET:HE2	6:F:135:ARG:HB2	1.85	0.58
2:B:956:THR:HG23	12:L:46:VAL:HB	1.86	0.58
3:C:148:ARG:NH2	10:J:64:ASN:HA	2.19	0.58
15:O:105:ARG:HD2	20:V:69:TYR:OH	2.03	0.57
18:T:48:DT:C2'	18:T:49:DA:C8	2.86	0.57
3:C:149:LYS:HG3	3:C:150:GLY:N	2.19	0.57
10:J:8:PHE:HB2	10:J:48:ARG:NH2	2.19	0.57
1:A:503:GLN:OE1	6:F:90:ARG:NH1	2.32	0.57
1:A:903:ASN:OD1	1:A:904:THR:N	2.37	0.57
2:B:911:ILE:HD11	2:B:941:LEU:HD12	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1106:ARG:CZ	2:B:1118:PRO:HB3	2.34	0.57
2:B:1187:ASN:ND2	2:B:1190:ASP:O	2.38	0.57
2:B:156:SER:O	2:B:163:GLY:N	2.37	0.57
2:B:369:GLY:C	16:Q:367:ALA:HB3	2.29	0.57
2:B:676:VAL:O	2:B:677:GLU:HG2	2.04	0.57
7:G:101:VAL:N	7:G:108:VAL:O	2.36	0.57
17:R:98:ASN:ND2	17:R:103:LYS:HE3	2.20	0.57
5:E:43:LYS:O	5:E:47:CYS:HB2	2.05	0.57
8:H:64:ASN:OD1	8:H:65:LEU:N	2.38	0.57
13:M:201:LYS:CA	14:N:23:DA:OP1	2.50	0.57
1:A:1445:ILE:HB	7:G:61:ILE:HD11	1.87	0.57
2:B:73:GLN:O	2:B:86:ARG:N	2.33	0.57
2:B:642:ASP:HA	2:B:649:LYS:HG2	1.86	0.57
5:E:65:THR:O	5:E:69:ILE:HD12	2.04	0.57
8:H:89:LEU:C	8:H:91:ASP:H	2.13	0.57
14:N:61:DC:H2'	14:N:62:DA:C8	2.40	0.57
1:A:34:LYS:NZ	1:A:85:ASP:OD2	2.38	0.57
1:A:365:GLY:HA2	1:A:461:LYS:O	2.05	0.57
1:A:471:ASN:OD1	1:A:472:LEU:N	2.37	0.57
2:B:209:GLU:OE2	2:B:788:ARG:NH2	2.37	0.57
17:R:120:TYR:CD1	17:R:226:PRO:HA	2.39	0.57
1:A:752:LYS:HG3	2:B:1015:HIS:HB3	1.85	0.56
2:B:259:TYR:HE2	2:B:270:LYS:HB2	1.69	0.56
2:B:365:THR:HG21	2:B:370:PHE:CG	2.40	0.56
9:I:31:THR:O	16:Q:401:TYR:CB	2.53	0.56
1:A:367:PRO:HG2	1:A:466:SER:O	2.04	0.56
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.88	0.56
1:A:545:GLN:HG2	1:A:549:MET:HE3	1.86	0.56
1:A:940:ARG:HH21	1:A:944:ARG:NH2	2.03	0.56
2:B:209:GLU:O	2:B:482:VAL:HA	2.06	0.56
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.19	0.56
8:H:56:THR:O	8:H:144:ILE:HA	2.06	0.56
13:M:177:LEU:HD22	13:M:207:LEU:HD11	1.85	0.56
17:R:64:SER:O	17:R:217:THR:HG23	2.06	0.56
18:T:52:DC:P	18:T:52:DC:C3'	2.94	0.56
5:E:179:GLN:HA	5:E:215:MET:HG2	1.86	0.56
15:O:91:ASN:HD22	19:U:285:TRP:HZ2	1.51	0.56
1:A:562:THR:O	1:A:576:GLN:NE2	2.37	0.56
16:Q:339:ALA:HB1	16:Q:343:ARG:NH1	2.20	0.56
1:A:29:ALA:HB1	2:B:1184:GLY:HA3	1.87	0.56
1:A:1146:VAL:HG23	1:A:1197:LEU:HD22	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:563:MET:HE1	2:B:587:HIS:HB2	1.88	0.56
7:G:119:LEU:HD11	7:G:130:TYR:HB3	1.87	0.56
1:A:1138:ILE:O	1:A:1276:VAL:N	2.34	0.56
13:M:243:CYS:O	13:M:247:GLY:N	2.39	0.56
16:Q:100:GLU:HA	17:R:96:ARG:HA	1.86	0.56
1:A:146:MET:O	1:A:171:GLN:N	2.38	0.56
3:C:6:PRO:HB3	3:C:25:VAL:CG2	2.35	0.56
1:A:203:SER:N	1:A:206:GLU:OE2	2.39	0.56
1:A:491:VAL:O	2:B:1150:ARG:NH2	2.39	0.56
2:B:29:ASP:OD2	2:B:658:ILE:HG13	2.05	0.56
2:B:108:VAL:HA	13:M:244:SER:OG	2.06	0.56
3:C:60:ASP:HB3	12:L:67:PHE:HE2	1.70	0.56
7:G:79:PHE:CE2	7:G:81:PRO:CG	2.86	0.56
17:R:262:THR:O	17:R:266:THR:HG23	2.04	0.56
1:A:475:THR:OG1	1:A:480:ALA:O	2.21	0.56
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.41	0.56
1:A:1342:GLU:OE1	5:E:200:ARG:NH2	2.29	0.56
2:B:211:VAL:O	2:B:480:SER:HA	2.06	0.56
2:B:861:ASP:OD1	2:B:862:GLN:N	2.38	0.56
13:M:238:TYR:HB3	13:M:242:PHE:CE2	2.40	0.56
2:B:170:LEU:HD12	2:B:171:PRO:HD2	1.88	0.55
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.71	0.55
13:M:180:CYS:SG	13:M:187:ARG:HG2	2.46	0.55
17:R:127:LYS:HA	17:R:220:HIS:CE1	2.41	0.55
14:N:24:DT:H2''	14:N:25:DA:C5'	2.17	0.55
2:B:923:GLU:HB2	2:B:928:ARG:HD2	1.88	0.55
7:G:50:ASP:OD2	7:G:53:ASN:HB2	2.07	0.55
13:M:267:LYS:HD3	15:O:239:LYS:HD3	1.87	0.55
19:U:245:LEU:HB3	20:V:9:LEU:HD22	1.89	0.55
1:A:778:GLY:HA3	2:B:516:ASN:HB2	1.86	0.55
1:A:1224:LEU:HD12	1:A:1241:ARG:O	2.05	0.55
19:U:25:PHE:O	19:U:30:ILE:HG22	2.05	0.55
19:U:30:ILE:O	19:U:31:ASP:HB2	2.06	0.55
1:A:666:ILE:HG23	2:B:1026:LEU:HB3	1.87	0.55
1:A:833:GLU:OE2	1:A:1102:LYS:HD2	2.06	0.55
1:A:1148:ILE:HA	9:I:49:ILE:HD12	1.87	0.55
2:B:46:GLN:HG2	2:B:408:LEU:HD21	1.88	0.55
2:B:557:PHE:CZ	2:B:603:LEU:HD11	2.41	0.55
2:B:35:SER:OG	2:B:811:TYR:OH	2.18	0.55
2:B:46:GLN:OE1	2:B:46:GLN:N	2.32	0.55
2:B:296:GLU:HG2	2:B:300:HIS:NE2	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:28:DA:C8	14:N:29:DT:H73	2.42	0.55
16:Q:366:GLU:CB	16:Q:392:VAL:HG13	2.36	0.55
17:R:122:LEU:HD21	17:R:222:CYS:HB3	1.89	0.55
20:V:60:LEU:HD21	20:V:87:VAL:HG22	1.89	0.55
1:A:566:ILE:O	8:H:96:VAL:HB	2.07	0.55
1:A:1364:ASN:OD1	1:A:1365:TYR:N	2.40	0.55
2:B:104:GLU:OE2	12:L:54:ARG:HD2	2.07	0.55
14:N:22:DT:C2'	14:N:23:DA:O5'	2.54	0.55
16:Q:119:LEU:HD22	16:Q:395:PHE:CE2	2.41	0.55
2:B:44:VAL:CG1	2:B:495:LEU:CD1	2.81	0.54
2:B:865:LYS:HZ1	13:M:145:ILE:CD1	2.19	0.54
14:N:29:DT:C2'	14:N:30:DA:C8	2.84	0.54
15:O:169:PRO:HG2	15:O:240:MET:SD	2.47	0.54
1:A:1386:ARG:HH21	18:T:13:DC:H4'	1.72	0.54
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.88	0.54
4:D:39:ASN:ND2	4:D:43:GLU:HB2	2.21	0.54
4:D:49:ALA:HB1	7:G:3:PHE:HE1	1.72	0.54
17:R:98:ASN:CB	17:R:103:LYS:O	2.53	0.54
1:A:434:ARG:HD2	1:A:437:MET:HE2	1.89	0.54
3:C:46:ILE:HA	3:C:159:ALA:HA	1.89	0.54
13:M:267:LYS:HZ2	15:O:169:PRO:HB3	1.64	0.54
1:A:225:ASN:N	1:A:229:SER:OG	2.28	0.54
1:A:1144:LYS:HE3	9:I:48:LEU:HD22	1.89	0.54
1:A:1386:ARG:O	1:A:1390:ASN:HB3	2.07	0.54
9:I:9:ASP:OD2	16:Q:125:LYS:HE3	2.07	0.54
1:A:436:ILE:HD11	1:A:491:VAL:HG21	1.89	0.54
1:A:441:PRO:HD2	1:A:498:ARG:NH1	2.22	0.54
1:A:570:PRO:O	1:A:571:LEU:HD12	2.07	0.54
3:C:6:PRO:HB3	3:C:25:VAL:HG23	1.90	0.54
3:C:254:LYS:O	3:C:257:SER:OG	2.21	0.54
7:G:62:LEU:HD12	7:G:63:PRO:O	2.08	0.54
14:N:22:DT:H2''	14:N:23:DA:O5'	2.04	0.54
4:D:49:ALA:HA	7:G:3:PHE:CE1	2.43	0.54
2:B:86:ARG:HG3	2:B:137:TYR:O	2.08	0.54
2:B:1073:TYR:CE1	2:B:1080:LYS:HG2	2.43	0.54
3:C:136:ASP:OD1	3:C:137:LYS:N	2.41	0.54
17:R:122:LEU:HD21	17:R:222:CYS:SG	2.47	0.54
1:A:798:GLY:HA2	1:A:815:PHE:CD2	2.43	0.54
2:B:298:LEU:HD23	2:B:311:LEU:HD22	1.89	0.54
2:B:368:GLU:OE2	16:Q:344:PHE:HD1	1.90	0.54
1:A:285:PRO:HD2	1:A:288:ALA:HB3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:756:ILE:HG12	2:B:770:GLN:HG2	1.89	0.53
2:B:1094:ARG:NH2	2:B:1098:MET:SD	2.82	0.53
13:M:177:LEU:HD11	13:M:189:PHE:CD1	2.43	0.53
1:A:821:ARG:HD2	2:B:514:LEU:H	1.73	0.53
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.88	0.53
4:D:134:THR:HG22	4:D:136:GLY:H	1.73	0.53
9:I:56:ALA:O	9:I:89:GLN:HG3	2.09	0.53
13:M:283:TYR:CZ	13:M:287:LEU:HD11	2.44	0.53
3:C:102:GLN:HG3	3:C:154:LYS:HG3	1.90	0.53
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.48	0.53
1:A:284:ALA:HB1	1:A:289:ILE:HD11	1.90	0.53
2:B:129:PHE:HA	2:B:165:VAL:O	2.09	0.53
13:M:43:VAL:O	13:M:52:LEU:N	2.39	0.53
17:R:105:THR:HG1	17:R:120:TYR:C	2.10	0.53
1:A:804:TYR:HH	1:A:816:HIS:CE1	2.26	0.53
4:D:183:LEU:HD11	7:G:86:VAL:O	2.08	0.53
7:G:81:PRO:HB3	7:G:106:MET:HE1	1.89	0.53
13:M:273:SER:HB2	15:O:188:GLU:HA	1.89	0.53
16:Q:98:TYR:HA	17:R:97:ILE:O	2.08	0.53
2:B:104:GLU:OE2	12:L:54:ARG:CD	2.55	0.53
5:E:26:ARG:NH2	5:E:133:GLU:OE1	2.42	0.53
1:A:977:LYS:O	1:A:1036:ARG:NH2	2.38	0.53
2:B:969:ARG:HH22	3:C:60:ASP:HB2	1.74	0.53
1:A:13:THR:OG1	1:A:1432:GLN:OE1	2.27	0.53
1:A:909:ASP:OD2	1:A:911:SER:OG	2.21	0.53
8:H:136:LYS:O	8:H:138:GLU:N	2.41	0.53
2:B:283:VAL:O	2:B:287:ARG:HG2	2.09	0.53
4:D:64:VAL:HG13	4:D:67:ARG:HH22	1.74	0.53
7:G:86:VAL:HA	7:G:146:LYS:HA	1.90	0.53
16:Q:99:ASN:O	17:R:97:ILE:N	2.37	0.53
1:A:806:ARG:NH2	2:B:729:ILE:HG13	2.24	0.53
9:I:103:CYS:SG	9:I:105:SER:OG	2.62	0.53
17:R:63:ARG:HD2	17:R:66:ARG:CZ	2.39	0.53
1:A:810:PRO:HB2	2:B:705:MET:HE2	1.91	0.52
1:A:839:ARG:NH2	1:A:1402:PHE:O	2.33	0.52
2:B:841:MET:O	2:B:993:THR:HA	2.09	0.52
13:M:255:SER:OG	13:M:285:ASN:OD1	2.17	0.52
1:A:208:LEU:HD21	1:A:212:LYS:HE3	1.90	0.52
2:B:451:LYS:O	2:B:455:SER:OG	2.17	0.52
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.74	0.52
2:B:499:ASN:OD1	2:B:500:THR:N	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.90	0.52
16:Q:365:TYR:CZ	16:Q:367:ALA:HA	2.45	0.52
1:A:826:ASP:OD1	1:A:827:THR:N	2.43	0.52
2:B:822:ASN:O	10:J:48:ARG:NH1	2.43	0.52
4:D:194:LEU:HD22	7:G:86:VAL:HG21	1.92	0.52
1:A:16:GLU:CG	1:A:1418:LEU:HD11	2.40	0.52
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.91	0.52
2:B:96:TYR:HB2	2:B:129:PHE:HB2	1.92	0.52
2:B:179:CYS:SG	2:B:180:TYR:N	2.82	0.52
2:B:296:GLU:OE2	16:Q:122:GLN:NE2	2.42	0.52
3:C:21:ILE:HG12	3:C:229:TYR:CD1	2.44	0.52
9:I:19:ASP:O	9:I:23:ASN:HA	2.10	0.52
9:I:28:GLU:HA	9:I:35:VAL:HG22	1.92	0.52
13:M:177:LEU:O	13:M:181:ARG:HG2	2.09	0.52
1:A:522:GLY:O	1:A:524:VAL:HG23	2.10	0.52
1:A:1350:LYS:O	1:A:1354:ASN:ND2	2.42	0.52
2:B:99:LYS:HB3	2:B:180:TYR:CE1	2.45	0.52
2:B:100:PRO:HD2	2:B:180:TYR:CZ	2.44	0.52
4:D:148:LEU:O	4:D:152:SER:OG	2.15	0.52
7:G:10:ASN:HA	7:G:70:PHE:O	2.10	0.52
1:A:367:PRO:HA	1:A:463:ILE:O	2.09	0.52
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.44	0.52
13:M:133:ILE:HG13	13:M:172:MET:HE3	1.92	0.52
13:M:174:ALA:O	13:M:178:ILE:HG12	2.10	0.52
1:A:873:MET:HE1	1:A:1053:PHE:CZ	2.45	0.52
2:B:637:LEU:HD12	2:B:693:ILE:HD13	1.91	0.52
7:G:95:SER:O	7:G:130:TYR:OH	2.27	0.52
8:H:130:ARG:O	8:H:133:ASN:ND2	2.41	0.52
15:O:191:PRO:HB3	18:T:52:DC:C5'	2.29	0.52
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.93	0.52
5:E:122:LYS:O	5:E:125:PRO:HD2	2.10	0.52
1:A:1132:LYS:HG2	1:A:1135:ARG:HH22	1.75	0.51
1:A:1151:GLU:OE2	9:I:42:LEU:HD13	2.10	0.51
10:J:6:ARG:HA	10:J:13:VAL:HA	1.92	0.51
13:M:267:LYS:HE2	15:O:208:VAL:HG12	1.84	0.51
17:R:121:ASP:O	17:R:225:MET:HB2	2.10	0.51
17:R:126:LYS:HD2	17:R:129:VAL:HG12	1.91	0.51
19:U:259:LYS:HA	19:U:281:VAL:O	2.10	0.51
1:A:407:ARG:NH1	1:A:413:ILE:HD11	2.25	0.51
4:D:70:PHE:HE2	4:D:133:THR:HA	1.75	0.51
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.90	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:757:PRO:HG3	2:B:983:ARG:HH21	1.75	0.51
4:D:118:THR:HG21	4:D:121:LYS:HG2	1.91	0.51
13:M:154:TYR:CE1	13:M:171:ILE:HD13	2.45	0.51
16:Q:103:LEU:HD23	16:Q:384:PHE:HB2	1.92	0.51
14:N:21:DG:H2'	14:N:22:DT:H71	1.93	0.51
18:T:49:DA:C2'	18:T:50:DT:C5'	2.85	0.51
6:F:147:SER:O	6:F:150:GLU:HG2	2.11	0.51
8:H:100:THR:OG1	8:H:139:ASN:OD1	2.20	0.51
10:J:21:TYR:CZ	10:J:25:LEU:HD11	2.45	0.51
1:A:137:ALA:O	1:A:140:THR:OG1	2.19	0.51
2:B:405:ARG:HH12	2:B:632:ARG:CG	1.99	0.51
2:B:776:GLN:HG3	2:B:1095:LEU:HD22	1.91	0.51
2:B:1168:LEU:HD22	2:B:1208:MET:HE3	1.92	0.51
7:G:21:ARG:HG3	7:G:25:TYR:HE1	1.75	0.51
1:A:407:ARG:NH2	13:M:26:GLU:OE2	2.44	0.51
1:A:996:ASN:HB3	1:A:1050:GLU:OE2	2.11	0.51
2:B:840:ILE:O	2:B:1010:LEU:HD12	2.10	0.51
4:D:49:ALA:HB1	7:G:3:PHE:CE1	2.45	0.51
8:H:36:CYS:HA	8:H:126:GLU:O	2.11	0.51
8:H:107:VAL:HG13	8:H:108:SER:H	1.75	0.51
10:J:48:ARG:O	10:J:52:THR:OG1	2.10	0.51
13:M:191:GLU:HB3	17:R:268:MET:SD	2.51	0.51
1:A:613:ILE:HG22	1:A:614:PHE:HD1	1.76	0.51
2:B:868:MET:CG	13:M:149:CYS:SG	2.99	0.51
2:B:1076:HIS:O	3:C:31:ASN:ND2	2.44	0.51
3:C:33:LEU:HG	3:C:37:MET:HE2	1.92	0.51
5:E:191:LYS:N	5:E:194:GLU:OE1	2.39	0.51
2:B:474:SER:O	2:B:475:SER:HB3	2.11	0.51
11:K:63:VAL:HG12	11:K:71:PHE:HB3	1.93	0.51
13:M:143:PRO:HG2	13:M:146:VAL:HG23	1.93	0.51
1:A:350:ARG:NE	1:A:486:GLU:OE1	2.44	0.51
7:G:151:ILE:HG13	21:W:134:LEU:CA	2.41	0.51
18:T:43:DT:H2''	18:T:44:DA:H8	1.67	0.51
1:A:209:ASN:OD1	1:A:213:HIS:NE2	2.44	0.50
1:A:597:LEU:HD13	8:H:103:LYS:HD3	1.93	0.50
