



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:41 PM UTC

PDB ID : 7AOE / pdb_00007aoe
EMDB ID : EMD-11842
Title : Schizosaccharomyces pombe RNA polymerase I (elongation complex)
Authors : Heiss, F.; Daiss, J.; Becker, P.; Engel, C.
Deposited on : 2020-10-14
Resolution : 3.90 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:

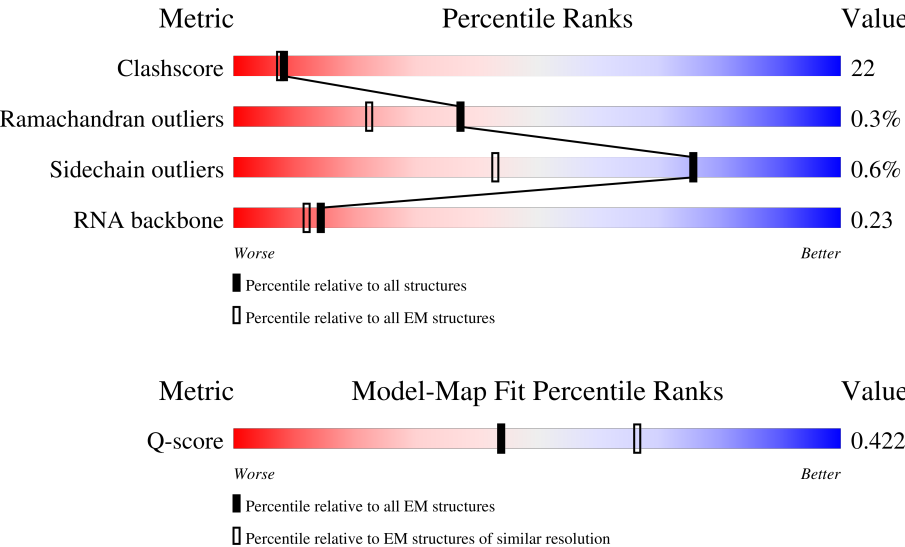
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.90 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	1689	23% 45% 37% 17%
2	B	1174	7% 56% 44% .
3	C	348	. 59% 31% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	147	
5	E	210	
6	F	142	
7	G	173	
8	H	125	
9	I	119	
10	J	71	
11	K	125	
12	L	63	
13	U	39	
14	T	39	
15	R	20	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 30828 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 I subunit rpa1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1401	Total	C	N	O	S	0	0
			11102	7039	1918	2086	59		

- Molecule 2 is a protein called Probable DNA-directed RNA polymerase I subunit RPA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1174	Total	C	N	O	S	0	0
			9254	5867	1618	1710	59		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	317	Total	C	N	O	S	0	0
			2533	1621	430	475	7		

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit rpa14.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	39	Total	C	N	O	S	0	0
			322	203	57	61	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	207	Total	C	N	O	S	0	0
			1663	1050	301	306	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S	0	0
			650	413	111	123	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit rpa43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	160	Total	C	N	O	S	0	0
			1267	817	210	236	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	123	Total	C	N	O	S	0	0
			990	628	166	193	3		

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	57	Total	C	N	O	S	0	0
			431	269	69	89	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	68	Total	C	N	O	S	0	0
			550	350	93	100	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	95	Total	C	N	O	S	0	0
			745	472	123	146	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			368	225	74	61	8		

- Molecule 13 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	14	Total	C	N	O	P	0	0
			285	138	51	83	13		

- Molecule 14 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	25	Total	C	N	O	P	0	0
			509	244	95	146	24		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	7	Total	C	N	O	P	0	0
			153	68	31	47	7		

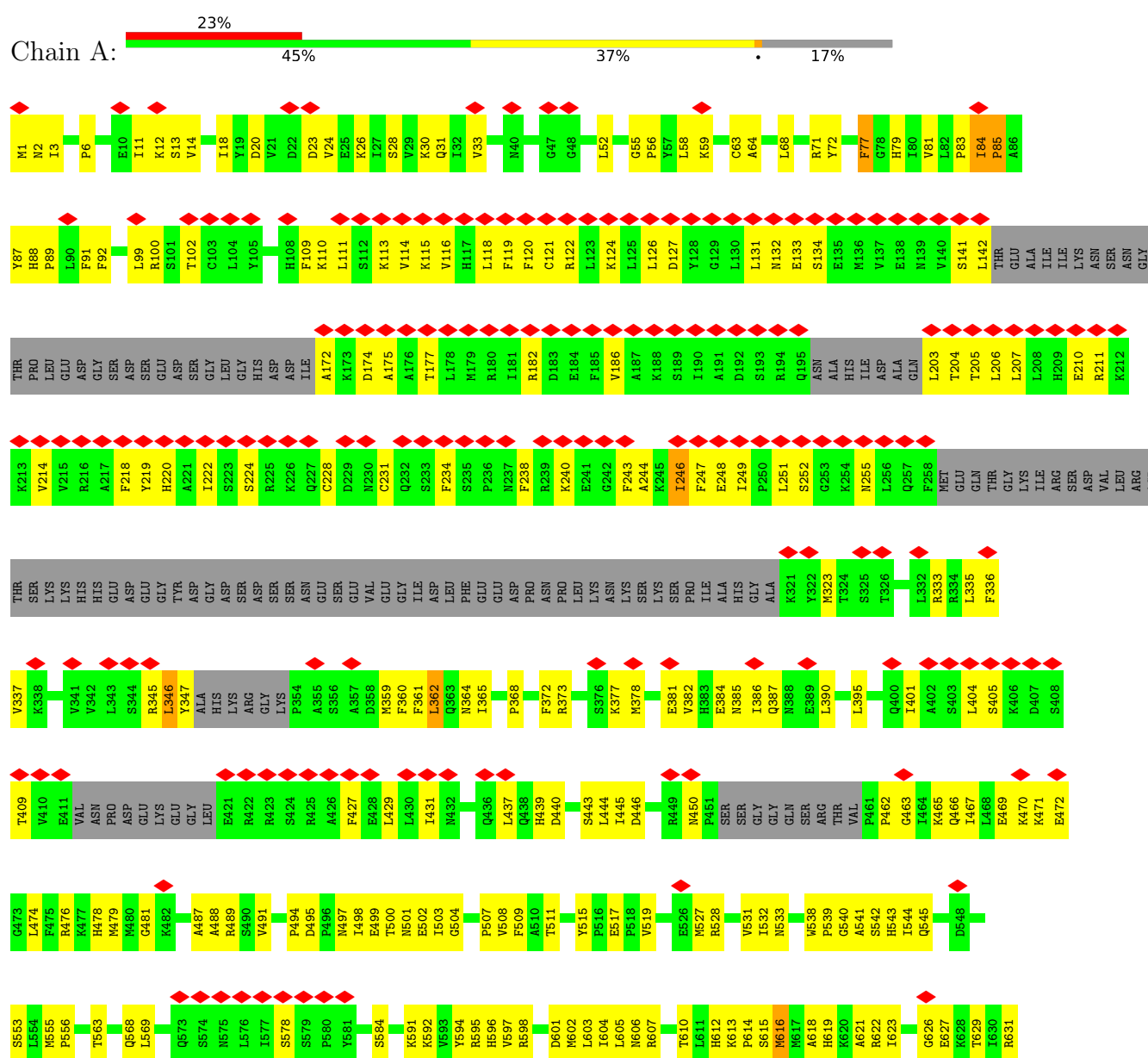
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

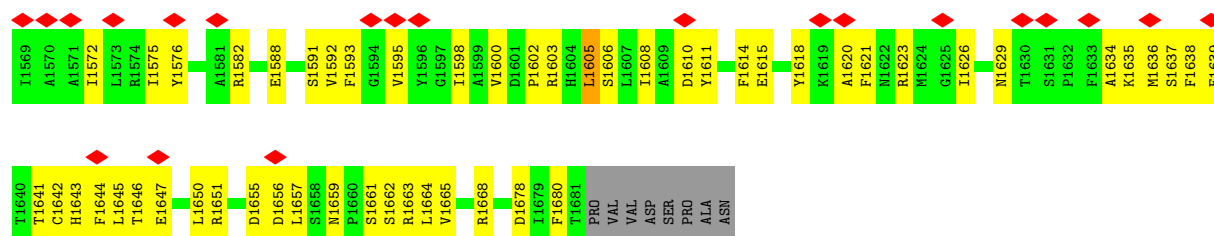
3 Residue-property plots

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

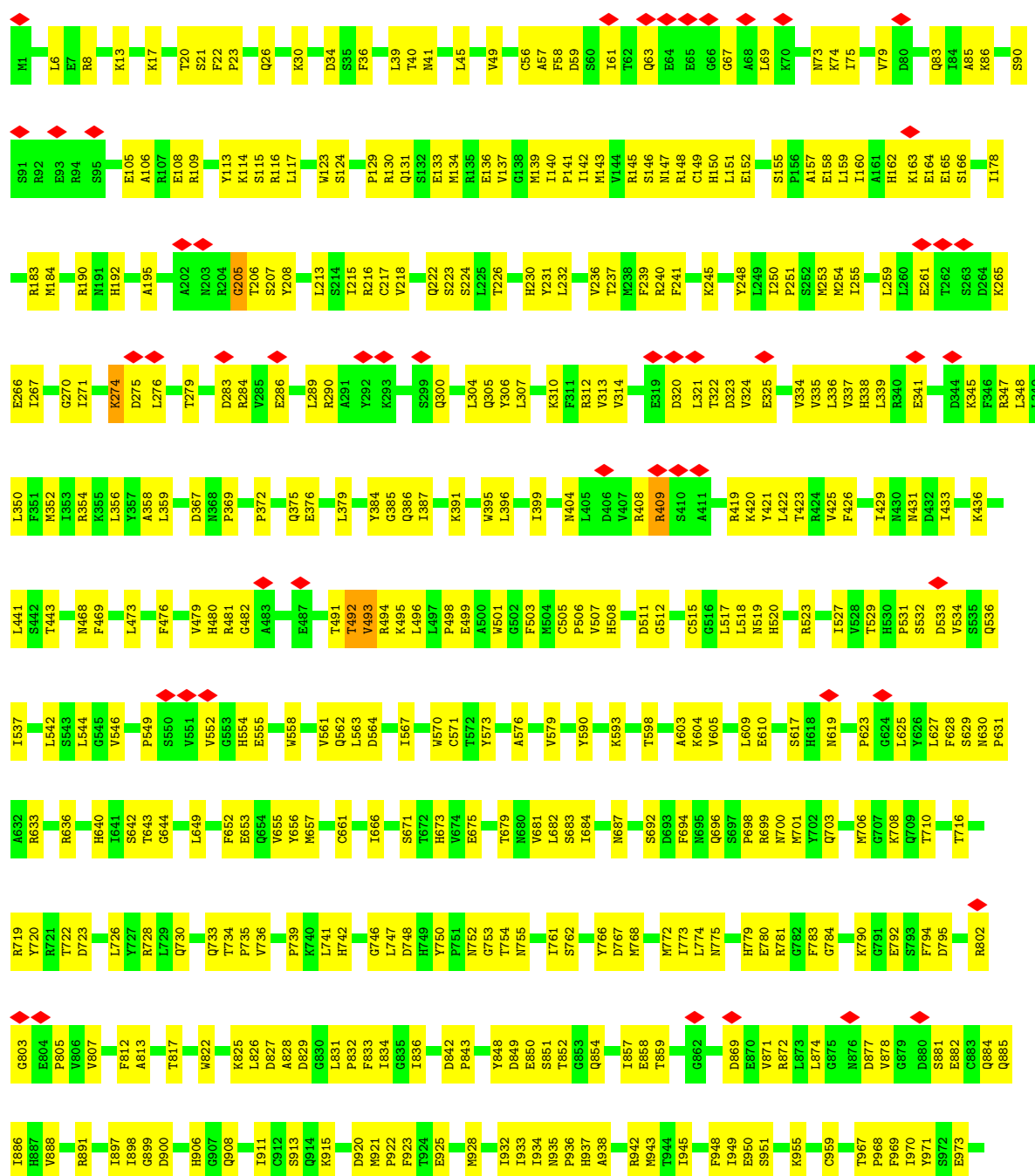
• Molecule 1: DNA-directed RNA polymerase I subunit rpa1