16:Q:399:ASN:OD1	16:Q:402:ALA:HA	2.11	0.50
1:A:871:ASP:CG	1:A:1366:ARG:HH21	2.18	0.50
2:B:87:LYS:HE3	2:B:147:LEU:HD11	1.92	0.50
2:B:187:SER:HA	2:B:190:TYR:HD2	1.76	0.50
2:B:311:LEU:HA	2:B:314:LEU:HD12	1.93	0.50
2:B:706:GLN:HB2	2:B:709:ASP:HB2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:99:LEU:O	6:F:102:SER:OG	2.19	0.50
1:A:23:SER:OG	1:A:25:GLU:OE1	2.28	0.50
1:A:225:ASN:H	1:A:229:SER:HG	1.55	0.50
1:A:1138:ILE:HG13	1:A:1139:GLU:N	2.27	0.50
1:A:1442:ASP:OD2	7:G:60:ARG:HD2	2.12	0.50
4:D:32:GLU:HB3	7:G:42:PHE:HE1	1.77	0.50
4:D:39:ASN:HA	7:G:6:ASP:OD2	2.10	0.50
13:M:306:GLU:O	13:M:309:ILE:HG12	2.11	0.50
13:M:325:ASP:HB3	13:M:326:PRO:HD3	1.92	0.50
1:A:1402:PHE:CD2	1:A:1403:GLU:HG2	2.45	0.50
5:E:161:LYS:NZ	5:E:193:GLY:O	2.41	0.50
7:G:101:VAL:HG21	7:G:145:VAL:HG21	1.93	0.50
13:M:134:THR:HG23	13:M:147:LYS:NZ	2.26	0.50
13:M:269:ILE:C	13:M:271:GLY:H	2.17	0.50
1:A:901:LEU:HB3	1:A:921:GLY:H	1.77	0.50
1:A:1402:PHE:CE2	1:A:1403:GLU:HG2	2.46	0.50
3:C:40:GLU:OE1	3:C:254:LYS:HE3	2.10	0.50
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.92	0.50
4:D:56:ARG:HB2	4:D:148:LEU:HB3	1.92	0.50
1:A:377:PRO:HB3	1:A:433:GLU:HG2	1.93	0.50
2:B:475:SER:O	2:B:476:ARG:CB	2.60	0.50
2:B:548:GLY:HA3	2:B:630:ALA:HB2	1.94	0.50
18:T:43:DT:P	18:T:43:DT:H6	2.33	0.50
1:A:736:ASN:C	1:A:736:ASN:HD22	2.19	0.50
2:B:55:VAL:O	17:R:252:ILE:HD12	2.12	0.50
2:B:496:ARG:NH2	2:B:540:SER:O	2.45	0.50
1:A:381:THR:OG1	1:A:382:PRO:HD2	2.11	0.50
2:B:368:GLU:OE2	16:Q:344:PHE:CD1	2.65	0.50
7:G:83:LYS:HE3	7:G:150:CYS:HB2	1.94	0.50
7:G:97:HIS:O	7:G:112:LYS:N	2.43	0.50
9:I:88:SER:O	9:I:91:ARG:NH1	2.45	0.50
15:O:169:PRO:HB2	15:O:239:LYS:HB2	1.93	0.50
1:A:663:SER:OG	1:A:664:THR:N	2.44	0.50
8:H:35:GLN:HB3	8:H:111:LEU:HD21	1.94	0.50
13:M:30:TYR:CD1	13:M:31:PRO:HD2	2.47	0.50
13:M:272:LYS:O	13:M:273:SER:OG	2.24	0.50
1:A:1116:LEU:HD12	1:A:1311:VAL:HG22	1.93	0.49
1:A:1155:ASP:OD2	1:A:1161:THR:HA	2.12	0.49
2:B:463:THR:C	2:B:465:ASN:OD1	2.55	0.49
2:B:486:TYR:HA	2:B:1096:ARG:HH21	1.76	0.49
16:Q:100:GLU:HG2	17:R:96:ARG:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:ARG:HD2	2:B:514:LEU:N	2.27	0.49
2:B:67:SER:HB2	2:B:92:PHE:HB2	1.94	0.49
2:B:149:TYR:HE2	2:B:151:LEU:HD23	1.78	0.49
3:C:25:VAL:HG12	3:C:26:ASP:O	2.13	0.49
3:C:125:MET:HB2	3:C:127:ARG:NH1	2.27	0.49
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.27	0.49
2:B:69:LEU:HD12	2:B:69:LEU:O	2.12	0.49
4:D:33:PHE:HZ	7:G:42:PHE:HA	1.77	0.49
5:E:202:SER:HB3	5:E:206:GLY:H	1.77	0.49
13:M:201:LYS:HE3	14:N:23:DA:O5'	2.12	0.49
1:A:51:GLY:H	1:A:55:ASP:HB3	1.77	0.49
2:B:53:GLN:HG3	2:B:57:TYR:HD2	1.77	0.49
2:B:570:VAL:HG23	2:B:573:GLN:HB3	1.94	0.49
3:C:35:ARG:NE	11:K:41:THR:OG1	2.35	0.49
5:E:48:ASP:OD1	5:E:51:GLY:N	2.45	0.49
7:G:114:LEU:HD23	7:G:162:SER:HB3	1.94	0.49
1:A:733:ALA:O	1:A:737:LEU:HG	2.11	0.49
3:C:52:GLU:HG2	3:C:53:THR:HG23	1.94	0.49
4:D:52:LEU:HA	4:D:55:ALA:HB3	1.95	0.49
8:H:101:ALA:HB2	8:H:116:TYR:CE1	2.47	0.49
9:I:59:VAL:HG12	9:I:61:ASP:H	1.76	0.49
13:M:22:LEU:O	13:M:32:PRO:HB3	2.13	0.49
13:M:157:CYS:HB3	13:M:210:MET:SD	2.52	0.49
20:V:25:THR:O	20:V:29:ASP:HB3	2.13	0.49
1:A:848:ILE:HG12	1:A:858:ASN:HB3	1.94	0.49
2:B:106:ASP:OD1	2:B:108:VAL:HG12	2.12	0.49
2:B:601:ARG:HD3	2:B:605:ARG:NH2	2.28	0.49
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.94	0.49
16:Q:133:PHE:HZ	16:Q:353:GLU:HA	1.77	0.49
20:V:34:ALA:C	20:V:36:LEU:H	2.21	0.49
2:B:325:GLN:HB3	16:Q:401:TYR:HH	1.72	0.49
2:B:1164:GLY:HA3	2:B:1190:ASP:OD2	2.13	0.49
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.95	0.49
3:C:169:LYS:NZ	12:L:69:ALA:HB3	2.28	0.49
5:E:16:PHE:CZ	5:E:20:LYS:HE3	2.46	0.49
9:I:71:SER:OG	9:I:83:ASN:OD1	2.25	0.49
16:Q:100:GLU:OE2	17:R:96:ARG:NH2	2.45	0.49
16:Q:139:LEU:HD12	16:Q:351:VAL:O	2.13	0.49
18:T:52:DC:H2''	18:T:53:DA:C5'	2.42	0.49
1:A:64:ASN:HA	13:M:20:ILE:HB	1.95	0.49
1:A:666:ILE:HD11	2:B:1030:LEU:HD22	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:778:MET:HA	2:B:1096:ARG:HH12	1.76	0.49
14:N:23:DA:N6	18:T:51:DA:N6	2.60	0.49
1:A:8:SER:OG	2:B:1178:ASN:ND2	2.45	0.49
1:A:1420:ASP:OD2	1:A:1422:ARG:NE	2.36	0.49
2:B:856:PHE:CE1	2:B:969:ARG:HB3	2.48	0.49
7:G:83:LYS:HG2	7:G:149:GLY:HA2	1.94	0.49
2:B:22:SER:O	2:B:654:ARG:NH1	2.44	0.49
3:C:80:LEU:HD12	3:C:94:LYS:O	2.13	0.49
4:D:188:ALA:HB2	4:D:208:GLU:HG3	1.95	0.49
5:E:23:VAL:HG12	5:E:28:TYR:HB2	1.95	0.49
7:G:115:MET:HB3	7:G:119:LEU:HD23	1.94	0.49
13:M:277:ILE:HA	13:M:280:VAL:HG22	1.94	0.49
21:W:43:LEU:O	21:W:47:LEU:N	2.44	0.49
1:A:446:ARG:HB2	1:A:487:MET:HE2	1.93	0.48
2:B:249:ARG:HH12	2:B:418:LYS:HB2	1.78	0.48
2:B:604:ARG:NH2	2:B:615:MET:HG2	2.28	0.48
2:B:619:ILE:O	9:I:59:VAL:HG21	2.12	0.48
2:B:807:ARG:HG2	2:B:1043:ASP:OD1	2.13	0.48
8:H:89:LEU:O	8:H:91:ASP:N	2.46	0.48
19:U:241:GLU:O	19:U:241:GLU:HG2	2.12	0.48
1:A:445:ASN:OD1	1:A:446:ARG:N	2.46	0.48
1:A:1444:MET:SD	6:F:135:ARG:NH2	2.84	0.48
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.45	0.48
2:B:569:TYR:CE2	2:B:571:PRO:HG3	2.48	0.48
3:C:59:ALA:O	3:C:62:PHE:HB3	2.13	0.48
4:D:194:LEU:HB3	7:G:86:VAL:HG21	1.95	0.48
13:M:199:LYS:O	13:M:200:THR:HB	2.13	0.48
13:M:267:LYS:HG3	13:M:268:GLU:N	2.27	0.48
1:A:1438:THR:HG23	6:F:92:ARG:HB2	1.95	0.48
8:H:13:SER:N	8:H:27:GLU:O	2.46	0.48
16:Q:121:PHE:CD1	16:Q:395:PHE:HB2	2.49	0.48
16:Q:344:PHE:O	16:Q:347:PHE:HD2	1.97	0.48
18:T:41:DA:H2"	18:T:42:DC:C6	2.47	0.48
22:X:261:LYS:O	22:X:265:ASN:N	2.47	0.48
1:A:113:LEU:HD11	1:A:218:ASP:HA	1.96	0.48
1:A:975:HIS:O	1:A:976:THR:OG1	2.24	0.48
2:B:856:PHE:CD1	2:B:969:ARG:HB3	2.47	0.48
2:B:1004:GLU:O	3:C:177:GLU:HG2	2.14	0.48
13:M:154:TYR:HE1	13:M:171:ILE:HD13	1.78	0.48
16:Q:121:PHE:HD1	16:Q:395:PHE:HB2	1.78	0.48
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:GLN:O	1:A:1134:ILE:HD12	2.12	0.48
13:M:147:LYS:HE2	13:M:151:LYS:HE3	1.95	0.48
14:N:24:DT:H3'	14:N:24:DT:H6	1.79	0.48
1:A:252:PHE:C	1:A:254:GLU:H	2.20	0.48
1:A:630:ILE:HG12	1:A:646:PHE:HE1	1.78	0.48
2:B:210:LYS:NZ	2:B:462:ALA:HA	2.28	0.48
2:B:801:LYS:HG2	10:J:52:THR:O	2.13	0.48
2:B:869:SER:HB3	13:M:152:GLU:OE2	2.14	0.48
3:C:98:VAL:HB	3:C:122:SER:HB3	1.95	0.48
8:H:93:TYR:CD1	8:H:143:LEU:HD23	2.48	0.48
13:M:267:LYS:HD3	15:O:239:LYS:HE3	1.95	0.48
16:Q:119:LEU:HD21	17:R:135:PHE:CE1	2.48	0.48
1:A:337:ARG:HH12	1:A:839:ARG:NE	2.11	0.48
1:A:380:VAL:HG22	1:A:388:LEU:HD13	1.96	0.48
1:A:704:ALA:HB2	1:A:710:LEU:HA	1.95	0.48
2:B:336:ARG:HD2	2:B:348:ARG:NH1	2.28	0.48
5:E:106:GLN:O	5:E:130:ALA:HA	2.14	0.48
18:T:50:DT:H3'	18:T:50:DT:H6	1.79	0.48
1:A:1153:TYR:HB2	1:A:1192:LEU:HD23	1.96	0.48
2:B:995:ARG:NH1	11:K:9:LEU:HD13	2.29	0.48
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.96	0.48
5:E:79:TRP:HE1	5:E:81:GLU:HG3	1.79	0.48
13:M:137:CYS:SG	13:M:147:LYS:HB2	2.54	0.48
1:A:11:LEU:HD12	2:B:1193:GLN:O	2.14	0.48
1:A:283:GLY:O	1:A:285:PRO:HD3	2.13	0.48
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.73	0.48
1:A:471:ASN:O	1:A:474:VAL:HG12	2.13	0.48
1:A:670:ILE:HG12	1:A:805:LEU:HD21	1.96	0.48
2:B:983:ARG:NH2	2:B:1028:GLU:OE2	2.46	0.48
4:D:64:VAL:HG12	4:D:68:ARG:NH1	2.29	0.48
1:A:412:ARG:O	13:M:51:VAL:HG12	2.14	0.48
1:A:597:LEU:O	8:H:102:TYR:OH	2.32	0.48
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.14	0.48
2:B:213:ILE:HG21	2:B:499:ASN:HB2	1.95	0.48
2:B:300:HIS:CE1	2:B:376:PHE:HE1	2.31	0.48
13:M:132:LYS:CG	13:M:172:MET:HE1	2.44	0.48
14:N:31:DG:H2''	14:N:32:DT:C6	2.49	0.48
2:B:70:ILE:HG21	16:Q:335:LEU:HD21	1.96	0.47
2:B:914:LYS:CB	2:B:937:ALA:O	2.53	0.47
7:G:143:ILE:HG13	7:G:170:ALA:HA	1.94	0.47
13:M:155:LYS:O	13:M:158:HIS:HB2	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:405:THR:CB	16:Q:409:ALA:HB2	2.44	0.47
17:R:133:TYR:CE1	17:R:217:THR:HG22	2.49	0.47
19:U:277:GLN:HG2	20:V:56:THR:OG1	2.14	0.47
1:A:1072:ILE:O	1:A:1075:PRO:HD2	2.14	0.47
2:B:1089:PRO:HD3	10:J:44:TYR:HE2	1.78	0.47
13:M:241:ARG:O	13:M:245:HIS:ND1	2.45	0.47
15:O:171:ARG:HD3	15:O:238:ARG:O	2.14	0.47
2:B:167:ILE:O	2:B:450:ALA:HA	2.14	0.47
2:B:713:ALA:HA	2:B:733:HIS:CD2	2.50	0.47
3:C:60:ASP:HB3	12:L:67:PHE:CE2	2.47	0.47
3:C:180:TYR:HB3	3:C:228:PHE:HD1	1.80	0.47
5:E:64:PRO:HB2	5:E:69:ILE:HD11	1.95	0.47
8:H:22:LYS:O	8:H:43:ASN:HA	2.13	0.47
13:M:293:ILE:O	13:M:294:THR:OG1	2.28	0.47
17:R:105:THR:CA	17:R:120:TYR:O	2.60	0.47
17:R:263:MET:O	17:R:266:THR:OG1	2.19	0.47
1:A:116:ASP:OD1	1:A:117:GLU:N	2.42	0.47
1:A:1032:LEU:O	1:A:1036:ARG:HD2	2.15	0.47
2:B:984:HIS:CD2	2:B:1025:HIS:HA	2.49	0.47
13:M:140:ALA:HB2	13:M:195:LEU:HD11	1.95	0.47
1:A:326:ARG:NE	1:A:1406:VAL:HG21	2.27	0.47
12:L:46:VAL:HG13	12:L:56:LEU:HD12	1.97	0.47
17:R:63:ARG:C	17:R:65:ASN:H	2.21	0.47
1:A:224:PHE:CE2	1:A:231:PRO:HG3	2.50	0.47
2:B:217:ARG:HH12	2:B:407:ASP:CG	2.22	0.47
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.96	0.47
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.95	0.47
2:B:839:MET:O	2:B:991:GLY:N	2.41	0.47
7:G:138:THR:O	7:G:141:SER:OG	2.23	0.47
13:M:16:PRO:HB3	21:W:127:CYS:HA	1.95	0.47
14:N:32:DT:P	17:R:325:PRO:CB	3.02	0.47
15:O:69:ASN:HB2	18:T:48:DT:O4'	2.14	0.47
16:Q:361:TRP:HA	16:Q:396:THR:O	2.15	0.47
18:T:47:DA:C8	18:T:48:DT:C4	3.02	0.47
1:A:792:TYR:HE2	9:I:87:GLN:HE22	1.63	0.47
1:A:1142:THR:O	1:A:1145:SER:OG	2.19	0.47
2:B:770:GLN:HG2	2:B:983:ARG:O	2.15	0.47
1:A:61:ILE:HG22	1:A:62:ASP:N	2.27	0.47
1:A:346:ASP:OD1	2:B:1106:ARG:NE	2.48	0.47
1:A:567:LYS:NZ	8:H:91:ASP:HA	2.30	0.47
2:B:898:LEU:HD21	2:B:964:VAL:HG11	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:214:ASN:ND2	3:C:217:ASP:OD2	2.46	0.47
13:M:171:ILE:HD12	13:M:172:MET:HG3	1.96	0.47
13:M:269:ILE:CG2	13:M:272:LYS:CE	2.83	0.47
16:Q:99:ASN:O	17:R:96:ARG:HA	2.15	0.47
16:Q:117:HIS:HB2	17:R:135:PHE:CE1	2.50	0.47
18:T:50:DT:C2'	18:T:51:DA:H5'	2.45	0.47
2:B:879:ARG:HG2	2:B:885:MET:SD	2.55	0.47
7:G:14:HIS:HB3	7:G:17:PHE:CE2	2.50	0.47
16:Q:140:HIS:O	16:Q:351:VAL:HG12	2.14	0.47
16:Q:376:LEU:O	17:R:69:TRP:N	2.39	0.47
1:A:879:GLU:OE1	1:A:959:ASN:HB2	2.15	0.46
2:B:617:ARG:NH1	2:B:619:ILE:HG12	2.30	0.46
2:B:923:GLU:HB3	2:B:925:LEU:HG	1.96	0.46
8:H:101:ALA:HA	8:H:115:TYR:O	2.15	0.46
16:Q:116:THR:O	16:Q:390:ASP:HB3	2.15	0.46
17:R:133:TYR:CD1	17:R:217:THR:HA	2.50	0.46
1:A:302:THR:HA	1:A:305:ASP:O	2.15	0.46
1:A:444:PHE:HE2	1:A:487:MET:SD	2.37	0.46
1:A:737:LEU:HD22	1:A:741:ASN:HD22	1.78	0.46
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.80	0.46
1:A:1208:THR:HB	1:A:1211:GLN:HG2	1.96	0.46
1:A:1444:MET:SD	6:F:135:ARG:NE	2.82	0.46
2:B:134:LYS:HD3	17:R:277:PHE:HB2	1.97	0.46
13:M:269:ILE:HG22	13:M:272:LYS:CG	2.34	0.46
15:O:170:ILE:HD13	15:O:234:LEU:HD22	1.96	0.46
16:Q:102:PRO:HB3	17:R:94:LYS:HG2	1.95	0.46
16:Q:375:LEU:HB2	16:Q:387:ILE:O	2.15	0.46
17:R:78:ALA:O	17:R:82:ARG:HG2	2.14	0.46
1:A:446:ARG:HB2	1:A:487:MET:HG2	1.96	0.46
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.46	0.46
2:B:944:THR:HG21	2:B:1122:ARG:HH22	1.80	0.46
3:C:133:ILE:HD12	3:C:237:SER:HA	1.97	0.46
4:D:208:GLU:HA	4:D:211:LEU:HB2	1.98	0.46
11:K:20:LYS:O	11:K:33:ILE:HA	2.15	0.46
13:M:273:SER:CB	15:O:188:GLU:HA	2.46	0.46
16:Q:117:HIS:NE2	16:Q:390:ASP:OD2	2.49	0.46
2:B:289:LEU:HD13	2:B:375:ALA:HA	1.96	0.46
2:B:820:GLY:N	2:B:1091:TYR:OH	2.48	0.46
3:C:148:ARG:HH21	10:J:64:ASN:HA	1.79	0.46
4:D:52:LEU:HD12	4:D:52:LEU:O	2.15	0.46
7:G:22:MET:HA	7:G:25:TYR:HD1	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:101:VAL:O	7:G:108:VAL:N	2.43	0.46
15:O:191:PRO:CG	18:T:52:DC:H5'	2.45	0.46
19:U:30:ILE:HD11	20:V:32:ILE:HG13	1.98	0.46
1:A:216:VAL:HA	1:A:219:PHE:CE2	2.51	0.46
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.81	0.46
2:B:20:ASP:OD1	2:B:21:GLU:N	2.42	0.46
2:B:604:ARG:NH2	2:B:615:MET:H	2.13	0.46
7:G:93:SER:OG	7:G:100:GLU:OE1	2.33	0.46
14:N:17:DC:H2''	14:N:18:DT:H72	1.97	0.46
17:R:108:LEU:HD11	17:R:120:TYR:HE2	1.80	0.46
20:V:32:ILE:HD12	20:V:32:ILE:N	2.30	0.46
1:A:465:TYR:CG	2:B:976:ILE:HD12	2.50	0.46
1:A:672:ASP:OD1	1:A:673:GLY:N	2.49	0.46
2:B:71:LEU:HB3	2:B:88:TYR:HB2	1.97	0.46
2:B:342:GLY:C	2:B:344:LYS:H	2.24	0.46
2:B:445:LYS:NZ	17:R:268:MET:HA	2.31	0.46
2:B:1163:CYS:HB3	2:B:1166:CYS:O	2.15	0.46
3:C:21:ILE:HG12	3:C:229:TYR:HD1	1.79	0.46
3:C:241:ASP:OD1	3:C:242:GLN:N	2.48	0.46
13:M:246:LEU:HD22	13:M:293:ILE:HD13	1.96	0.46
17:R:63:ARG:HD2	17:R:66:ARG:NH1	2.31	0.46
1:A:668:ASP:OD2	1:A:742:ASN:HB2	2.15	0.46
8:H:56:THR:HB	8:H:145:ARG:HG2	1.97	0.46
1:A:1120:LEU:HD21	1:A:1131:ALA:HA	1.98	0.46
2:B:862:GLN:HA	2:B:963:PHE:HB2	1.98	0.46
2:B:952:VAL:HG22	2:B:966:VAL:HG22	1.96	0.46
3:C:76:ASP:OD2	3:C:127:ARG:HB2	2.16	0.46
4:D:50:LEU:HB2	7:G:2:PHE:O	2.16	0.46
9:I:70:ARG:HD3	9:I:84:VAL:HG22	1.97	0.46
13:M:267:LYS:HD3	15:O:239:LYS:CE	2.45	0.46
16:Q:114:MET:HE2	17:R:138:GLN:HE21	1.80	0.46
17:R:257:GLU:OE1	17:R:257:GLU:N	2.48	0.46
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.98	0.46
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.81	0.46
4:D:33:PHE:CZ	7:G:42:PHE:HA	2.50	0.46
17:R:68:VAL:O	17:R:69:TRP:HD1	1.99	0.46
2:B:280:ILE:HD13	2:B:334:ILE:HG13	1.97	0.46
3:C:66:ARG:NH1	10:J:2:ILE:O	2.48	0.46
8:H:5:LEU:HD11	8:H:61:SER:HB3	1.97	0.46
15:O:94:TYR:CZ	15:O:96:PRO:HG3	2.51	0.46
1:A:212:LYS:HA	1:A:232:GLU:OE2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ASP:HA	2:B:989:THR:HG23	1.97	0.45
2:B:357:GLN:CD	2:B:368:GLU:HG2	2.40	0.45
4:D:53:SER:HB2	4:D:154:PHE:HB2	1.97	0.45
17:R:104:ILE:HD11	17:R:122:LEU:HD22	1.98	0.45
1:A:526:ASP:OD1	2:B:1015:HIS:ND1	2.49	0.45
2:B:286:PHE:CD2	2:B:297:ILE:HG23	2.51	0.45
2:B:300:HIS:CE1	2:B:376:PHE:CE1	3.04	0.45
4:D:32:GLU:HG2	7:G:41:LYS:HE2	1.98	0.45
4:D:49:ALA:HA	7:G:3:PHE:HD1	1.72	0.45
1:A:353:ILE:HG21	1:A:487:MET:SD	2.56	0.45
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.16	0.45
1:A:1390:ASN:HD21	1:A:1408:ILE:HD11	1.81	0.45
2:B:336:ARG:HD2	2:B:348:ARG:HH11	1.81	0.45
20:V:11:ARG:NH1	20:V:41:LEU:HD13	2.31	0.45
20:V:34:ALA:O	20:V:35:SER:HB2	2.16	0.45
1:A:1132:LYS:HG2	1:A:1135:ARG:HH12	1.80	0.45
1:A:1170:ILE:HG23	1:A:1174:PHE:CE2	2.51	0.45
2:B:69:LEU:HD23	2:B:425:THR:HG23	1.99	0.45
3:C:182:PRO:HB2	3:C:207:CYS:SG	2.56	0.45
7:G:149:GLY:O	7:G:159:ALA:HB1	2.16	0.45
8:H:122:LEU:HD23	8:H:122:LEU:HA	1.77	0.45
14:N:24:DT:H2'	14:N:25:DA:C8	2.51	0.45
1:A:358:ASN:OD1	2:B:833:TYR:OH	2.24	0.45
1:A:526:ASP:HB2	2:B:835:GLN:OE1	2.16	0.45
1:A:786:HIS:NE2	2:B:705:MET:SD	2.90	0.45
1:A:1277:GLU:O	1:A:1279:ILE:HD12	2.16	0.45
2:B:432:MET:O	2:B:436:VAL:HG12	2.17	0.45
2:B:569:TYR:CE1	2:B:589:VAL:HG11	2.51	0.45
2:B:923:GLU:HB2	2:B:928:ARG:CD	2.46	0.45
3:C:6:PRO:O	11:K:104:ASN:ND2	2.49	0.45
6:F:105:ALA:HA	7:G:16:SER:HA	1.98	0.45
13:M:137:CYS:SG	13:M:142:LEU:HB2	2.56	0.45
13:M:198:VAL:HG11	13:M:203:PHE:HD1	1.81	0.45
19:U:244:MET:HB2	19:U:267:VAL:HG13	1.99	0.45
2:B:676:VAL:C	2:B:678:GLU:H	2.23	0.45
2:B:776:GLN:O	2:B:1096:ARG:HG2	2.16	0.45
3:C:67:LEU:HD13	3:C:157:CYS:SG	2.56	0.45
6:F:82:THR:HG22	6:F:84:TYR:H	1.80	0.45
16:Q:117:HIS:HD2	16:Q:391:LYS:HB2	1.80	0.45
18:T:44:DA:C2'	18:T:45:DT:O5'	2.64	0.45
18:T:47:DA:C5	18:T:48:DT:O4	2.70	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.80	0.45
1:A:998:LEU:HD23	1:A:1001:ARG:HG2	1.98	0.45
1:A:1352:VAL:O	1:A:1355:VAL:HG12	2.16	0.45
2:B:460:ALA:O	2:B:464:GLY:N	2.38	0.45
2:B:597:MET:HE1	2:B:615:MET:HG3	1.99	0.45
18:T:52:DC:C2'	18:T:53:DA:H5'	2.45	0.45
1:A:660:ASN:OD1	2:B:1082:MET:HB3	2.16	0.45
7:G:98:GLY:HA3	7:G:110:VAL:O	2.16	0.45
8:H:25:ARG:NH2	8:H:41:ASP:OD2	2.50	0.45
11:K:59:ALA:HA	11:K:74:ARG:O	2.17	0.45
13:M:267:LYS:NZ	15:O:208:VAL:CG1	2.78	0.45
13:M:295:ALA:O	13:M:298:VAL:HG12	2.16	0.45
15:O:239:LYS:O	15:O:240:MET:HG3	2.16	0.45
1:A:1295:THR:HG23	1:A:1297:GLU:OE1	2.17	0.45
2:B:331:LEU:HA	2:B:334:ILE:HG22	1.99	0.45
8:H:24:CYS:SG	8:H:44:VAL:HG21	2.57	0.45
11:K:7:PHE:HB2	11:K:11:LEU:HD13	1.98	0.45
13:M:134:THR:HA	13:M:147:LYS:HE3	1.99	0.45
16:Q:103:LEU:O	17:R:92:LEU:HB2	2.16	0.45
2:B:842:ASN:HB3	2:B:845:SER:HB2	1.99	0.45
4:D:56:ARG:HD3	4:D:149:THR:HA	1.99	0.45
16:Q:373:TYR:CD1	17:R:70:LEU:HD11	2.51	0.45
2:B:601:ARG:HD3	2:B:605:ARG:CZ	2.47	0.44
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.81	0.44
12:L:58:LYS:O	12:L:58:LYS:HG3	2.17	0.44
1:A:72:GLU:HB3	1:A:76:GLU:HB3	1.98	0.44
4:D:130:LEU:HD13	4:D:142:LYS:HG2	1.99	0.44
5:E:26:ARG:NH1	5:E:189:GLY:HA3	2.29	0.44
13:M:167:SER:O	13:M:168:MET:HB2	2.18	0.44
16:Q:405:THR:O	16:Q:409:ALA:N	2.44	0.44
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.57	0.44
2:B:244:LEU:HD13	2:B:250:PHE:CE2	2.52	0.44
4:D:24:ALA:CA	7:G:83:LYS:HB2	2.45	0.44
8:H:4:THR:HA	8:H:60:ALA:HA	1.99	0.44
14:N:25:DA:C8	14:N:25:DA:O5'	2.71	0.44
17:R:133:TYR:HD1	17:R:217:THR:HA	1.82	0.44
18:T:55:DA:H2''	18:T:56:DG:C8	2.52	0.44
2:B:101:MET:HE3	2:B:127:GLY:H	1.82	0.44
2:B:446:LEU:HD23	2:B:446:LEU:HA	1.83	0.44
2:B:512:ARG:NH1	2:B:533:CYS:O	2.50	0.44
2:B:867:GLY:C	2:B:869:SER:H	2.25	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ARG:HD3	1:A:469:ARG:HA	1.75	0.44
1:A:1217:LYS:HE2	1:A:1228:TRP:HZ3	1.82	0.44
1:A:1235:LYS:HG2	1:A:1237:ILE:HD11	1.99	0.44
2:B:322:PHE:HA	2:B:325:GLN:OE1	2.18	0.44
2:B:580:VAL:O	2:B:586:TRP:HD1	2.00	0.44
2:B:785:TYR:HA	2:B:788:ARG:HG2	1.99	0.44
6:F:133:VAL:HG11	7:G:58:ARG:NH2	2.33	0.44
7:G:7:LEU:HB2	7:G:74:TYR:CZ	2.53	0.44
13:M:199:LYS:O	13:M:199:LYS:HG3	2.17	0.44
14:N:28:DA:H8	14:N:29:DT:H73	1.81	0.44
16:Q:374:VAL:HB	17:R:71:VAL:HB	1.98	0.44
1:A:849:MET:HB3	1:A:1063:MET:SD	2.58	0.44
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	2.00	0.44
2:B:500:THR:OG1	2:B:537:LYS:NZ	2.48	0.44
3:C:148:ARG:NH2	10:J:64:ASN:OD1	2.51	0.44
7:G:160:ILE:HG22	7:G:161:GLY:N	2.33	0.44
14:N:27:DA:H2'	14:N:28:DA:C8	2.52	0.44
18:T:49:DA:H2'	18:T:50:DT:C5'	2.47	0.44
1:A:408:ASP:H	1:A:430:TRP:CD1	2.35	0.44
1:A:411:ASP:CG	13:M:50:LEU:HD11	2.43	0.44
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	2.18	0.44
1:A:1207:LEU:HA	1:A:1211:GLN:NE2	2.32	0.44
1:A:1444:MET:HB2	6:F:133:VAL:HG13	1.99	0.44
9:I:7:CYS:SG	9:I:8:ARG:N	2.90	0.44
16:Q:128:ASN:HB2	17:R:131:ASN:OD1	2.18	0.44
21:W:39:ALA:C	21:W:41:ASP:H	2.21	0.44
2:B:996:ARG:HH22	3:C:175:ALA:HA	1.82	0.44
2:B:1119:VAL:HG23	2:B:1126:GLY:HA2	1.99	0.44
2:B:1175:LEU:HD12	2:B:1175:LEU:O	2.16	0.44
4:D:177:VAL:HA	4:D:180:LEU:HD12	2.00	0.44
6:F:136:ARG:O	6:F:143:PHE:HA	2.18	0.44
7:G:15:PRO:HA	7:G:18:PHE:CZ	2.52	0.44
8:H:10:PHE:CD1	8:H:30:SER:HA	2.52	0.44
13:M:177:LEU:HD11	13:M:189:PHE:CE1	2.53	0.44
13:M:191:GLU:CD	13:M:241:ARG:HH22	2.25	0.44
13:M:285:ASN:O	13:M:288:LEU:HB3	2.18	0.44
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.18	0.44
1:A:1189:SER:OG	1:A:1256:GLU:OE2	2.22	0.44
2:B:799:PRO:CB	2:B:818:PRO:HG2	2.48	0.44
10:J:30:LEU:HD13	10:J:38:ARG:NH1	2.32	0.44
1:A:455:MET:HE2	1:A:455:MET:HB3	1.90	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:LEU:HB2	2:B:276:ILE:HD13	2.00	0.43
4:D:65:GLU:HA	4:D:68:ARG:HH11	1.81	0.43
8:H:42:ILE:HG23	8:H:95:TYR:CZ	2.52	0.43
17:R:69:TRP:CD1	17:R:219:CYS:HB3	2.53	0.43
2:B:195:CYS:SG	2:B:197:PHE:HD2	2.41	0.43
2:B:274:PRO:O	2:B:276:ILE:HD12	2.18	0.43
2:B:839:MET:SD	2:B:1010:LEU:HD11	2.58	0.43
4:D:140:ASP:O	4:D:144:THR:N	2.46	0.43
5:E:43:LYS:HG3	5:E:47:CYS:SG	2.58	0.43
7:G:79:PHE:CE2	7:G:81:PRO:HD3	2.53	0.43
2:B:149:TYR:CE2	2:B:151:LEU:HD23	2.53	0.43
2:B:365:THR:HG21	2:B:370:PHE:CB	2.48	0.43
2:B:850:LEU:HG	2:B:851:PHE:HD2	1.83	0.43
2:B:924:GLU:HG3	2:B:929:THR:HB	2.00	0.43
2:B:1187:ASN:OD1	2:B:1190:ASP:N	2.51	0.43
7:G:127:PRO:HG3	7:G:139:ILE:HD12	2.00	0.43
8:H:95:TYR:HE2	8:H:97:MET:HE2	1.83	0.43
19:U:21:VAL:HG12	19:U:25:PHE:CD1	2.54	0.43
1:A:372:LYS:HA	1:A:435:HIS:HD2	1.80	0.43
1:A:845:LEU:O	1:A:1065:GLY:HA3	2.19	0.43
2:B:850:LEU:HG	2:B:851:PHE:CD2	2.54	0.43
2:B:865:LYS:CE	13:M:145:ILE:HD12	2.38	0.43
3:C:4:GLU:O	3:C:24:ASN:ND2	2.51	0.43
3:C:56:THR:HG22	3:C:147:LEU:CD2	2.47	0.43
13:M:132:LYS:O	13:M:136:LEU:HG	2.18	0.43
1:A:857:ARG:HB2	1:A:862:ASN:O	2.17	0.43
1:A:1208:THR:O	1:A:1211:GLN:HG2	2.18	0.43
2:B:68:THR:CB	16:Q:335:LEU:HD13	2.46	0.43
2:B:839:MET:HG2	2:B:989:THR:O	2.18	0.43
6:F:137:TYR:HD1	6:F:143:PHE:HB3	1.83	0.43
8:H:98:TYR:C	8:H:118:PHE:HD1	2.25	0.43
2:B:310:MET:O	2:B:314:LEU:HG	2.19	0.43
2:B:635:ARG:NH1	2:B:637:LEU:HD21	2.34	0.43
3:C:133:ILE:CD1	3:C:237:SER:HA	2.48	0.43
4:D:194:LEU:HD22	7:G:86:VAL:HG11	2.00	0.43
11:K:46:ILE:O	11:K:49:GLU:N	2.51	0.43
15:O:99:PHE:CE1	18:T:45:DT:H1'	2.53	0.43
19:U:9:VAL:HG13	20:V:51:THR:HG22	1.99	0.43
22:X:168:ARG:O	22:X:181:LEU:N	2.48	0.43
1:A:737:LEU:HD11	1:A:758:ILE:HG21	2.00	0.43
1:A:915:SER:O	1:A:919:ILE:HG12	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:SER:HB3	2:B:250:PHE:CE2	2.54	0.43
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.99	0.43
2:B:445:LYS:HZ3	17:R:268:MET:HA	1.83	0.43
2:B:1022:THR:HG23	2:B:1022:THR:O	2.18	0.43
8:H:75:ALA:C	8:H:77:ARG:H	2.27	0.43
9:I:54:GLU:HB3	9:I:100:PHE:HE2	1.84	0.43
12:L:38:LEU:HD21	12:L:48:CYS:HA	2.00	0.43
13:M:39:SER:OG	13:M:40:GLU:OE1	2.37	0.43
13:M:44:VAL:HG22	13:M:51:VAL:HA	2.01	0.43
17:R:129:VAL:HG21	17:R:218:VAL:HG12	2.01	0.43
19:U:262:LEU:HB2	19:U:279:ALA:HB3	2.01	0.43
2:B:103:ASN:O	2:B:958:GLN:OE1	2.36	0.43
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.47	0.43
3:C:18:VAL:HG12	3:C:20:PHE:HD1	1.83	0.43
3:C:41:ILE:HB	3:C:172:PRO:HG3	2.00	0.43
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.49	0.43
13:M:132:LYS:HG2	13:M:172:MET:HE1	2.00	0.43
1:A:106:VAL:HG22	1:A:107:CYS:H	1.83	0.43
1:A:412:ARG:HB3	13:M:51:VAL:HG11	2.01	0.43
1:A:737:LEU:HD22	1:A:741:ASN:ND2	2.34	0.43
1:A:770:VAL:HA	1:A:822:GLU:OE1	2.19	0.43
2:B:199:MET:CE	2:B:492:LEU:HD23	2.48	0.43
2:B:918:ILE:HG12	2:B:933:SER:O	2.18	0.43
2:B:979:LYS:HA	2:B:989:THR:HA	2.01	0.43
2:B:1187:ASN:OD1	2:B:1189:ILE:N	2.48	0.43
7:G:1:MET:HE2	7:G:85:GLU:OE2	2.18	0.43
13:M:16:PRO:O	13:M:18:LEU:HG	2.19	0.43
13:M:239:ILE:HB	13:M:240:PRO:HD3	2.01	0.43
15:O:99:PHE:CZ	18:T:45:DT:O2	2.72	0.43
16:Q:108:LYS:O	16:Q:112:GLU:HG3	2.19	0.43
1:A:404:TYR:OH	13:M:40:GLU:HG2	2.19	0.43
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.53	0.43
2:B:457:LEU:HD23	2:B:457:LEU:HA	1.81	0.43
2:B:823:ALA:O	2:B:825:VAL:HG23	2.18	0.43
4:D:126:ILE:HD13	4:D:145:MET:HE3	2.01	0.43
6:F:94:LEU:HD23	6:F:94:LEU:HA	1.66	0.43
1:A:105:CYS:SG	1:A:139:TRP:HD1	2.41	0.42
1:A:444:PHE:CE2	1:A:487:MET:SD	3.12	0.42
1:A:710:LEU:HD23	9:I:96:SER:HA	2.00	0.42
1:A:1144:LYS:HB2	1:A:1268:LEU:HB3	2.01	0.42
3:C:54:ASN:HD21	3:C:63:ILE:HD12	1.84	0.42