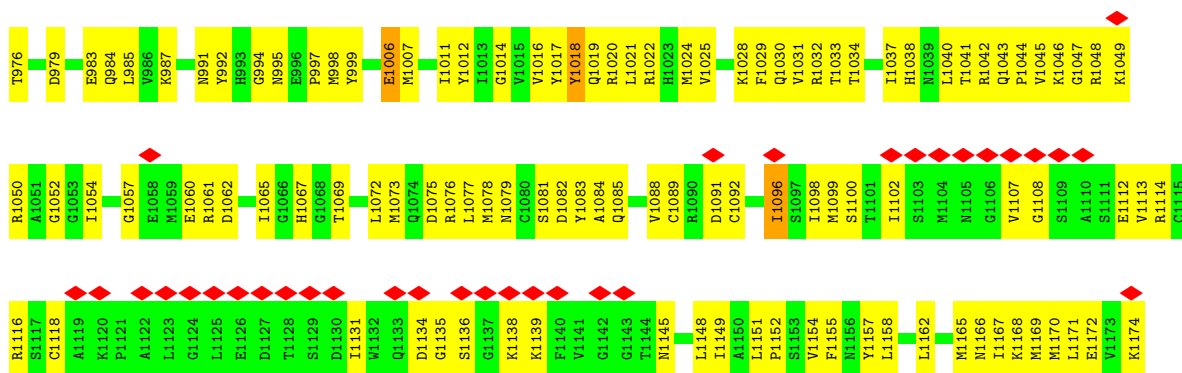






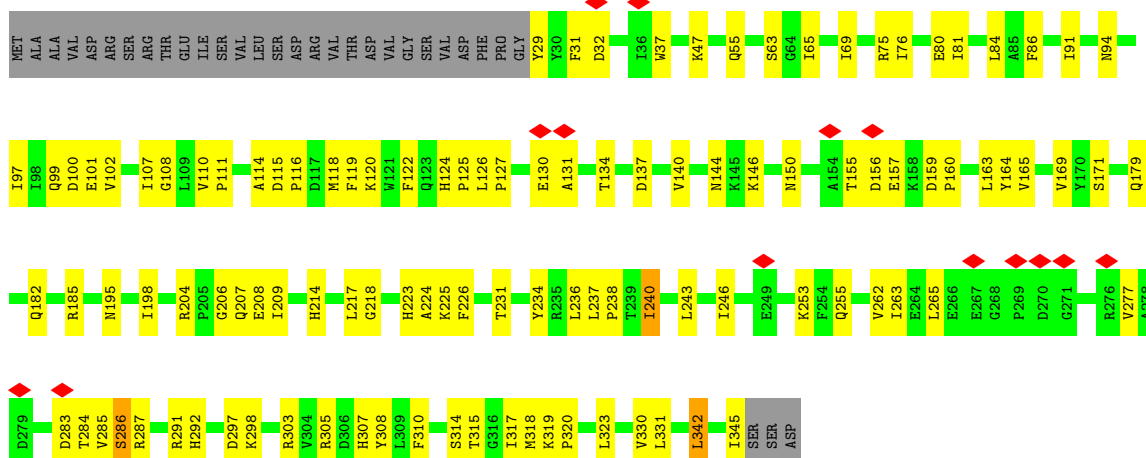
• Molecule 2: Probable DNA-directed RNA polymerase I subunit RPA2





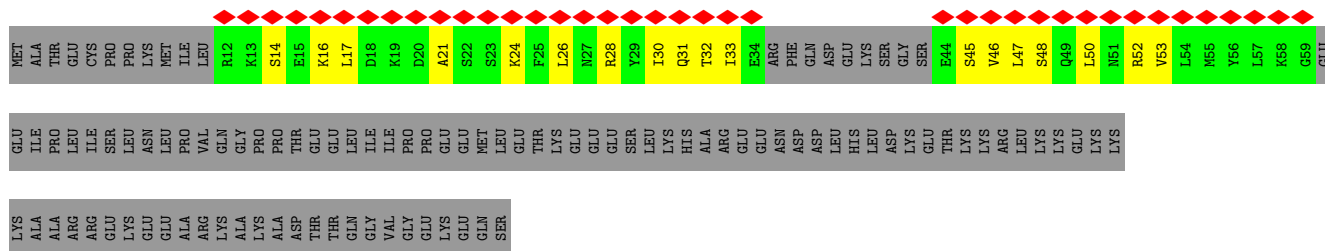
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C: 59% 31% 9%



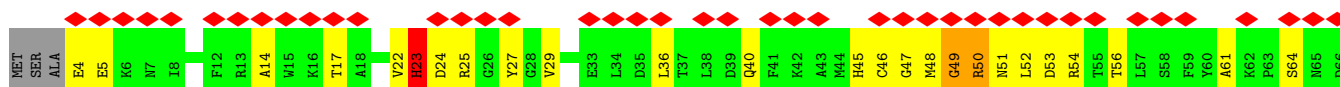
• Molecule 4: DNA-directed RNA polymerase I subunit rpa14

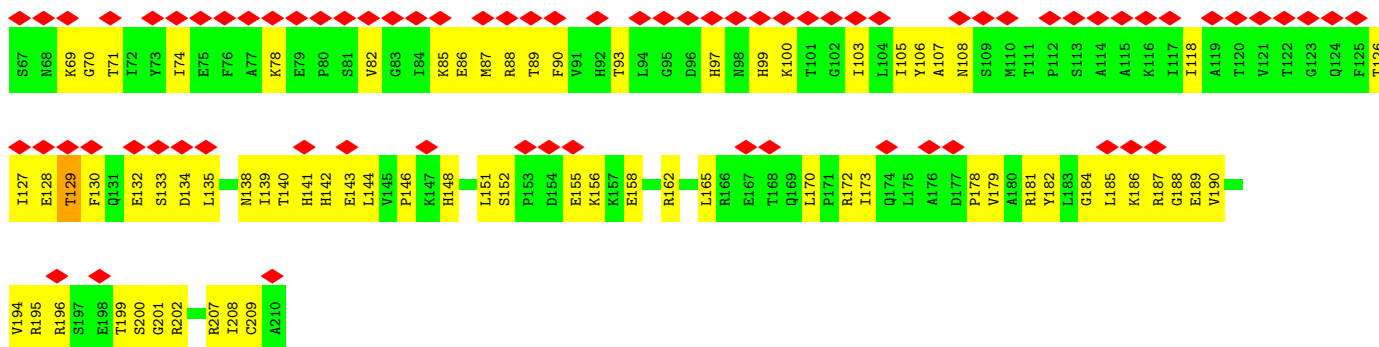
Chain D: 27% 14% 12% 73%



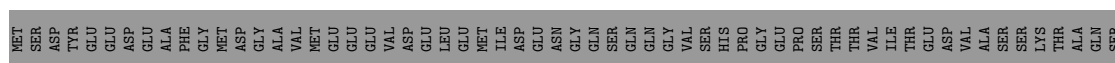
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 55% 53% 44% 2%

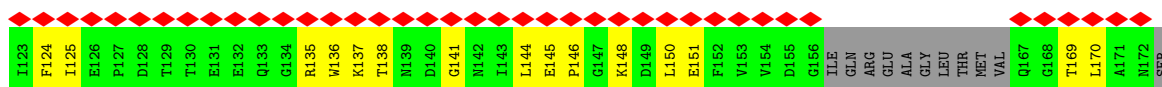
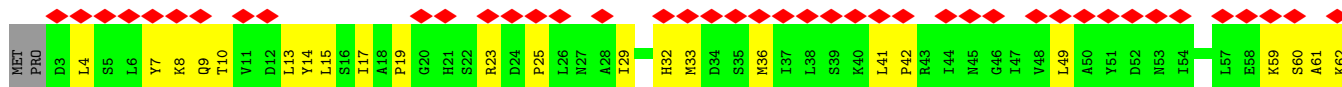
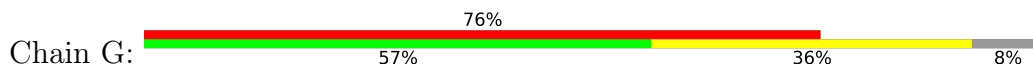




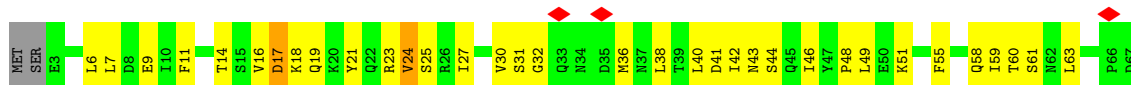
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



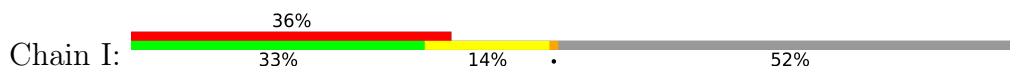
- Molecule 7: DNA-directed RNA polymerase I subunit rpa43

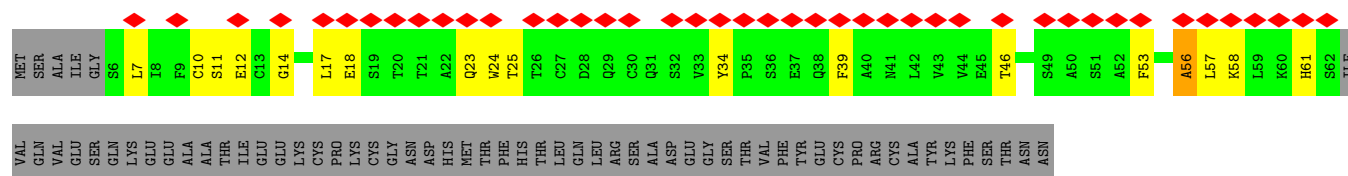


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 9: DNA-directed RNA polymerase I subunit RPA12

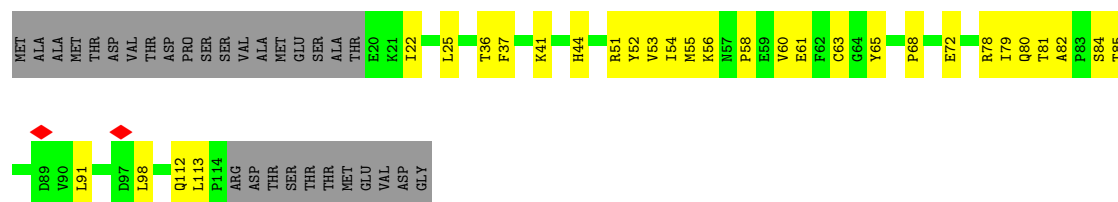




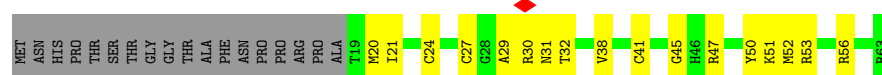
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



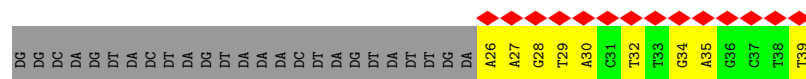
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2



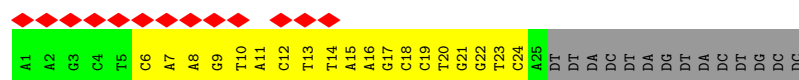
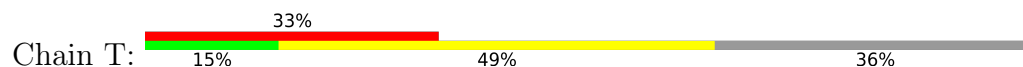
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 13: non-template DNA



- Molecule 14: template DNA



- Molecule 15: RNA



U	A	U	C	U	G	C	C	A	U	G	U	A	G13	A14	C15	C16	A17	G18	G19	C
---	---	---	---	---	---	---	---	---	---	---	---	---	-----	-----	-----	-----	-----	-----	-----	---

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61954	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	88.28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.371	Depositor
Minimum map value	-0.231	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.06	Depositor
Map size ($\text{\AA}$)	272.256, 272.256, 272.256	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0635, 1.0635, 1.0635	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.33	0/11323	0.57	4/15297 (0.0%)
2	B	0.38	0/9463	0.56	0/12794
3	C	0.35	0/2588	0.51	0/3505
4	D	0.14	0/323	0.40	0/427
5	E	0.24	0/1695	0.60	4/2287 (0.2%)
6	F	0.30	0/660	0.44	0/893
7	G	0.23	0/1295	0.48	0/1755
8	H	0.33	0/1004	0.64	2/1355 (0.1%)
9	I	0.20	0/439	0.47	1/596 (0.2%)
10	J	0.43	0/558	0.60	0/751
11	K	0.36	0/759	0.54	2/1030 (0.2%)
12	L	0.34	0/371	0.57	0/491
13	U	0.23	0/319	0.43	0/491
14	T	0.31	0/571	0.44	0/879
15	R	0.30	0/171	0.48	0/265
All	All	0.34	0/31539	0.55	13/42816 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
2	B	0	5
5	E	0	3
All	All	0	15

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1065	GLU	CA-C-N	6.50	133.95	121.54
1	A	1065	GLU	C-N-CA	6.50	133.95	121.54
11	K	112	GLN	CA-C-N	-6.40	108.87	123.15
11	K	112	GLN	C-N-CA	-6.40	108.87	123.15
5	E	49	GLY	CA-C-N	5.90	132.32	121.70
5	E	49	GLY	C-N-CA	5.90	132.32	121.70
8	H	17	ASP	CA-C-N	5.75	132.04	121.70
8	H	17	ASP	C-N-CA	5.75	132.04	121.70
1	A	1067	SER	CA-C-N	5.24	131.55	121.54
1	A	1067	SER	C-N-CA	5.24	131.55	121.54
5	E	23	HIS	CA-C-N	5.09	130.86	121.70
5	E	23	HIS	C-N-CA	5.09	130.86	121.70
9	I	56	ALA	N-CA-C	-5.01	108.20	114.56

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1068	LEU	Peptide
1	A	1566	THR	Peptide
1	A	1656	ASP	Peptide
1	A	246	ILE	Peptide
1	A	6	PRO	Peptide
1	A	686	ILE	Peptide
1	A	84	ILE	Peptide
2	B	205	GLY	Peptide
2	B	274	LYS	Peptide
2	B	320	ASP	Peptide
2	B	409	ARG	Peptide
2	B	498	PRO	Peptide
5	E	129	THR	Peptide
5	E	23	HIS	Peptide
5	E	50	ARG	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	11102	0	11105	575	0
2	B	9254	0	9225	469	0
3	C	2533	0	2540	99	0
4	D	322	0	338	19	0
5	E	1663	0	1684	79	0
6	F	650	0	674	31	0
7	G	1267	0	1278	55	0
8	H	990	0	1001	56	0
9	I	431	0	410	16	0
10	J	550	0	566	34	0
11	K	745	0	745	27	0
12	L	368	0	377	21	0
13	U	285	0	161	8	0
14	T	509	0	283	20	0
15	R	153	0	78	3	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	I	1	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
All	All	30828	0	30465	1328	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 22.