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	2.18	0.42
16:Q:25:ASP:C	16:Q:27:MET:H	2.27	0.42
1:A:48:ALA:HB3	1:A:56:PRO:HD3	2.01	0.42
1:A:412:ARG:HH22	13:M:54:ASP:CG	2.27	0.42
1:A:1376:THR:O	1:A:1378:GLN:N	2.52	0.42
2:B:199:MET:CE	2:B:491:THR:HG21	2.21	0.42
3:C:190:ASP:OD1	3:C:191:TYR:N	2.52	0.42
11:K:18:LYS:NZ	11:K:38:GLU:OE2	2.47	0.42
13:M:279:VAL:HG11	13:M:304:VAL:HG21	2.01	0.42
15:O:171:ARG:HG3	15:O:239:LYS:HG2	2.00	0.42
16:Q:101:PHE:CD1	16:Q:382:GLY:HA3	2.54	0.42
16:Q:121:PHE:HE1	16:Q:395:PHE:HD2	1.66	0.42
17:R:94:LYS:O	17:R:106:LEU:HD12	2.19	0.42
1:A:206:GLU:O	1:A:210:ILE:HG12	2.18	0.42
1:A:982:THR:HG22	1:A:983:ILE:N	2.34	0.42
1:A:1144:LYS:NZ	2:B:262:GLU:OE2	2.51	0.42
2:B:44:VAL:HG11	2:B:199:MET:SD	2.59	0.42
2:B:106:ASP:OD1	2:B:106:ASP:N	2.52	0.42
2:B:199:MET:HG3	2:B:200:GLY:O	2.18	0.42
2:B:254:LEU:HD23	2:B:381:MET:HE1	2.00	0.42
2:B:515:HIS:CE1	2:B:517:THR:HG23	2.54	0.42
2:B:755:ILE:HG22	2:B:983:ARG:HD2	2.00	0.42
3:C:12:GLU:HB2	3:C:19:ASP:HB3	2.01	0.42
7:G:138:THR:HG22	7:G:139:ILE:N	2.32	0.42
13:M:237:THR:O	13:M:240:PRO:HD2	2.18	0.42
17:R:135:PHE:HA	17:R:215:VAL:HG23	2.01	0.42
17:R:251:ARG:HG3	17:R:252:ILE:N	2.35	0.42
1:A:951:GLU:O	1:A:954:TRP:NE1	2.52	0.42
2:B:1067:ARG:HA	2:B:1067:ARG:HD3	1.87	0.42
5:E:153:HIS:CD2	5:E:184:VAL:HG11	2.55	0.42
9:I:27:PHE:O	9:I:35:VAL:HA	2.20	0.42
13:M:198:VAL:HG12	13:M:202:GLU:OE1	2.20	0.42
16:Q:130:VAL:O	16:Q:133:PHE:HB3	2.18	0.42
16:Q:363:GLY:HA2	16:Q:394:LYS:O	2.19	0.42
17:R:70:LEU:HD12	17:R:71:VAL:H	1.84	0.42
1:A:337:ARG:HH12	1:A:839:ARG:HE	1.67	0.42
1:A:344:ARG:HA	2:B:1129:ARG:HA	2.00	0.42
2:B:1113:VAL:HG22	13:M:57:VAL:HB	2.02	0.42
3:C:174:ALA:N	3:C:233:GLU:O	2.52	0.42
11:K:19:LEU:HD22	11:K:35:PHE:CD1	2.54	0.42
13:M:187:ARG:NH1	13:M:241:ARG:HE	2.16	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:118:HIS:HB2	17:R:120:TYR:CE2	2.54	0.42
1:A:333:GLU:HA	1:A:338:GLY:HA3	2.01	0.42
1:A:356:ASP:OD2	11:K:65:HIS:NE2	2.28	0.42
1:A:673:GLY:N	1:A:674:PRO:HD2	2.34	0.42
1:A:854:ASN:HB2	1:A:1000:LEU:HD21	2.01	0.42
2:B:53:GLN:HG3	2:B:57:TYR:CD2	2.54	0.42
2:B:120:ARG:CG	12:L:55:ILE:HD11	2.50	0.42
2:B:309:GLN:HE22	9:I:50:THR:HG21	1.85	0.42
2:B:642:ASP:OD1	2:B:643:ASP:N	2.52	0.42
5:E:180:ARG:HH21	5:E:192:ARG:HG3	1.85	0.42
12:L:31:CYS:SG	12:L:32:ALA:N	2.93	0.42
13:M:183:ALA:C	13:M:185:VAL:H	2.28	0.42
1:A:94:GLY:HA3	1:A:1410:PHE:CE2	2.54	0.42
1:A:1210:GLY:HA2	1:A:1228:TRP:CE2	2.54	0.42
1:A:1395:GLY:HA3	1:A:1426:GLU:OE2	2.19	0.42
1:A:1418:LEU:HA	1:A:1418:LEU:HD12	1.85	0.42
2:B:435:THR:O	2:B:439:ALA:N	2.53	0.42
3:C:83:SER:OG	3:C:160:LYS:HD3	2.20	0.42
4:D:192:LYS:HB3	4:D:199:ASN:OD1	2.20	0.42
9:I:42:LEU:HD12	9:I:43:VAL:N	2.34	0.42
13:M:267:LYS:HZ1	15:O:169:PRO:HB3	1.70	0.42
20:V:38:MET:O	20:V:42:GLU:HG3	2.19	0.42
1:A:185:TRP:HB2	1:A:198:GLU:HB3	2.02	0.42
1:A:399:HIS:O	1:A:401:GLY:N	2.53	0.42
1:A:1267:MET:HA	1:A:1271:ILE:HD12	2.01	0.42
1:A:1421:CYS:HA	1:A:1426:GLU:OE1	2.18	0.42
2:B:1094:ARG:HH21	2:B:1098:MET:HG2	1.84	0.42
17:R:68:VAL:HG21	17:R:134:VAL:HG21	2.01	0.42
1:A:300:VAL:O	1:A:303:TYR:HB3	2.20	0.42
1:A:1214:GLU:O	1:A:1218:GLN:HG2	2.19	0.42
2:B:59:LEU:O	2:B:63:ILE:HG12	2.19	0.42
2:B:134:LYS:HG2	2:B:154:GLU:O	2.20	0.42
2:B:213:ILE:CG2	2:B:499:ASN:HB2	2.49	0.42
3:C:167:HIS:HB3	3:C:170:TRP:CZ3	2.55	0.42
4:D:214:LEU:O	4:D:218:GLU:HG3	2.20	0.42
7:G:34:VAL:CG1	7:G:45:ILE:HG21	2.46	0.42
13:M:140:ALA:HB1	13:M:142:LEU:HD13	2.01	0.42
13:M:198:VAL:HG11	13:M:203:PHE:CD1	2.54	0.42
13:M:272:LYS:HD3	18:T:52:DC:H3'	2.01	0.42
18:T:48:DT:H2'	18:T:49:DA:C5	2.54	0.42
1:A:1293:SER:HB3	1:A:1299:VAL:HG23	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:ARG:HB2	2:B:122:LEU:HG	2.01	0.42
3:C:222:LYS:HA	3:C:222:LYS:HD2	1.91	0.42
7:G:23:LYS:O	7:G:26:LEU:HB2	2.19	0.42
13:M:248:LEU:HD23	13:M:248:LEU:HA	1.79	0.42
15:O:191:PRO:HG3	18:T:52:DC:C4'	2.50	0.42
16:Q:119:LEU:HA	16:Q:119:LEU:HD23	1.76	0.42
1:A:635:ARG:NH2	1:A:877:HIS:HA	2.35	0.41
1:A:855:THR:HG21	1:A:863:VAL:HG22	2.01	0.41
1:A:1154:TYR:HB2	1:A:1191:TRP:CZ3	2.55	0.41
1:A:1212:VAL:O	1:A:1216:ILE:HD12	2.20	0.41
2:B:185:THR:O	2:B:188:ASP:HB3	2.19	0.41
4:D:194:LEU:CB	7:G:86:VAL:HG21	2.50	0.41
7:G:43:GLY:HA2	7:G:157:ILE:HD11	2.02	0.41
7:G:142:ARG:HB3	7:G:171:ILE:HD12	2.01	0.41
7:G:151:ILE:HG13	21:W:134:LEU:HA	2.00	0.41
8:H:89:LEU:C	8:H:91:ASP:N	2.76	0.41
9:I:101:PHE:CZ	9:I:112:SER:HB3	2.55	0.41
13:M:132:LYS:HB3	13:M:172:MET:HE1	2.02	0.41
13:M:164:LYS:O	13:M:164:LYS:HG2	2.20	0.41
16:Q:115:ARG:HD3	16:Q:390:ASP:OD2	2.20	0.41
22:X:225:GLU:CB	22:X:232:VAL:H	2.33	0.41
2:B:136:THR:HB	2:B:151:LEU:HD12	2.01	0.41
2:B:369:GLY:O	16:Q:367:ALA:HB3	2.20	0.41
2:B:529:GLU:OE1	2:B:529:GLU:N	2.53	0.41
13:M:171:ILE:CD1	13:M:172:MET:HG3	2.50	0.41
13:M:269:ILE:O	13:M:271:GLY:N	2.53	0.41
14:N:28:DA:H2'	14:N:29:DT:C6	2.55	0.41
16:Q:379:GLU:HG2	16:Q:383:SER:O	2.20	0.41
17:R:277:PHE:CE2	17:R:278:LEU:HD13	2.56	0.41
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.82	0.41
2:B:760:ASP:OD1	2:B:760:ASP:N	2.53	0.41
2:B:1159:ARG:HD2	2:B:1193:GLN:OE1	2.19	0.41
8:H:142:LEU:C	8:H:143:LEU:HD12	2.45	0.41
17:R:63:ARG:O	17:R:64:SER:OG	2.27	0.41
1:A:80:HIS:H	1:A:243:PRO:HB3	1.85	0.41
1:A:215:SER:O	1:A:218:ASP:HB2	2.20	0.41
2:B:137:TYR:C	2:B:138:GLU:HG3	2.45	0.41
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.50	0.41
2:B:977:GLY:HA3	2:B:1099:VAL:HB	2.03	0.41
2:B:1069:PHE:HE2	3:C:192:TRP:CD2	2.38	0.41
3:C:40:GLU:CD	3:C:254:LYS:HE3	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:155:ARG:HB3	4:D:219:THR:HG21	2.01	0.41
5:E:163:GLU:O	5:E:167:ARG:HG2	2.20	0.41
15:O:227:PHE:HA	15:O:230:ILE:HG22	2.01	0.41
1:A:1194:ARG:HA	1:A:1238:ILE:O	2.20	0.41
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.50	0.41
2:B:1171:VAL:HG22	2:B:1182:CYS:HB2	2.02	0.41
11:K:35:PHE:CD2	11:K:71:PHE:CZ	3.07	0.41
13:M:200:THR:HG22	13:M:201:LYS:N	2.35	0.41
13:M:251:GLN:HA	13:M:254:THR:HG22	2.02	0.41
16:Q:115:ARG:O	17:R:136:THR:HA	2.20	0.41
18:T:51:DA:N3	18:T:52:DC:C2	2.89	0.41
2:B:796:LEU:HD11	2:B:851:PHE:HA	2.02	0.41
7:G:150:CYS:SG	7:G:159:ALA:HB2	2.61	0.41
9:I:74:GLU:HB3	9:I:81:ARG:HG2	2.01	0.41
10:J:2:ILE:O	10:J:2:ILE:HG23	2.21	0.41
14:N:28:DA:C8	14:N:29:DT:C7	3.04	0.41
16:Q:129:PRO:HG2	16:Q:132:ASP:HB2	2.03	0.41
1:A:913:LEU:HD23	1:A:1032:LEU:HD13	2.03	0.41
1:A:960:ILE:O	1:A:964:ILE:HD12	2.21	0.41
1:A:1397:LEU:HA	1:A:1400:CYS:SG	2.60	0.41
7:G:121:PHE:CE2	7:G:123:ALA:HB2	2.56	0.41
16:Q:369:ASN:HB2	16:Q:392:VAL:HG11	2.02	0.41
1:A:353:ILE:H	1:A:353:ILE:HG13	1.66	0.41
1:A:516:SER:O	1:A:517:ASN:OD1	2.39	0.41
2:B:238:ALA:HB3	2:B:256:VAL:HB	2.02	0.41
2:B:429:PHE:HA	2:B:432:MET:HE2	2.02	0.41
4:D:30:GLY:O	4:D:34:GLN:N	2.54	0.41
5:E:169:ARG:HD3	6:F:140:ASP:OD2	2.20	0.41
10:J:41:LEU:HD22	10:J:46:CYS:HB3	2.01	0.41
13:M:162:THR:HG23	13:M:213:ILE:HD11	2.03	0.41
14:N:25:DA:O5'	14:N:25:DA:H8	2.03	0.41
1:A:514:PRO:HG2	1:A:1067:LEU:HD11	2.01	0.41
1:A:722:LEU:HD23	1:A:722:LEU:HA	1.93	0.41
2:B:70:ILE:HG22	2:B:89:GLU:HG3	2.02	0.41
2:B:98:THR:OG1	2:B:127:GLY:N	2.54	0.41
2:B:171:PRO:O	2:B:172:ILE:HD13	2.21	0.41
2:B:339:THR:HG21	2:B:351:TYR:OH	2.20	0.41
2:B:378:LEU:HD12	2:B:381:MET:HE3	2.03	0.41
2:B:412:LEU:HD23	2:B:476:ARG:HH12	1.85	0.41
2:B:451:LYS:HD2	13:M:138:ASP:CG	2.45	0.41
2:B:705:MET:H	2:B:710:LEU:HD12	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:117:SER:HA	8:H:122:LEU:HD23	2.02	0.41
13:M:27:CYS:C	13:M:29:VAL:H	2.29	0.41
13:M:168:MET:HA	13:M:171:ILE:CG1	2.50	0.41
15:O:99:PHE:HB2	18:T:45:DT:H4'	2.01	0.41
16:Q:378:VAL:HA	16:Q:384:PHE:CD1	2.56	0.41
18:T:43:DT:P	18:T:43:DT:O4'	2.79	0.41
19:U:5:GLU:O	19:U:9:VAL:HG23	2.21	0.41
1:A:242:PRO:HB2	1:A:246:VAL:HB	2.01	0.41
1:A:306:ASN:ND2	1:A:322:VAL:O	2.49	0.41
1:A:369:SER:HB3	11:K:2:ASN:OD1	2.20	0.41
2:B:593:PRO:HB2	2:B:617:ARG:NE	2.32	0.41
2:B:724:ASP:OD1	2:B:725:PRO:HD2	2.21	0.41
10:J:18:TRP:O	10:J:21:TYR:HB3	2.21	0.41
16:Q:361:TRP:CH2	16:Q:397:ALA:HB2	2.56	0.41
17:R:61:LEU:HD21	17:R:63:ARG:O	2.20	0.41
17:R:118:HIS:HB2	17:R:120:TYR:CZ	2.56	0.41
20:V:119:LYS:N	20:V:119:LYS:HD3	2.36	0.41
2:B:243:ALA:HA	2:B:250:PHE:HB2	2.02	0.40
2:B:826:ALA:HB2	2:B:1087:PHE:HD1	1.86	0.40
3:C:101:LEU:HB2	3:C:118:LEU:HD23	2.02	0.40
9:I:43:VAL:HG23	9:I:44:TYR:H	1.86	0.40
11:K:35:PHE:O	11:K:70:ARG:HB2	2.21	0.40
13:M:158:HIS:CG	13:M:159:ASP:N	2.87	0.40
17:R:73:LEU:HD12	17:R:74:PRO:CD	2.44	0.40
1:A:244:PRO:O	1:A:247:ARG:N	2.54	0.40
1:A:544:ASP:HB2	11:K:47:ARG:HH12	1.85	0.40
2:B:240:ILE:HG23	2:B:254:LEU:HB3	2.03	0.40
2:B:786:ASN:O	2:B:967:ARG:NH1	2.46	0.40
2:B:914:LYS:O	2:B:937:ALA:O	2.39	0.40
5:E:37:LEU:HA	5:E:38:PRO:HD3	1.93	0.40
7:G:59:GLY:HA2	7:G:70:PHE:HD1	1.85	0.40
8:H:97:MET:HE3	8:H:142:LEU:HD23	2.02	0.40
13:M:44:VAL:HG13	13:M:50:LEU:O	2.21	0.40
13:M:157:CYS:SG	13:M:158:HIS:N	2.93	0.40
13:M:267:LYS:CE	15:O:239:LYS:HE3	2.52	0.40
14:N:24:DT:C2'	14:N:25:DA:C5'	2.90	0.40
16:Q:103:LEU:CD2	16:Q:384:PHE:HB2	2.51	0.40
1:A:175:ARG:O	1:A:182:VAL:HG12	2.20	0.40
2:B:290:GLY:HA2	2:B:327:ARG:HD2	2.03	0.40
2:B:420:LEU:HD23	2:B:420:LEU:HA	1.87	0.40
7:G:132:SER:OG	7:G:133:SER:N	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:106:GLU:HG2	8:H:112:ILE:HD13	2.04	0.40
13:M:267:LYS:CD	15:O:239:LYS:HE3	2.52	0.40
1:A:474:VAL:C	1:A:477:PRO:HD2	2.47	0.40
1:A:540:PHE:CG	1:A:571:LEU:HD23	2.56	0.40
1:A:1132:LYS:HE2	1:A:1284:MET:HE1	2.03	0.40
1:A:1368:MET:O	1:A:1372:VAL:HG23	2.21	0.40
2:B:88:TYR:CD1	2:B:136:THR:HG23	2.56	0.40
2:B:546:SER:OG	2:B:632:ARG:N	2.54	0.40
2:B:604:ARG:HH22	2:B:615:MET:H	1.69	0.40
3:C:235:VAL:HG13	10:J:13:VAL:HG13	2.04	0.40
4:D:32:GLU:CB	7:G:42:PHE:HE1	2.34	0.40
4:D:126:ILE:O	4:D:130:LEU:HG	2.22	0.40
4:D:138:ASN:ND2	7:G:36:GLY:CA	2.84	0.40
5:E:11:ARG:NH2	5:E:141:VAL:HG21	2.36	0.40
10:J:34:THR:HG22	10:J:38:ARG:HH12	1.87	0.40
17:R:98:ASN:O	17:R:102:SER:N	2.54	0.40
19:U:256:ALA:HB1	19:U:285:TRP:O	2.21	0.40
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.57	0.40
1:A:727:ASP:HB3	1:A:731:ARG:HH12	1.85	0.40
1:A:809:THR:O	1:A:812:GLU:HB2	2.22	0.40
1:A:1132:LYS:HA	1:A:1135:ARG:NH1	2.35	0.40
1:A:1157:ASP:OD2	1:A:1160:SER:OG	2.27	0.40
8:H:10:PHE:HD1	8:H:30:SER:HA	1.86	0.40
10:J:16:ASP:OD1	10:J:16:ASP:N	2.54	0.40
13:M:162:THR:CG2	13:M:213:ILE:HD11	2.52	0.40
13:M:274:PRO:CG	15:O:188:GLU:OE2	2.61	0.40
15:O:239:LYS:C	15:O:240:MET:HG3	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1386/1733 (80%)	1306 (94%)	77 (6%)	3 (0%)	43	77
2	B	1139/1224 (93%)	1086 (95%)	48 (4%)	5 (0%)	30	66
3	C	260/318 (82%)	246 (95%)	14 (5%)	0	100	100
4	D	153/221 (69%)	145 (95%)	8 (5%)	0	100	100
5	E	211/215 (98%)	209 (99%)	2 (1%)	0	100	100
6	F	81/155 (52%)	76 (94%)	5 (6%)	0	100	100
7	G	169/171 (99%)	160 (95%)	8 (5%)	1 (1%)	21	58
8	H	132/146 (90%)	114 (86%)	14 (11%)	4 (3%)	3	23
9	I	114/122 (93%)	105 (92%)	9 (8%)	0	100	100
10	J	63/70 (90%)	57 (90%)	5 (8%)	1 (2%)	7	37
11	K	110/120 (92%)	107 (97%)	3 (3%)	0	100	100
12	L	43/70 (61%)	37 (86%)	6 (14%)	0	100	100
13	M	225/345 (65%)	202 (90%)	20 (9%)	3 (1%)	9	41
15	O	178/240 (74%)	174 (98%)	4 (2%)	0	100	100
16	Q	140/735 (19%)	124 (89%)	13 (9%)	3 (2%)	5	30
17	R	181/400 (45%)	171 (94%)	9 (5%)	1 (1%)	21	58
19	U	88/286 (31%)	82 (93%)	3 (3%)	3 (3%)	3	21
20	V	96/122 (79%)	87 (91%)	8 (8%)	1 (1%)	12	47
21	W	162/482 (34%)	154 (95%)	7 (4%)	1 (1%)	21	58
22	X	135/328 (41%)	125 (93%)	9 (7%)	1 (1%)	18	55
All	All	5066/7503 (68%)	4767 (94%)	272 (5%)	27 (0%)	26	62