All (1328) 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:1092:CYS:HB3	2:B:1118:CYS:SG	1.94	1.08
1:A:1297:TYR:HB3	1:A:1494:LEU:O	1.61	1.00
1:A:466:GLN:O	1:A:470:LYS:HB2	1.63	0.96
1:A:1297:TYR:OH	1:A:1505:MET:SD	2.24	0.94
5:E:23:HIS:HA	5:E:25:ARG:H	1.34	0.93
1:A:1135:GLY:HA2	1:A:1180:GLN:HE21	1.33	0.92
2:B:802:ARG:HE	2:B:803:GLY:H	1.18	0.91
1:A:1664:LEU:HD11	2:B:1077:LEU:HD12	1.53	0.91
1:A:1324:PHE:O	1:A:1328:PHE:HB3	1.71	0.90
2:B:630:ASN:O	2:B:633:ARG:NH1	2.07	0.88
1:A:1228:ILE:HG13	1:A:1229:PRO:HD3	1.55	0.87
1:A:114:VAL:HG11	1:A:175:ALA:HB1	1.57	0.87
1:A:56:PRO:HG3	1:A:63:CYS:HB3	1.57	0.87
2:B:728:ARG:NH2	2:B:730:GLN:OE1	2.09	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1068:LEU:HD13	1:A:1072:LYS:HB2	1.57	0.85
7:G:61:ALA:HB2	7:G:72:ILE:HD12	1.58	0.84
2:B:1025:VAL:HA	2:B:1028:LYS:HG2	1.58	0.83
5:E:196:ARG:HA	5:E:202:ARG:HB2	1.61	0.83
1:A:842:THR:HG21	2:B:1011:ILE:HA	1.58	0.83
1:A:1312:GLU:HB2	9:I:57:LEU:HD21	1.60	0.83
2:B:767:ASP:O	2:B:935:ASN:ND2	2.12	0.82
2:B:687:ASN:HD21	2:B:741:LEU:HD12	1.42	0.81
2:B:761:ILE:HD12	2:B:1011:ILE:HD13	1.61	0.81
1:A:491:VAL:O	1:A:629:THR:OG1	1.97	0.81
1:A:826:SER:OG	1:A:830:ARG:NH1	2.12	0.81
2:B:555:GLU:HB2	2:B:558:TRP:HD1	1.46	0.81
1:A:1036:LEU:O	1:A:1199:SER:OG	2.00	0.80
1:A:723:MET:SD	1:A:823:ARG:NH2	2.56	0.79
5:E:93:THR:O	5:E:97:HIS:ND1	2.14	0.79
2:B:348:LEU:HD12	2:B:562:GLN:HE22	1.47	0.79
10:J:44:CYS:SG	10:J:45:CYS:N	2.56	0.78
5:E:190:VAL:HG22	5:E:208:ILE:HG22	1.66	0.78
8:H:17:ASP:HA	8:H:18:LYS:HB2	1.64	0.78
1:A:1320:ILE:O	1:A:1324:PHE:HB3	1.84	0.78
1:A:373:ARG:HB3	1:A:385:ASN:HD21	1.49	0.77
2:B:906:HIS:NE2	2:B:950:GLU:OE1	2.17	0.77
1:A:619:HIS:NE2	1:A:640:TYR:OH	2.11	0.77
8:H:24:VAL:HG12	8:H:43:ASN:HA	1.66	0.77
1:A:613:LYS:HD3	1:A:676:PRO:HG2	1.65	0.77
2:B:636:ARG:NH2	2:B:675:GLU:OE2	2.14	0.77
1:A:977:LYS:HE2	1:A:980:PRO:HA	1.67	0.76
2:B:190:ARG:HD3	2:B:218:VAL:HG11	1.67	0.76
11:K:36:THR:HG22	11:K:78:ARG:HD3	1.67	0.76
3:C:234:TYR:HB3	3:C:310:PHE:CD1	2.20	0.76
1:A:1068:LEU:HD23	1:A:1069:ASP:H	1.51	0.75
1:A:1063:TYR:HB3	1:A:1066:ASP:HB3	1.67	0.75
10:J:35:LEU:HA	10:J:38:LEU:HD13	1.68	0.75
2:B:239:PHE:N	2:B:250:ILE:O	2.16	0.75
1:A:1336:ILE:HG22	1:A:1508:LEU:HD13	1.68	0.75
1:A:497:ASN:ND2	2:B:766:TYR:OH	2.20	0.74
1:A:700:ASP:OD2	8:H:23:ARG:NH1	2.20	0.74
2:B:322:THR:HG21	2:B:325:GLU:HB2	1.69	0.74
2:B:653:GLU:N	2:B:653:GLU:OE1	2.20	0.74
1:A:859:ARG:NH1	2:B:973:GLU:OE1	2.21	0.73
2:B:852:THR:HG23	2:B:854:GLN:H	1.53	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PHE:HE2	1:A:323:MET:HB2	1.53	0.73
2:B:1024:MET:SD	2:B:1024:MET:N	2.62	0.73
1:A:1205:PRO:HB3	1:A:1598:ILE:HD12	1.69	0.73
5:E:61:ALA:O	5:E:71:THR:OG1	2.06	0.73
2:B:768:MET:SD	2:B:935:ASN:ND2	2.61	0.73
2:B:781:ARG:NH1	10:J:10:CYS:O	2.22	0.73
1:A:920:ILE:HD11	1:A:959:LEU:HD13	1.71	0.72
1:A:1001:THR:HG23	2:B:976:THR:HG22	1.70	0.72
1:A:893:GLU:OE2	2:B:617:SER:OG	2.06	0.72
2:B:265:LYS:HZ3	9:I:14:GLY:HA2	1.53	0.72
2:B:728:ARG:HH22	3:C:99:GLN:NE2	1.87	0.72
1:A:540:GLY:O	1:A:596:HIS:ND1	2.23	0.72
2:B:762:SER:HB2	2:B:768:MET:HE1	1.72	0.72
1:A:445:ILE:HG23	2:B:1165:MET:HE2	1.69	0.72
1:A:700:ASP:O	8:H:23:ARG:NH1	2.23	0.72
2:B:1046:LYS:NZ	14:T:19:DC:OP1	2.18	0.72
1:A:731:PRO:O	1:A:745:GLN:NE2	2.21	0.72
2:B:231:TYR:OH	2:B:284:ARG:NH2	2.22	0.72
1:A:28:SER:OG	1:A:79:HIS:ND1	2.18	0.72
2:B:259:LEU:HD21	2:B:345:LYS:HB2	1.72	0.71
2:B:1037:ILE:HD12	2:B:1042:ARG:HG3	1.70	0.71
8:H:41:ASP:OD2	8:H:101:LEU:N	2.22	0.71
3:C:223:HIS:HD2	3:C:225:LYS:HG2	1.55	0.71
2:B:270:GLY:HA3	2:B:350:LEU:HD13	1.71	0.71
1:A:1066:ASP:C	1:A:1068:LEU:H	1.99	0.71
1:A:1140:LYS:HB2	5:E:201:GLY:H	1.56	0.71
1:A:610:THR:HG23	1:A:615:SER:HB3	1.73	0.71
1:A:826:SER:HG	1:A:830:ARG:HH12	1.37	0.71
1:A:12:LYS:HE3	2:B:1174:LYS:HB3	1.73	0.71
2:B:755:ASN:O	10:J:47:ARG:NH1	2.24	0.71
1:A:1549:LEU:HD13	1:A:1575:ILE:HD11	1.72	0.70
7:G:105:ILE:HG23	7:G:109:PHE:HB2	1.73	0.70
1:A:494:PRO:HG3	1:A:644:PHE:CD1	2.27	0.70
1:A:1479:HIS:HB3	1:A:1493:GLU:HB3	1.74	0.70
2:B:1099:MET:HE3	2:B:1116:ARG:HD2	1.73	0.70
7:G:10:THR:HG22	7:G:77:ASP:HB3	1.72	0.70
8:H:11:PHE:HB2	8:H:55:PHE:HB2	1.73	0.70
3:C:234:TYR:HB3	3:C:310:PHE:HD1	1.56	0.70
7:G:117:SER:HB3	7:G:169:THR:HA	1.74	0.70
2:B:511:ASP:OD1	2:B:512:GLY:N	2.25	0.70
1:A:1050:THR:HG23	1:A:1061:PHE:HA	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:SER:HB2	1:A:584:SER:HB2	1.73	0.69
1:A:470:LYS:O	1:A:471:LYS:HG2	1.91	0.69
1:A:936:ASN:OD1	1:A:939:GLN:N	2.22	0.69
7:G:33:MET:HE3	7:G:76:VAL:HG21	1.73	0.69
1:A:781:GLU:O	1:A:783:SER:N	2.25	0.69
2:B:753:GLY:N	2:B:1017:TYR:OH	2.20	0.69
1:A:498:ILE:HG13	1:A:499:GLU:H	1.58	0.68
2:B:1091:ASP:OD1	2:B:1145:ASN:ND2	2.26	0.68
1:A:1038:LYS:HB2	1:A:1638:PHE:CE2	2.28	0.68
1:A:1034:ARG:NH1	14:T:15:DA:OP1	2.27	0.68
2:B:147:ASN:O	2:B:148:ARG:NH1	2.27	0.68
1:A:1477:CYS:HA	1:A:1494:LEU:HD22	1.75	0.68
2:B:734:THR:HG1	10:J:51:THR:HG1	1.35	0.68
1:A:1038:LYS:HE2	1:A:1626:ILE:HG23	1.75	0.67
8:H:48:PRO:O	8:H:125:ARG:NH2	2.27	0.67
1:A:685:LEU:HD21	1:A:829:SER:HB2	1.75	0.67
2:B:149:CYS:SG	2:B:150:HIS:N	2.67	0.67
2:B:34:ASP:HB3	2:B:529:THR:HG21	1.76	0.67
1:A:1521:ILE:HG21	1:A:1551:ALA:HB2	1.76	0.67
12:L:31:ASN:HD21	12:L:41:CYS:HA	1.59	0.67
2:B:794:PHE:HB2	2:B:886:ILE:HG22	1.76	0.67
1:A:1020:ILE:HD11	2:B:491:THR:HG23	1.77	0.67
1:A:476:ARG:HH22	1:A:1034:ARG:CZ	2.08	0.67
1:A:479:MET:HE1	2:B:1158:LEU:HD22	1.77	0.67
2:B:231:TYR:HD1	2:B:237:THR:HG22	1.59	0.67
2:B:643:THR:HG22	2:B:644:GLY:H	1.60	0.67
3:C:240:ILE:HB	3:C:277:VAL:HG11	1.77	0.67
2:B:20:THR:OG1	2:B:26:GLN:NE2	2.28	0.67
3:C:204:ARG:H	3:C:207:GLN:HE21	1.43	0.67
1:A:603:LEU:HD22	1:A:621:ALA:HB2	1.78	0.66
4:D:30:ILE:HG23	4:D:47:LEU:HD11	1.78	0.66
11:K:55:MET:HE2	11:K:63:CYS:HB3	1.78	0.66
1:A:1052:ARG:HG2	1:A:1058:ILE:HD13	1.77	0.66
2:B:90:SER:HB2	2:B:878:VAL:HB	1.77	0.66
6:F:76:THR:OG1	6:F:79:GLU:OE1	2.09	0.66
2:B:734:THR:HG23	10:J:53:VAL:HG23	1.78	0.66
3:C:317:ILE:HG22	3:C:318:MET:HG3	1.78	0.66
2:B:164:GLU:N	2:B:164:GLU:OE2	2.29	0.66
2:B:719:ARG:O	2:B:872:ARG:NH2	2.29	0.66
6:F:121:PRO:HB2	6:F:122:LEU:HD12	1.77	0.65
5:E:134:ASP:OD1	5:E:135:LEU:N	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:ARG:HB2	1:A:649:MET:HG2	1.79	0.65
1:A:1634:ALA:HB2	1:A:1659:ASN:ND2	2.12	0.65
3:C:146:LYS:HG3	3:C:208:GLU:HB2	1.78	0.65
6:F:72:THR:O	6:F:126:ARG:NH1	2.23	0.65
1:A:1238:ALA:HB1	1:A:1618:TYR:HE2	1.60	0.65
1:A:736:ARG:HG3	8:H:75:ILE:HD12	1.79	0.65
2:B:555:GLU:HB2	2:B:558:TRP:CD1	2.29	0.65
3:C:47:LYS:HG3	3:C:63:SER:HB2	1.78	0.65
6:F:93:MET:HG3	7:G:68:PRO:HG3	1.78	0.65
1:A:687:GLN:HB3	2:B:937:HIS:CD2	2.32	0.65
3:C:150:ASN:HB2	3:C:165:VAL:HG13	1.79	0.65
8:H:14:THR:O	8:H:51:LYS:NZ	2.30	0.65
1:A:52:LEU:HG	1:A:64:ALA:HB2	1.78	0.64
15:R:13:G:H2'	15:R:14:A:H8	1.62	0.64
1:A:1037:MET:HE3	2:B:1061:ARG:HH22	1.62	0.64
1:A:89:PRO:HG2	1:A:445:ILE:HB	1.78	0.64
1:A:1645:LEU:HD11	2:B:1162:LEU:HD11	1.79	0.64
2:B:433:ILE:HA	2:B:436:LYS:HD2	1.79	0.64
6:F:123:LEU:HD12	6:F:135:ASP:HB2	1.80	0.64
2:B:216:ARG:NH2	2:B:224:SER:OG	2.30	0.64
2:B:347:ARG:HB3	2:B:567:ILE:HD12	1.80	0.64
2:B:780:GLU:OE2	3:C:224:ALA:N	2.30	0.64
2:B:849:ASP:OD1	2:B:850:GLU:N	2.31	0.64
2:B:1047:GLY:H	2:B:1052:GLY:HA3	1.63	0.64
2:B:998:MET:HB2	2:B:1011:ILE:HD12	1.79	0.64
2:B:205:GLY:O	2:B:207:SER:N	2.31	0.64
1:A:688:ASP:HB2	2:B:768:MET:SD	2.38	0.64
2:B:192:HIS:HB2	2:B:628:PHE:HZ	1.62	0.64
2:B:395:TRP:HE3	2:B:396:LEU:HD12	1.63	0.64
5:E:74:ILE:HA	5:E:103:ILE:HG12	1.79	0.64
1:A:732:PRO:HG2	1:A:735:GLN:HG2	1.79	0.64
2:B:312:ARG:NH2	2:B:322:THR:O	2.24	0.64
2:B:133:GLU:OE2	2:B:419:ARG:NH2	2.30	0.64
15:R:13:G:H2'	15:R:14:A:C8	2.32	0.64
2:B:399:ILE:HG22	2:B:429:ILE:HG21	1.79	0.63
2:B:696:GLN:HG2	2:B:698:PRO:HD2	1.79	0.63
2:B:692:SER:OG	2:B:700:ASN:ND2	2.31	0.63
5:E:151:LEU:HD22	5:E:155:GLU:HB3	1.79	0.63
1:A:697:THR:HG21	1:A:796:LEU:HG	1.81	0.63
7:G:118:ILE:HG12	7:G:170:LEU:HD13	1.81	0.63
1:A:247:PHE:CE2	1:A:323:MET:HB2	2.33	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:LYS:NZ	1:A:781:GLU:OE1	2.30	0.63
1:A:211:ARG:HD3	1:A:1651:ARG:NH2	2.14	0.63
1:A:736:ARG:NH1	8:H:72:ALA:O	2.31	0.63
1:A:1041:GLU:N	1:A:1041:GLU:OE1	2.30	0.63
14:T:6:DC:H2'	14:T:7:DA:C8	2.32	0.63
2:B:160:ILE:HD11	2:B:166:SER:HB3	1.80	0.63
9:I:10:CYS:SG	9:I:11:SER:N	2.71	0.63
1:A:248:GLU:HG2	1:A:249:ILE:H	1.64	0.62
1:A:517:GLU:OE1	1:A:595:ARG:NE	2.30	0.62
1:A:896:TYR:HB3	1:A:902:LEU:HD21	1.80	0.62
1:A:1135:GLY:HA2	1:A:1180:GLN:NE2	2.11	0.62
1:A:1610:ASP:OD1	5:E:195:ARG:NH1	2.32	0.62
1:A:1623:ARG:HA	1:A:1626:ILE:HD12	1.81	0.62
2:B:494:ARG:HD2	2:B:515:CYS:O	1.99	0.62
9:I:58:LYS:HA	9:I:61:HIS:HB2	1.81	0.62
1:A:501:ASN:HA	1:A:669:THR:HG21	1.82	0.62
1:A:1281:VAL:HG11	1:A:1505:MET:HB3	1.81	0.62
2:B:426:PHE:O	2:B:431:ASN:ND2	2.31	0.62
2:B:531:PRO:HB3	2:B:631:PRO:HD3	1.81	0.62
1:A:487:ALA:HB1	2:B:1054:ILE:HD11	1.82	0.62
2:B:1089:CYS:CB	2:B:1092:CYS:SG	2.85	0.62
3:C:63:SER:OG	3:C:307:HIS:ND1	2.32	0.62
1:A:99:LEU:O	1:A:102:THR:OG1	2.13	0.62
1:A:720:GLU:N	1:A:720:GLU:OE2	2.32	0.62
1:A:1297:TYR:HD2	1:A:1494:LEU:HB2	1.65	0.62
2:B:404:ASN:OD1	2:B:408:ARG:NH1	2.33	0.62
2:B:13:LYS:NZ	3:C:159:ASP:O	2.30	0.62
2:B:871:VAL:HG12	2:B:888:VAL:HG13	1.80	0.62
2:B:158:GLU:O	2:B:162:HIS:ND1	2.31	0.62
2:B:1007:MET:HG3	2:B:1011:ILE:HD11	1.80	0.62
2:B:184:MET:HB2	2:B:479:VAL:HG12	1.80	0.61
1:A:127:ASP:OD2	1:A:345:ARG:NH1	2.32	0.61
1:A:1193:SER:OG	2:B:1065:ILE:O	2.17	0.61
1:A:1638:PHE:HB3	1:A:1639:GLU:OE2	1.99	0.61
2:B:473:LEU:O	2:B:476:PHE:N	2.32	0.61
1:A:1154:ASP:OD1	1:A:1155:LYS:N	2.32	0.61
2:B:492:THR:O	2:B:494:ARG:N	2.32	0.61
6:F:125:ARG:NH2	7:G:60:SER:OG	2.33	0.61
14:T:20:DT:H2'	14:T:21:DG:H8	1.65	0.61
4:D:16:LYS:HZ1	7:G:4:LEU:HD22	1.66	0.61
4:D:14:SER:HB3	7:G:9:GLN:HE21	1.65	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:HIS:N	1:A:360:PHE:O	2.26	0.61
1:A:730:LEU:HD11	1:A:752:LEU:HD13	1.83	0.61
2:B:146:SER:OG	2:B:147:ASN:N	2.30	0.61
1:A:606:ASN:ND2	2:B:1060:GLU:OE1	2.34	0.61
2:B:920:ASP:OD1	3:C:75:ARG:NH2	2.33	0.61
2:B:716:THR:HG21	10:J:58:LYS:HD3	1.83	0.61
2:B:900:ASP:OD1	2:B:1020:ARG:NH2	2.31	0.61
2:B:141:PRO:HG2	2:B:441:LEU:HD12	1.82	0.61
1:A:131:LEU:O	1:A:134:SER:OG	2.18	0.60
2:B:1151:LEU:HD12	2:B:1152:PRO:HD2	1.82	0.60
1:A:634:TYR:HB3	1:A:686:ILE:HD11	1.82	0.60
5:E:49:GLY:HA3	5:E:51:ASN:H	1.66	0.60
1:A:515:TYR:OH	1:A:595:ARG:NH1	2.34	0.60
2:B:323:ASP:N	2:B:323:ASP:OD1	2.32	0.60
1:A:726:ARG:HA	11:K:78:ARG:HH21	1.66	0.60
1:A:962:GLN:NE2	1:A:992:GLY:O	2.31	0.60
5:E:49:GLY:HA2	5:E:50:ARG:HB2	1.82	0.60
8:H:80:VAL:HB	8:H:95:VAL:HG22	1.82	0.60
1:A:500:THR:HG23	1:A:826:SER:HB2	1.84	0.60
1:A:1563:ASP:HB2	1:A:1565:TYR:HE1	1.67	0.60
12:L:21:ILE:HG23	12:L:30:ARG:HG3	1.81	0.60
1:A:706:ASP:HB3	11:K:51:ARG:HH12	1.66	0.60
2:B:959:CYS:O	10:J:46:ARG:NH2	2.32	0.60
1:A:528:ARG:O	1:A:532:ILE:HG12	2.02	0.60
1:A:812:VAL:HG11	1:A:824:LEU:HD13	1.84	0.60
1:A:891:ASN:O	1:A:895:VAL:HG23	2.01	0.60
1:A:111:LEU:HD22	1:A:115:LYS:HD2	1.83	0.60
1:A:965:LEU:HD11	1:A:971:PRO:HD3	1.84	0.60
1:A:1068:LEU:HD23	1:A:1069:ASP:N	2.16	0.60
1:A:1238:ALA:HB1	1:A:1618:TYR:CE2	2.36	0.60
2:B:747:LEU:O	2:B:750:TYR:N	2.26	0.60
2:B:1041:THR:HB	2:B:1154:VAL:HG22	1.84	0.60
1:A:372:PHE:HE1	2:B:1157:TYR:HA	1.66	0.59
1:A:627:GLU:N	1:A:627:GLU:OE1	2.34	0.59
1:A:977:LYS:NZ	2:B:657:MET:O	2.35	0.59
2:B:773:ILE:HG22	2:B:774:LEU:H	1.67	0.59
2:B:923:PHE:CE1	2:B:999:TYR:HB2	2.37	0.59
1:A:390:LEU:HD22	1:A:444:LEU:HB2	1.83	0.59
1:A:87:TYR:HA	1:A:361:PHE:HA	1.84	0.59
6:F:64:VAL:HB	6:F:134:GLU:HG3	1.85	0.59
8:H:17:ASP:N	8:H:17:ASP:OD1	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LEU:HB2	1:A:182:ARG:CZ	2.33	0.59