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	343	ILE
2	B	476	ARG
8	H	132	LEU
13	M	269	ILE
17	R	259	VAL
22	X	231	LEU
2	B	221	ASN
8	H	131	ASN
8	H	137	GLN
13	M	200	THR
19	U	31	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	U	264	ASP
20	V	6	TYR
21	W	40	GLU
2	B	364	ILE
7	G	63	PRO
8	H	90	ALA
16	Q	26	ARG
16	Q	406	ILE
2	B	743	ILE
13	M	31	PRO
1	A	958	VAL
1	A	50	ILE
16	Q	127	ILE
19	U	30	ILE
10	J	2	ILE
1	A	569	LYS

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	1221/1520 (80%)	1215 (100%)	6 (0%)	81	81
2	B	1000/1061 (94%)	998 (100%)	2 (0%)	87	85
3	C	230/274 (84%)	230 (100%)	0	100	100
4	D	139/200 (70%)	139 (100%)	0	100	100
5	E	195/197 (99%)	195 (100%)	0	100	100
6	F	73/137 (53%)	72 (99%)	1 (1%)	59	71
7	G	152/152 (100%)	149 (98%)	3 (2%)	48	65
8	H	119/128 (93%)	119 (100%)	0	100	100
9	I	110/116 (95%)	110 (100%)	0	100	100
10	J	60/65 (92%)	60 (100%)	0	100	100
11	K	97/102 (95%)	97 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	201/299 (67%)	200 (100%)	1 (0%)	81	81
15	O	152/205 (74%)	142 (93%)	10 (7%)	15	37
16	Q	109/641 (17%)	109 (100%)	0	100	100
17	R	107/363 (30%)	107 (100%)	0	100	100
19	U	84/260 (32%)	80 (95%)	4 (5%)	23	45
20	V	90/108 (83%)	85 (94%)	5 (6%)	19	41
All	All	4179/5885 (71%)	4147 (99%)	32 (1%)	70	77