2:B:784:GLY:O	2:B:1020:ARG:NH1	2.36	0.59
7:G:13:LEU:HD21	7:G:33:MET:HE1	1.85	0.59
1:A:770:VAL:HG11	1:A:795:ILE:HD11	1.83	0.59
1:A:1269:LYS:HE2	1:A:1517:VAL:HG21	1.85	0.59
2:B:1049:LYS:HG3	2:B:1050:ARG:HG3	1.83	0.59
5:E:22:VAL:HG11	5:E:29:VAL:HG23	1.84	0.59
1:A:404:LEU:HD21	1:A:429:LEU:HG	1.84	0.58
2:B:61:ILE:O	2:B:69:LEU:HB2	2.02	0.58
5:E:107:ALA:HB2	5:E:132:GLU:HG3	1.85	0.58
1:A:597:VAL:HG23	1:A:623:ILE:HD11	1.83	0.58
1:A:612:HIS:CD2	1:A:614:PRO:HD2	2.38	0.58
5:E:71:THR:HG23	5:E:99:HIS:HD2	1.68	0.58
1:A:1309:TYR:O	1:A:1313:TYR:HB2	2.02	0.58
2:B:59:ASP:OD2	2:B:73:ASN:ND2	2.31	0.58
2:B:991:ASN:OD1	2:B:992:TYR:N	2.36	0.58
11:K:37:PHE:CE2	11:K:91:LEU:HD22	2.38	0.58
6:F:91:ILE:HA	6:F:95:ALA:HB3	1.85	0.58
13:U:28:DG:N2	14:T:13:DT:H3	2.01	0.58
1:A:704:THR:HG22	1:A:705:ARG:H	1.67	0.58
1:A:1171:ASN:HB3	1:A:1174:LYS:HB2	1.86	0.58
2:B:152:GLU:N	2:B:152:GLU:OE1	2.36	0.58
2:B:1089:CYS:HB3	2:B:1092:CYS:SG	2.44	0.58
4:D:26:LEU:HD11	4:D:50:LEU:HD22	1.86	0.58
5:E:155:GLU:HA	5:E:158:GLU:CD	2.29	0.58
1:A:372:PHE:CE1	2:B:1157:TYR:HA	2.39	0.58
5:E:152:SER:N	5:E:155:GLU:OE1	2.27	0.58
8:H:7:LEU:HB2	8:H:59:ILE:HG12	1.84	0.58
11:K:25:LEU:HB2	11:K:36:THR:OG1	2.04	0.58
1:A:1066:ASP:C	1:A:1068:LEU:N	2.61	0.58
3:C:255:GLN:HB2	3:C:265:LEU:HD21	1.85	0.58
2:B:1081:SER:OG	2:B:1082:ASP:OD1	2.21	0.57
4:D:14:SER:HA	7:G:9:GLN:HG3	1.86	0.57
2:B:730:GLN:NE2	3:C:102:VAL:HG11	2.19	0.57
2:B:997:PRO:HG2	3:C:285:VAL:HB	1.87	0.57
1:A:463:GLY:O	1:A:467:ILE:HG23	2.03	0.57
2:B:83:GLN:HE22	2:B:134:MET:HE2	1.68	0.57
8:H:31:SER:OG	8:H:32:GLY:N	2.33	0.57
1:A:541:ALA:HA	1:A:595:ARG:HA	1.85	0.57
3:C:86:PHE:HB2	3:C:108:GLY:HA2	1.86	0.57
1:A:960:LEU:HD21	1:A:999:PHE:CE1	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:GLY:O	2:B:208:TYR:N	2.37	0.57
1:A:13:SER:OG	2:B:1172:GLU:OE2	2.22	0.57
1:A:1277:ARG:HB3	1:A:1302:ASP:HB3	1.85	0.57
3:C:231:THR:HG21	10:J:42:ARG:HH22	1.70	0.57
7:G:103:LEU:HD21	7:G:150:LEU:HB3	1.87	0.57
1:A:1270:LEU:HD21	1:A:1518:ILE:HB	1.86	0.57
1:A:11:ILE:O	1:A:1668:ARG:NH1	2.38	0.57
2:B:683:SER:OG	2:B:684:ILE:N	2.34	0.57
3:C:99:GLN:NE2	3:C:99:GLN:H	2.03	0.57
5:E:165:LEU:HD13	5:E:170:LEU:HG	1.86	0.57
10:J:7:CYS:HB3	10:J:14:ILE:HD13	1.87	0.57
1:A:100:ARG:NH2	1:A:238:PHE:O	2.22	0.57
2:B:123:TRP:CZ2	2:B:422:LEU:HD22	2.39	0.57
3:C:223:HIS:CD2	3:C:225:LYS:HG2	2.39	0.57
3:C:285:VAL:HG21	3:C:303:ARG:HH21	1.70	0.57
7:G:115:ARG:HA	7:G:118:ILE:HD12	1.86	0.57
2:B:261:GLU:OE2	2:B:300:GLN:NE2	2.37	0.56
1:A:474:LEU:HD23	1:A:478:HIS:HB2	1.86	0.56
1:A:1016:ARG:NE	2:B:496:LEU:HD23	2.20	0.56
4:D:17:LEU:HD22	7:G:79:LEU:HD22	1.86	0.56
5:E:146:PRO:HB3	5:E:194:VAL:O	2.04	0.56
1:A:26:LYS:O	2:B:1116:ARG:NH2	2.37	0.56
1:A:519:VAL:HG21	1:A:569:LEU:HD21	1.87	0.56
1:A:784:VAL:HA	1:A:794:GLY:HA3	1.87	0.56
2:B:155:SER:OG	2:B:158:GLU:OE2	2.18	0.56
2:B:1033:THR:HG23	2:B:1034:THR:H	1.70	0.56
5:E:156:LYS:NZ	5:E:188:GLY:O	2.30	0.56
7:G:93:ILE:HG22	7:G:103:LEU:HG	1.87	0.56
1:A:481:GLY:HA3	2:B:1057:GLY:HA3	1.87	0.56
1:A:1066:ASP:OD1	1:A:1067:SER:N	2.39	0.56
2:B:869:ASP:OD1	2:B:891:ARG:NE	2.34	0.56
12:L:31:ASN:ND2	12:L:41:CYS:HA	2.21	0.56
1:A:853:GLN:HA	1:A:856:ASN:HD21	1.70	0.56
1:A:1046:GLN:HG3	6:F:129:PRO:HB3	1.87	0.56
2:B:230:HIS:CD2	2:B:240:ARG:HB2	2.40	0.56
2:B:813:ALA:HB2	2:B:848:TYR:CG	2.40	0.56
1:A:543:HIS:HB2	1:A:553:SER:HA	1.87	0.56
1:A:1678:ASP:HB2	6:F:127:TYR:HE2	1.71	0.56
4:D:24:LYS:O	4:D:28:ARG:HG2	2.05	0.56
1:A:925:ILE:HG22	1:A:958:CYS:SG	2.45	0.56
1:A:998:ARG:NE	1:A:1001:THR:OG1	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1131:SER:HB2	6:F:72:THR:HB	1.88	0.56
6:F:89:LEU:O	6:F:92:SER:OG	2.20	0.56
8:H:19:GLN:OE1	8:H:19:GLN:N	2.39	0.56
1:A:1655:ASP:OD1	1:A:1655:ASP:N	2.38	0.56
5:E:23:HIS:HA	5:E:25:ARG:N	2.14	0.56
1:A:1086:TYR:HD1	1:A:1178:LEU:HD22	1.71	0.55
1:A:114:VAL:O	1:A:182:ARG:NH1	2.39	0.55
1:A:1045:VAL:HG23	1:A:1190:PRO:HA	1.88	0.55
2:B:518:LEU:H	2:B:518:LEU:HD23	1.70	0.55
3:C:195:ASN:ND2	10:J:16:ASP:OD2	2.39	0.55
1:A:612:HIS:HA	1:A:1200:GLN:HG2	1.89	0.55
1:A:1039:HIS:HB3	1:A:1611:TYR:HE2	1.71	0.55
1:A:1476:ASN:O	1:A:1478:LYS:NZ	2.38	0.55
2:B:780:GLU:HB2	3:C:223:HIS:CE1	2.41	0.55
2:B:129:PRO:C	2:B:130:ARG:HD3	2.31	0.55
2:B:1168:LYS:HZ1	2:B:1170:MET:HE2	1.72	0.55
3:C:231:THR:HG21	10:J:42:ARG:HH12	1.72	0.55
5:E:142:HIS:CD2	5:E:144:LEU:H	2.23	0.55
1:A:598:ARG:N	1:A:601:ASP:OD2	2.24	0.55
1:A:877:VAL:HG21	1:A:891:ASN:HB3	1.88	0.55
1:A:1156:LEU:HA	1:A:1170:LEU:HD13	1.89	0.55
2:B:266:GLU:HG2	2:B:552:VAL:HG21	1.88	0.55
2:B:739:PRO:O	2:B:742:HIS:N	2.31	0.55
12:L:45:GLY:O	12:L:47:ARG:NH1	2.40	0.55
1:A:705:ARG:NH1	11:K:60:VAL:O	2.37	0.55
2:B:1082:ASP:OD1	2:B:1082:ASP:N	2.39	0.55
7:G:94:ASN:OD1	7:G:95:LEU:N	2.39	0.55
2:B:105:GLU:CD	12:L:47:ARG:HH21	2.15	0.55
7:G:89:LEU:HD23	7:G:105:ILE:HD13	1.88	0.55
2:B:1022:ARG:HA	2:B:1024:MET:HE1	1.89	0.55
1:A:346:LEU:HB3	1:A:347:TYR:CD1	2.42	0.55
1:A:1137:VAL:HG12	1:A:1183:TYR:CD2	2.42	0.55
1:A:1510:GLU:HG2	9:I:53:PHE:CE1	2.41	0.55
1:A:1526:ARG:HB3	1:A:1545:GLU:HB2	1.89	0.55
1:A:1602:PRO:O	1:A:1606:SER:OG	2.20	0.55
12:L:30:ARG:HH21	12:L:52:MET:HE1	1.72	0.55
2:B:505:CYS:SG	2:B:683:SER:N	2.80	0.54
7:G:124:PHE:HB2	7:G:136:TRP:CZ3	2.42	0.54
1:A:83:PRO:C	1:A:85:PRO:HD3	2.33	0.54
1:A:532:ILE:HD12	1:A:563:THR:HG22	1.89	0.54
1:A:1168:SER:O	1:A:1169:LEU:HD23	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:843:PRO:HA	2:B:859:THR:HA	1.89	0.54
3:C:157:GLU:O	3:C:157:GLU:HG2	2.07	0.54
1:A:372:PHE:HD1	2:B:1157:TYR:HD1	1.55	0.54
1:A:1057:SER:HB3	1:A:1614:PHE:HZ	1.73	0.54
1:A:1559:ILE:HG12	1:A:1561:MET:H	1.71	0.54
8:H:60:THR:OG1	8:H:61:SER:N	2.40	0.54
10:J:3:ILE:HD12	10:J:3:ILE:H	1.72	0.54
1:A:748:SER:OG	1:A:790:GLU:HA	2.07	0.54
1:A:1052:ARG:NH1	1:A:1056:GLY:O	2.40	0.54
11:K:52:TYR:OH	11:K:56:LYS:NZ	2.32	0.54
1:A:437:LEU:HA	1:A:440:ASP:OD1	2.07	0.54
1:A:717:LYS:NZ	11:K:68:PRO:HA	2.23	0.54
1:A:868:PHE:HB3	1:A:913:MET:HE1	1.88	0.54
1:A:1055:ASP:OD1	1:A:1056:GLY:N	2.41	0.54
1:A:1279:VAL:HG11	1:A:1509:VAL:HG11	1.90	0.54
2:B:8:ARG:HD2	2:B:748:ASP:HB3	1.89	0.54
1:A:1063:TYR:CE1	1:A:1194:VAL:HG11	2.43	0.54
1:A:568:GLN:O	1:A:591:LYS:NZ	2.40	0.54
1:A:1277:ARG:HG2	1:A:1278:GLN:H	1.72	0.54
1:A:1575:ILE:C	5:E:178:PRO:HG2	2.33	0.54
2:B:421:TYR:O	2:B:425:VAL:HG23	2.07	0.54
2:B:703:GLN:HE22	2:B:1019:GLN:NE2	2.05	0.54
2:B:1092:CYS:CB	2:B:1118:CYS:SG	2.72	0.54
5:E:82:VAL:HG13	5:E:86:GLU:HB3	1.90	0.54
1:A:1041:GLU:HG3	1:A:1659:ASN:HB3	1.89	0.54
1:A:1270:LEU:HD22	1:A:1519:HIS:CE1	2.43	0.54
2:B:137:VAL:HG12	2:B:433:ILE:HG12	1.89	0.54
2:B:279:THR:OG1	9:I:46:THR:HG23	2.08	0.54
1:A:79:HIS:CD2	1:A:364:ASN:HD21	2.26	0.54
1:A:1108:SER:HB2	1:A:1180:GLN:HE22	1.72	0.54
8:H:43:ASN:OD1	8:H:46:ILE:N	2.26	0.54
1:A:1615:GLU:OE2	5:E:172:ARG:NH1	2.40	0.53
8:H:25:SER:OG	8:H:44:SER:OG	2.07	0.53
1:A:132:ASN:CG	5:E:187:ARG:HB2	2.34	0.53
2:B:142:ILE:HD13	2:B:148:ARG:HB3	1.90	0.53
1:A:1281:VAL:HG23	1:A:1299:ILE:HG13	1.89	0.53
7:G:93:ILE:HG12	7:G:148:LYS:HA	1.90	0.53
1:A:405:SER:O	1:A:409:THR:HG23	2.08	0.53
1:A:1657:LEU:HG	1:A:1663:ARG:HE	1.74	0.53
2:B:195:ALA:HB1	2:B:359:LEU:HD22	1.89	0.53
2:B:253:MET:HE1	2:B:267:ILE:HG13	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ILE:HD12	1:A:605:LEU:HD11	1.90	0.53
1:A:610:THR:HG23	1:A:615:SER:CB	2.38	0.53
1:A:799:SER:HA	1:A:804:SER:HB3	1.91	0.53
1:A:1237:THR:HG22	1:A:1239:SER:HB2	1.91	0.53
1:A:1297:TYR:CD2	1:A:1494:LEU:HB2	2.44	0.53
2:B:271:ILE:O	2:B:354:ARG:HD3	2.09	0.53
3:C:320:PRO:HA	3:C:323:LEU:HD23	1.91	0.53
8:H:63:LEU:HD22	8:H:120:TYR:HB3	1.90	0.53
1:A:1139:GLU:OE2	5:E:202:ARG:NH1	2.42	0.53
1:A:31:GLN:HG2	1:A:33:VAL:HG13	1.90	0.53
1:A:762:LEU:HD22	1:A:786:PHE:CE2	2.44	0.53
2:B:190:ARG:HD2	2:B:630:ASN:HD22	1.72	0.53
1:A:1066:ASP:O	1:A:1068:LEU:N	2.33	0.53
1:A:1297:TYR:HE2	1:A:1494:LEU:HD12	1.74	0.53
2:B:443:THR:HG22	14:T:24:DC:H4'	1.91	0.53
5:E:132:GLU:O	5:E:133:SER:OG	2.20	0.53
8:H:6:LEU:HB2	8:H:59:ILE:HG13	1.89	0.53
1:A:443:SER:HB2	1:A:450:ASN:HD22	1.73	0.53
2:B:544:LEU:HD23	2:B:579:VAL:HG22	1.91	0.53
2:B:710:THR:HG21	2:B:752:ASN:HB3	1.90	0.53
1:A:84:ILE:HD12	1:A:84:ILE:H	1.74	0.53
1:A:1100:SER:OG	1:A:1101:ALA:N	2.42	0.53
2:B:733:GLN:HE21	2:B:755:ASN:H	1.56	0.53
5:E:173:ILE:HB	5:E:209:CYS:SG	2.49	0.53
1:A:1634:ALA:O	1:A:1637:SER:N	2.41	0.52
5:E:173:ILE:HG12	5:E:207:ARG:HD3	1.91	0.52
13:U:26:DA:H1'	13:U:27:DA:H5'	1.91	0.52
8:H:30:VAL:HA	8:H:36:MET:O	2.10	0.52
8:H:19:GLN:HG2	8:H:19:GLN:O	2.08	0.52
1:A:33:VAL:HA	1:A:395:LEU:HD11	1.90	0.52
2:B:367:ASP:O	2:B:369:PRO:HD3	2.09	0.52
3:C:81:ILE:HG22	3:C:330:VAL:HG21	1.90	0.52
1:A:210:GLU:O	1:A:214:VAL:HG13	2.10	0.52
1:A:1041:GLU:HG2	1:A:1042:GLY:H	1.73	0.52
2:B:145:ARG:HH21	2:B:159:LEU:HD11	1.73	0.52
1:A:1:MET:HB2	2:B:1079:ASN:CG	2.35	0.52
1:A:762:LEU:HD23	1:A:763:ASN:N	2.25	0.52
1:A:977:LYS:HE3	1:A:982:PHE:O	2.10	0.52
1:A:1635:LYS:HB3	1:A:1644:PHE:CD2	2.43	0.52
2:B:1047:GLY:N	2:B:1052:GLY:HA3	2.24	0.52
5:E:105:ILE:HD12	5:E:132:GLU:HB3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:185:LEU:HD13	5:E:209:CYS:SG	2.49	0.52
7:G:93:ILE:HD11	7:G:145:GLU:HA	1.91	0.52
1:A:733:ALA:N	1:A:745:GLN:HE22	2.08	0.52
1:A:1041:GLU:HG2	1:A:1042:GLY:N	2.24	0.52
1:A:1478:LYS:NZ	1:A:1495:VAL:H	2.08	0.52
2:B:22:PHE:CD2	2:B:746:GLY:HA3	2.45	0.52
3:C:171:SER:HB3	3:C:198:ILE:HB	1.91	0.52
5:E:129:THR:HG21	5:E:181:ARG:HB2	1.91	0.52
6:F:135:ASP:OD1	6:F:135:ASP:N	2.33	0.52
1:A:722:GLY:O	1:A:723:MET:HG2	2.10	0.52
1:A:744:LYS:NZ	1:A:794:GLY:H	2.08	0.52
2:B:1149:ILE:HD11	2:B:1151:LEU:HD22	1.92	0.52
7:G:15:LEU:HD13	7:G:32:HIS:CE1	2.44	0.52
1:A:2:ASN:HD21	1:A:545:GLN:HE22	1.55	0.52
1:A:219:TYR:HA	1:A:222:ILE:HG12	1.92	0.52
1:A:662:GLU:OE2	2:B:1072:LEU:HB2	2.10	0.52
1:A:1015:GLY:HA3	2:B:698:PRO:HD3	1.91	0.52
1:A:1095:VAL:HA	1:A:1098:VAL:HG12	1.91	0.52
2:B:6:LEU:HD11	10:J:25:LEU:C	2.35	0.52
2:B:36:PHE:O	2:B:39:LEU:HB2	2.09	0.52
2:B:970:ILE:HB	2:B:971:TYR:CD2	2.45	0.52
2:B:1102:ILE:HD13	2:B:1135:GLY:HA2	1.92	0.52
3:C:101:GLU:OE1	3:C:101:GLU:N	2.37	0.52
6:F:95:ALA:HB1	6:F:96:PRO:HD2	1.92	0.52
1:A:498:ILE:HG13	1:A:499:GLU:N	2.25	0.51
2:B:999:TYR:HA	2:B:1006:GLU:HA	1.92	0.51
3:C:76:ILE:HG12	3:C:80:GLU:CD	2.36	0.51
3:C:122:PHE:HE2	3:C:125:PRO:HD3	1.75	0.51
11:K:54:ILE:HD13	11:K:79:ILE:HD11	1.92	0.51
1:A:688:ASP:HA	2:B:937:HIS:CE1	2.45	0.51
1:A:1142:GLN:HA	1:A:1145:VAL:HG12	1.91	0.51
7:G:19:PRO:HD3	7:G:69:PHE:HB3	1.92	0.51
8:H:88:ASP:HB3	8:H:90:LYS:HB2	1.91	0.51
1:A:121:CYS:HB3	1:A:186:VAL:HG21	1.92	0.51
1:A:1009:TYR:O	1:A:1013:MET:HG3	2.11	0.51
1:A:1521:ILE:HD13	1:A:1551:ALA:HB1	1.92	0.51
2:B:8:ARG:NH2	10:J:53:VAL:HA	2.26	0.51
6:F:109:GLN:HA	6:F:112:MET:HE3	1.91	0.51
10:J:53:VAL:HG12	10:J:55:LEU:HB2	1.92	0.51
1:A:102:THR:HG22	1:A:335:LEU:HD22	1.93	0.51
1:A:768:ALA:HB1	1:A:797:ASP:OD1	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:844:ARG:HD2	2:B:995:ASN:OD1	2.11	0.51
2:B:590:TYR:HE1	2:B:603:ALA:HA	1.74	0.51
2:B:736:VAL:HG23	2:B:755:ASN:ND2	2.25	0.51
4:D:48:SER:O	4:D:52:ARG:HG3	2.11	0.51
1:A:646:GLY:N	2:B:911:ILE:HD11	2.25	0.51
2:B:610:GLU:OE2	2:B:633:ARG:NE	2.44	0.51
3:C:115:ASP:HB2	3:C:118:MET:HE2	1.92	0.51
8:H:91:VAL:HG23	8:H:111:LEU:HD23	1.92	0.51
1:A:1:MET:HE3	2:B:1079:ASN:OD1	2.11	0.51
1:A:810:HIS:ND1	1:A:1075:HIS:HE1	2.08	0.51
2:B:1030:GLN:OE1	2:B:1048:ARG:HB2	2.10	0.51
2:B:1040:LEU:HD23	2:B:1157:TYR:CZ	2.46	0.51
3:C:206:GLY:HA3	10:J:65:LEU:HD13	1.92	0.51
3:C:314:SER:OG	3:C:315:THR:N	2.44	0.51
14:T:9:DG:H2'	14:T:10:DT:H71	1.92	0.51
1:A:1645:LEU:HD21	2:B:1167:ILE:HD11	1.93	0.51
2:B:217:CYS:SG	2:B:337:VAL:HG22	2.51	0.51