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	353	ILE
1	A	613	ILE
1	A	1170	ILE
1	A	1279	ILE
1	A	1356	ILE
2	B	465	ASN
2	B	693	ILE
6	F	93	ILE
7	G	61	ILE
7	G	150	CYS
7	G	160	ILE
13	M	202	GLU
15	O	70	ILE
15	O	108	GLU
15	O	130	ASP
15	O	134	LEU
15	O	175	LEU
15	O	199	LYS
15	O	219	GLN
15	O	225	GLN
15	O	235	SER
15	O	240	MET
19	U	241	GLU
19	U	250	LYS
19	U	253	ARG
19	U	267	VAL
20	V	9	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	V	33	GLU
20	V	57	GLN
20	V	59	LYS
20	V	108	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	397	ASN
1	A	451	HIS
1	A	490	HIS
1	A	611	GLN
1	A	706	HIS
1	A	877	HIS
1	A	953	ASN
1	A	1059	HIS
1	A	1390	ASN
2	B	73	GLN
2	B	325	GLN
2	B	583	ASN
2	B	686	ASN
2	B	958	GLN
2	B	1178	ASN
2	B	1205	GLN
3	C	131	HIS
4	D	143	ASN
4	D	173	HIS
5	E	54	GLN
5	E	114	ASN
7	G	97	HIS
7	G	153	GLN
9	I	79	HIS
9	I	87	GLN
9	I	108	HIS
11	K	40	HIS
13	M	197	HIS
13	M	235	ASN
15	O	95	ASN
15	O	158	GLN
15	O	219	GLN
16	Q	122	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	U	272	ASN
19	U	280	GLN
20	V	55	ASN
20	V	57	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 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
8	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	131:ASN	C	132:LEU	N	1.04

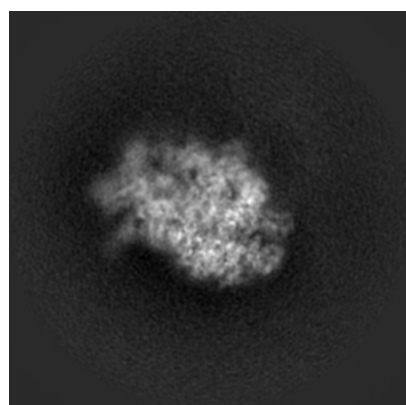
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3378. These allow visual inspection of the internal detail of the map and identification of artifacts.

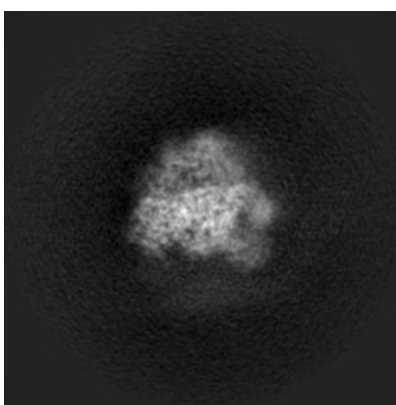
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

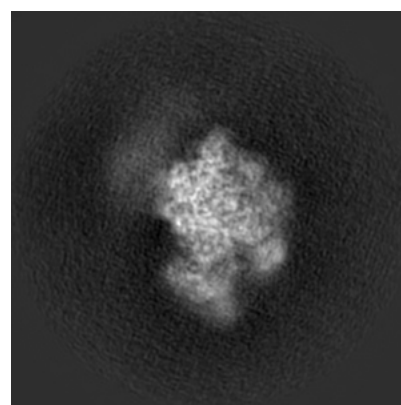
6.1.1 Primary map



X



Y

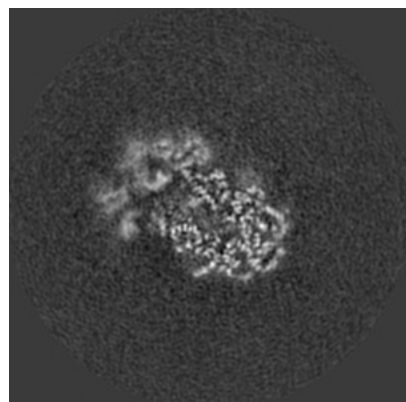


Z

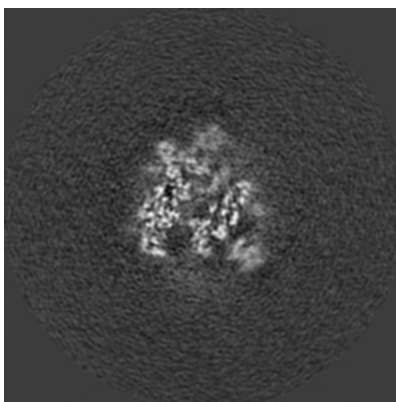
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

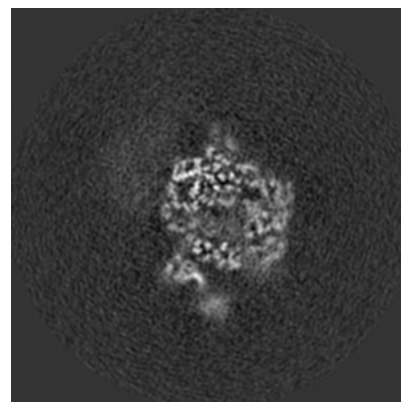
6.2.1 Primary map



X Index: 150



Y Index: 150

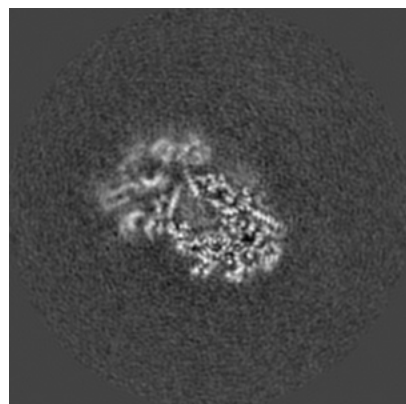


Z Index: 150

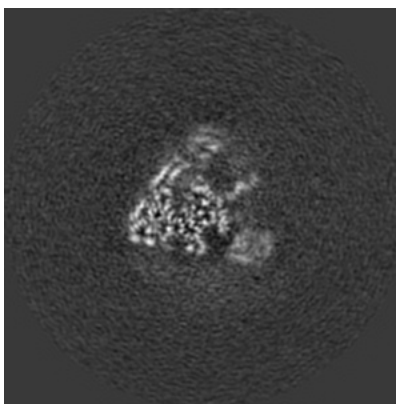
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

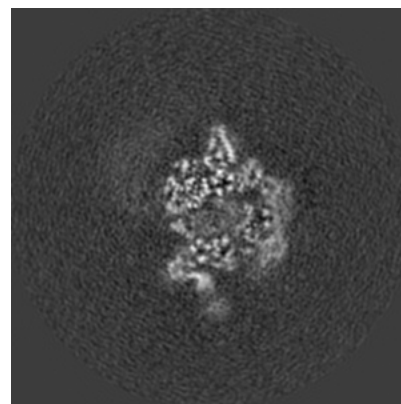
6.3.1 Primary map



X Index: 146



Y Index: 165

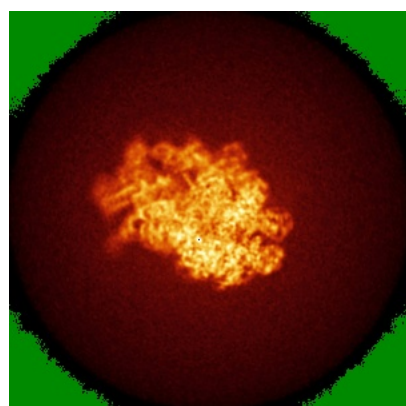


Z Index: 146

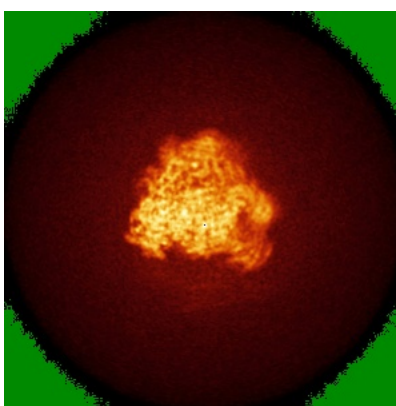
The images above show the largest variance slices of the map in three orthogonal directions.

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

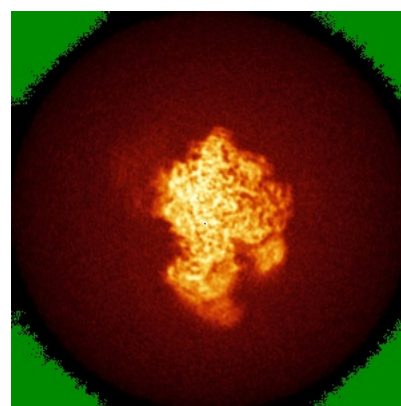
6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.0325. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

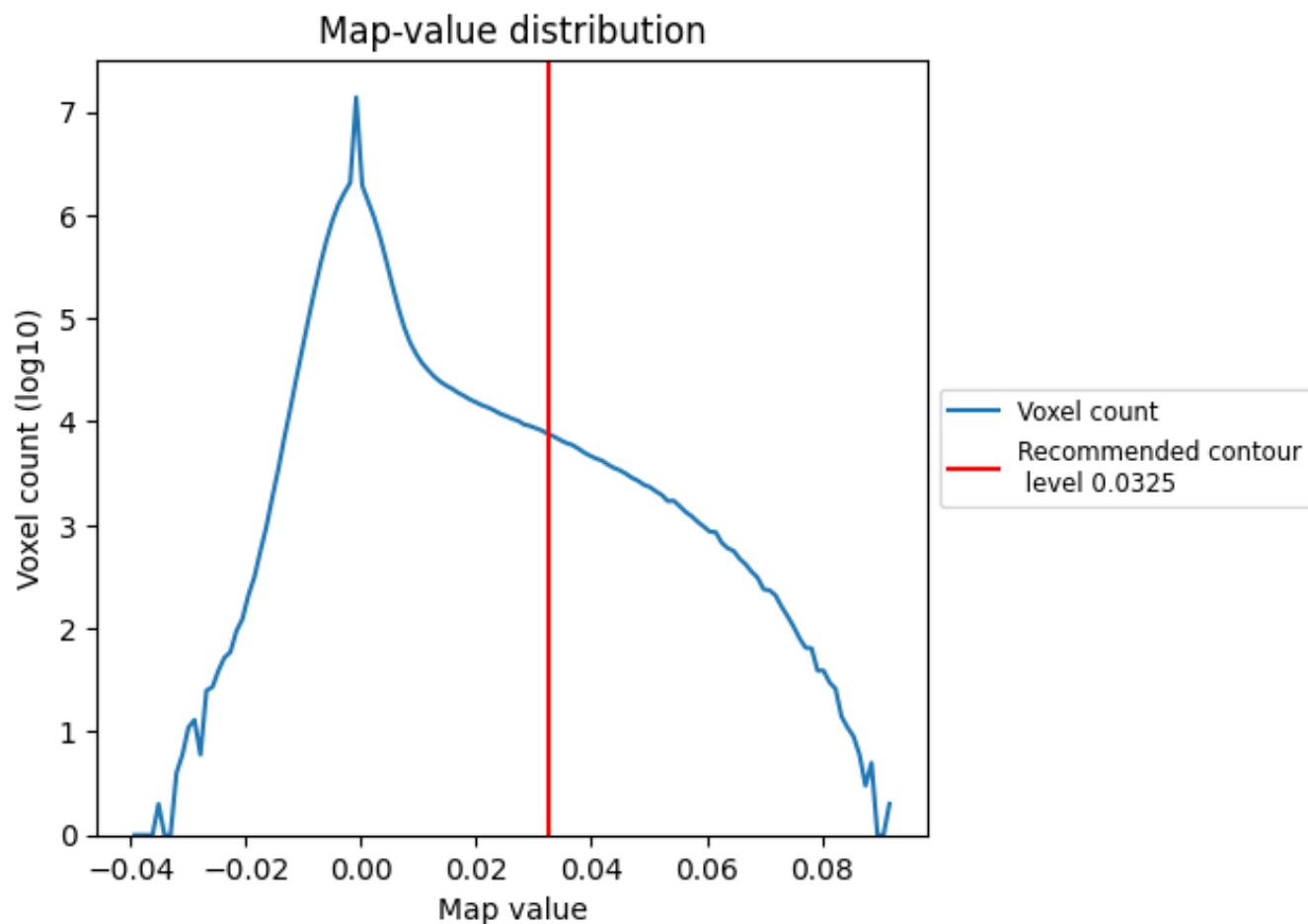
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

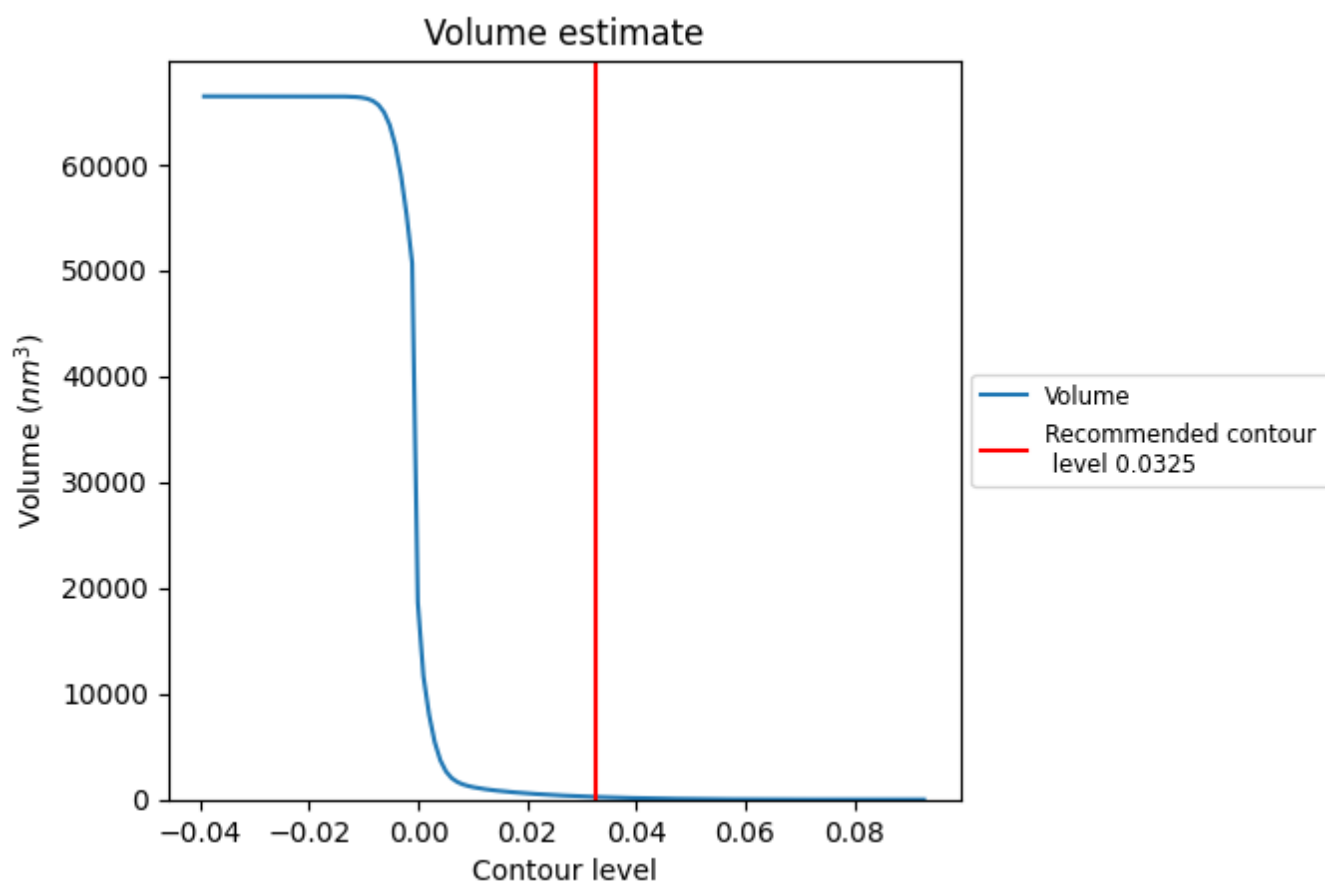
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

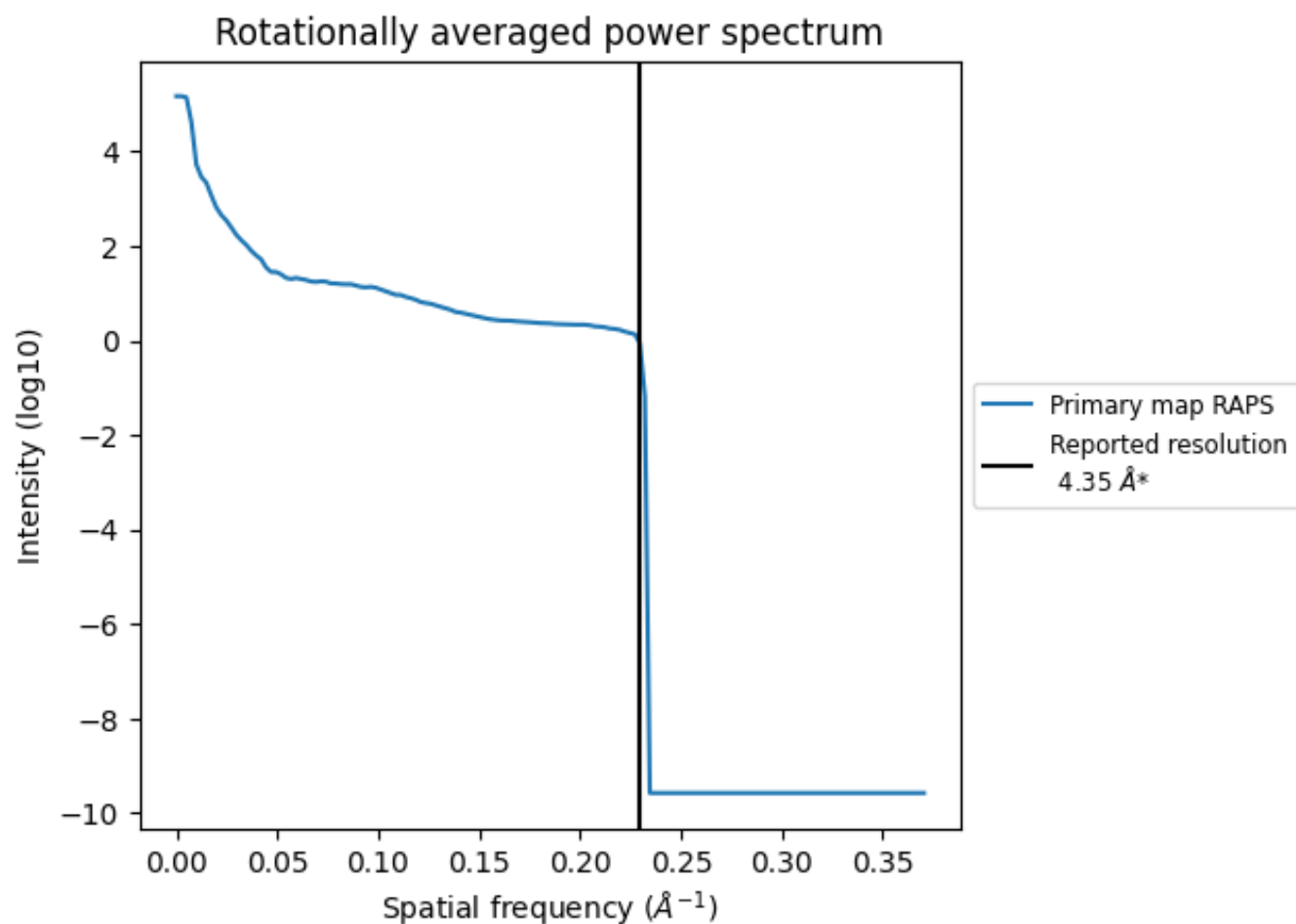
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 250 nm³; this corresponds to an approximate mass of 226 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.230 $\text{\AA}^{-1}$

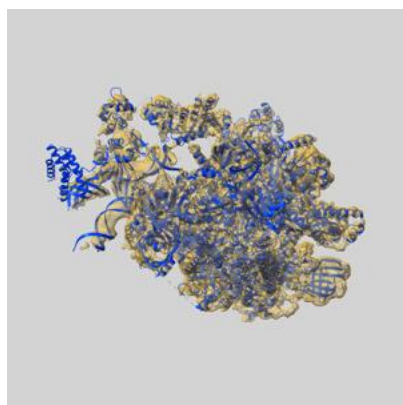
8 Fourier-Shell correlation ⓘ

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

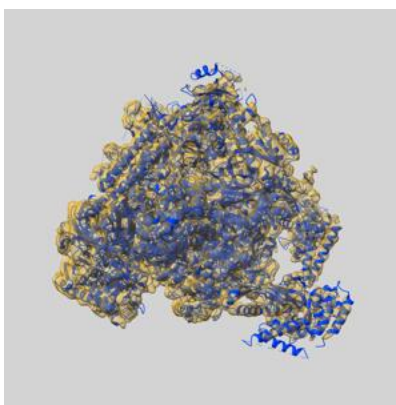
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3378 and PDB model 5FYW. Per-residue inclusion information can be found in section [3](#) on page [8](#).

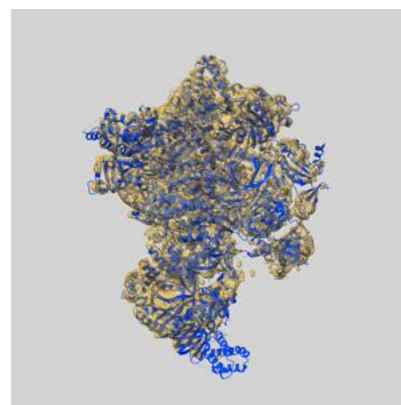
9.1 Map-model overlay [i](#)



X



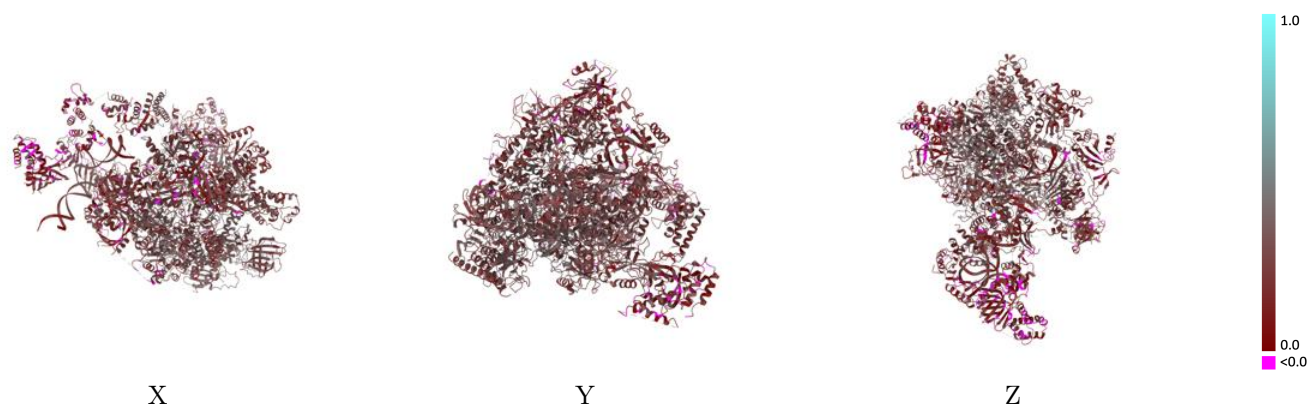
Y



Z

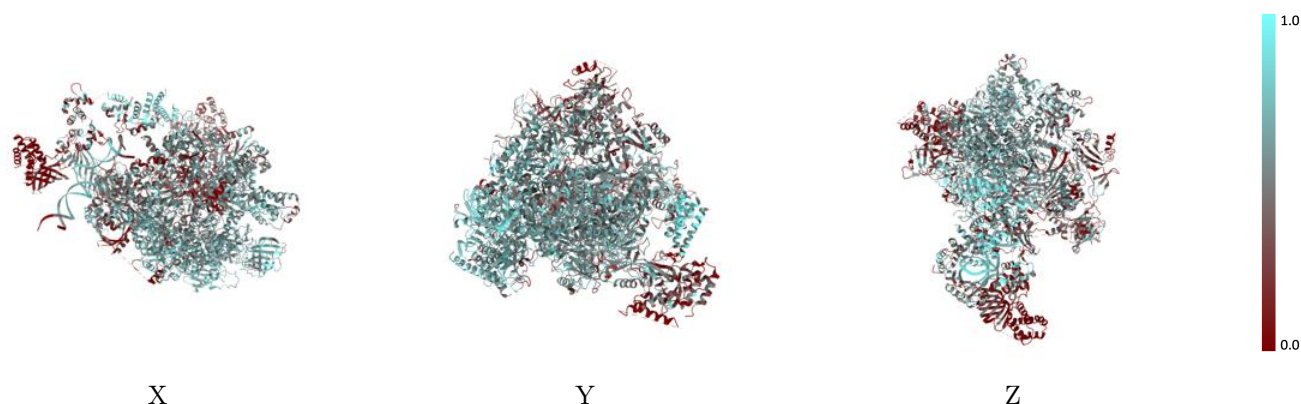
The images above show the 3D surface view of the map at the recommended contour level 0.0325 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



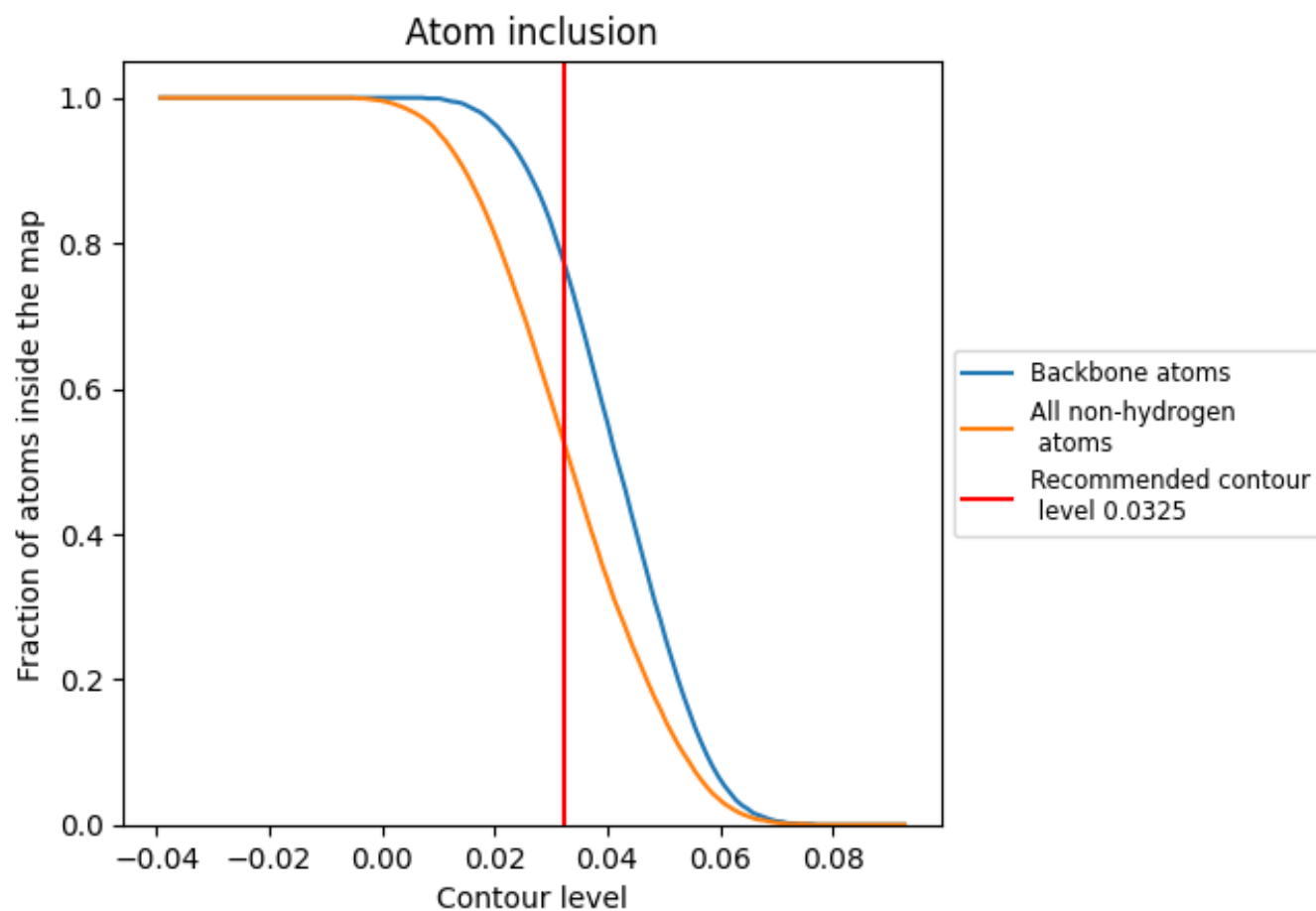
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.0325).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 52% 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 (0.0325) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5210	 0.2600
A	 0.5660	 0.2900
B	 0.5770	 0.3040
C	 0.6790	 0.3190
D	 0.1920	 0.1420
E	 0.5400	 0.2590
F	 0.6170	 0.2990
G	 0.3910	 0.2230
H	 0.6470	 0.2980
I	 0.3760	 0.2100
J	 0.6690	 0.3070
K	 0.5470	 0.2990
L	 0.6160	 0.3150
M	 0.5350	 0.2430
N	 0.5680	 0.2020
O	 0.4430	 0.1560
Q	 0.3080	 0.1880
R	 0.3630	 0.2010
T	 0.5970	 0.1930
U	 0.0890	 0.0950
V	 0.0930	 0.1140
W	 0.6520	 0.2270
X	 0.5030	 0.1730