2:B:537:ILE:HD11	2:B:605:VAL:HG22	1.92	0.51
3:C:169:VAL:HG21	3:C:209:ILE:HD12	1.92	0.51
1:A:1308:GLU:HA	1:A:1311:ASP:HB2	1.92	0.51
2:B:872:ARG:HE	12:L:50:TYR:HE1	1.59	0.51
1:A:705:ARG:O	1:A:709:GLN:HG2	2.11	0.51
2:B:117:LEU:HD22	2:B:140:ILE:HG21	1.93	0.51
8:H:60:THR:HG21	8:H:63:LEU:HD13	1.92	0.51
1:A:23:ASP:N	1:A:23:ASP:OD1	2.37	0.50
1:A:204:THR:HG22	1:A:205:THR:H	1.76	0.50
1:A:508:VAL:HG23	1:A:509:PHE:CD2	2.46	0.50
1:A:531:VAL:HG21	1:A:544:ILE:HD11	1.93	0.50
1:A:1038:LYS:HZ1	1:A:1629:ASN:HB2	1.77	0.50
1:A:555:MET:HB2	1:A:556:PRO:HD3	1.94	0.50
1:A:1210:THR:HG22	1:A:1228:ILE:HG12	1.92	0.50
2:B:610:GLU:OE1	2:B:633:ARG:NH2	2.45	0.50
2:B:858:GLU:OE2	2:B:859:THR:N	2.45	0.50
2:B:922:PRO:HB2	2:B:998:MET:HE2	1.93	0.50
4:D:28:ARG:NH1	4:D:31:GLN:OE1	2.44	0.50
1:A:68:LEU:HD13	1:A:72:TYR:HB2	1.94	0.50
1:A:796:LEU:HD22	1:A:800:SER:OG	2.10	0.50
1:A:1189:ASP:OD2	6:F:77:LYS:N	2.43	0.50
2:B:884:GLN:O	2:B:885:GLN:HG3	2.12	0.50
2:B:1042:ARG:NH2	2:B:1084:ALA:HB2	2.26	0.50
3:C:29:TYR:OH	11:K:58:PRO:O	2.20	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:85:LYS:NZ	5:E:88:ARG:HH21	2.09	0.50
1:A:471:LYS:HE3	14:T:14:DT:H3'	1.93	0.50
1:A:504:GLY:N	1:A:631:ARG:O	2.33	0.50
1:A:1189:ASP:OD1	6:F:76:THR:HB	2.12	0.50
1:A:1231:LEU:HA	1:A:1234:ILE:HG22	1.93	0.50
2:B:114:LYS:HB2	2:B:139:MET:HB3	1.93	0.50
5:E:148:HIS:CE1	5:E:179:VAL:HG11	2.47	0.50
1:A:386:ILE:HG13	1:A:387:GLN:N	2.26	0.50
1:A:1001:THR:HG21	2:B:973:GLU:HG3	1.93	0.50
1:A:1269:LYS:HD3	1:A:1525:THR:HB	1.94	0.50
2:B:703:GLN:HE22	2:B:1019:GLN:HE22	1.58	0.50
2:B:843:PRO:HB3	2:B:857:ILE:HD11	1.94	0.50
5:E:48:MET:SD	5:E:48:MET:N	2.84	0.50
6:F:128:LEU:HG	6:F:129:PRO:HD2	1.94	0.50
7:G:25:PRO:O	7:G:29:ILE:HG13	2.11	0.50
9:I:10:CYS:HB2	9:I:17:LEU:HD21	1.93	0.50
1:A:664:GLN:O	1:A:668:ASN:HB3	2.12	0.50
1:A:699:LYS:NZ	8:H:21:TYR:OH	2.44	0.50
1:A:1011:HIS:HE2	2:B:696:GLN:HA	1.76	0.50
1:A:1267:VAL:HG13	1:A:1527:CYS:SG	2.52	0.50
2:B:561:VAL:HG23	2:B:625:LEU:HD23	1.93	0.50
3:C:157:GLU:OE1	3:C:157:GLU:N	2.45	0.50
1:A:1086:TYR:CD1	1:A:1178:LEU:HD22	2.47	0.50
1:A:1147:GLU:O	1:A:1151:LYS:CB	2.59	0.50
1:A:1517:VAL:HG21	1:A:1520:GLU:HB2	1.94	0.50
3:C:65:ILE:HG23	3:C:69:ILE:HB	1.94	0.50
3:C:122:PHE:HA	3:C:137:ASP:OD1	2.11	0.50
10:J:10:CYS:SG	10:J:42:ARG:NH1	2.85	0.50
1:A:3:ILE:O	7:G:67:SER:OG	2.30	0.50
1:A:507:PRO:HG2	1:A:626:GLY:H	1.77	0.50
1:A:1270:LEU:HD21	1:A:1518:ILE:HD12	1.94	0.50
1:A:92:PHE:CZ	1:A:244:ALA:HA	2.47	0.50
2:B:116:ARG:NH1	2:B:136:GLU:OE2	2.45	0.50
2:B:593:LYS:O	2:B:598:THR:OG1	2.30	0.50
1:A:77:PHE:CD1	1:A:368:PRO:HA	2.47	0.49
1:A:174:ASP:O	1:A:177:THR:OG1	2.27	0.49
1:A:743:GLY:O	1:A:746:ILE:N	2.44	0.49
2:B:754:THR:OG1	2:B:755:ASN:N	2.45	0.49
2:B:812:PHE:CG	2:B:817:THR:HG21	2.47	0.49
3:C:155:THR:OG1	3:C:156:ASP:N	2.45	0.49
3:C:284:THR:C	3:C:286:SER:H	2.19	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1039:HIS:HB3	1:A:1611:TYR:CE2	2.47	0.49
1:A:1317:GLN:HA	1:A:1320:ILE:HD12	1.94	0.49
2:B:286:GLU:HG2	9:I:7:LEU:HD21	1.93	0.49
2:B:805:PRO:O	2:B:807:VAL:HG23	2.12	0.49
5:E:142:HIS:CG	5:E:143:GLU:N	2.80	0.49
8:H:71:ALA:HA	8:H:124:ARG:HD3	1.93	0.49
11:K:81:THR:OG1	11:K:82:ALA:N	2.45	0.49
14:T:20:DT:H2'	14:T:21:DG:C8	2.46	0.49
1:A:118:LEU:O	1:A:122:ARG:HG3	2.12	0.49
1:A:1680:PHE:CE1	6:F:125:ARG:HD2	2.48	0.49
1:A:378:MET:HB3	1:A:381:GLU:OE1	2.12	0.49
2:B:473:LEU:HD13	2:B:684:ILE:HG21	1.94	0.49
3:C:126:LEU:HD12	3:C:127:PRO:O	2.12	0.49
1:A:708:TYR:CE1	1:A:746:ILE:HG12	2.47	0.49
1:A:1045:VAL:HG23	1:A:1191:GLY:H	1.77	0.49
1:A:1559:ILE:HG23	1:A:1562:ASN:H	1.77	0.49
3:C:234:TYR:HB3	3:C:310:PHE:CE1	2.47	0.49
1:A:1238:ALA:HB3	1:A:1620:ALA:HB2	1.93	0.49
1:A:1575:ILE:HA	5:E:178:PRO:HG2	1.93	0.49
2:B:420:LYS:HA	2:B:423:THR:HG22	1.95	0.49
1:A:465:LYS:HG3	1:A:1642:CYS:SG	2.52	0.49
1:A:776:SER:HB2	1:A:779:SER:HB2	1.93	0.49
1:A:853:GLN:HA	1:A:856:ASN:ND2	2.27	0.49
1:A:975:SER:HB2	2:B:656:TYR:CE2	2.46	0.49
2:B:1067:HIS:HB3	2:B:1069:THR:HG23	1.95	0.49
2:B:1078:MET:HE2	2:B:1083:TYR:CE2	2.47	0.49
1:A:336:PHE:HZ	1:A:360:PHE:HE2	1.59	0.49
1:A:538:TRP:NE1	1:A:623:ILE:HD13	2.28	0.49
1:A:595:ARG:NH2	1:A:598:ARG:HG2	2.27	0.49
2:B:190:ARG:HG3	2:B:376:GLU:OE1	2.13	0.49
2:B:908:GLN:HG2	2:B:934:ILE:HD11	1.94	0.49
3:C:91:ILE:O	3:C:91:ILE:HG13	2.11	0.49
8:H:38:LEU:HD12	8:H:104:ILE:HD13	1.95	0.49
1:A:622:ARG:NH2	11:K:72:GLU:OE2	2.46	0.49
1:A:968:ARG:HG3	1:A:969:ARG:H	1.78	0.49
2:B:468:ASN:HD21	2:B:752:ASN:ND2	2.10	0.49
2:B:955:LYS:NZ	2:B:994:GLY:O	2.44	0.49
1:A:1309:TYR:CE2	1:A:1320:ILE:HD11	2.48	0.49
2:B:232:LEU:HD11	2:B:236:VAL:HB	1.95	0.49
2:B:1024:MET:HG2	2:B:1025:VAL:H	1.78	0.49
5:E:27:TYR:HA	5:E:64:SER:H	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLN:HB2	1:A:79:HIS:CE1	2.47	0.48
1:A:234:PHE:O	1:A:251:LEU:HD21	2.13	0.48
2:B:239:PHE:HB3	2:B:250:ILE:HG13	1.95	0.48
2:B:640:HIS:CE1	2:B:642:SER:HB2	2.48	0.48
2:B:687:ASN:ND2	2:B:741:LEU:HD12	2.21	0.48
2:B:795:ASP:OD1	2:B:795:ASP:N	2.45	0.48
2:B:833:PHE:HE2	12:L:56:ARG:HD3	1.77	0.48
3:C:236:LEU:HD21	3:C:308:TYR:CZ	2.48	0.48
1:A:1063:TYR:HE1	1:A:1194:VAL:HG21	1.77	0.48
3:C:84:LEU:HD12	3:C:114:ALA:HB3	1.94	0.48
1:A:721:THR:HB	1:A:823:ARG:HH12	1.78	0.48
1:A:855:ASP:OD1	1:A:856:ASN:N	2.46	0.48
2:B:967:THR:HB	2:B:970:ILE:HD11	1.95	0.48
7:G:59:LYS:HD3	7:G:73:TRP:CD1	2.49	0.48
10:J:19:ASP:OD1	10:J:19:ASP:N	2.43	0.48
1:A:1320:ILE:O	1:A:1324:PHE:CB	2.58	0.48
1:A:1582:ARG:HE	1:A:1610:ASP:CG	2.21	0.48
2:B:108:GLU:HA	2:B:722:THR:HG21	1.94	0.48
5:E:45:HIS:ND1	5:E:56:THR:HG23	2.29	0.48
8:H:16:VAL:HG22	8:H:27:ILE:HG22	1.95	0.48
11:K:44:HIS:ND1	11:K:65:TYR:OH	2.33	0.48
1:A:885:ILE:HD12	1:A:885:ILE:H	1.78	0.48
1:A:1147:GLU:O	1:A:1151:LYS:HB2	2.14	0.48
3:C:150:ASN:HB3	3:C:163:LEU:O	2.14	0.48
15:R:14:A:H2'	15:R:15:C:C6	2.49	0.48
1:A:652:HIS:HB3	2:B:1076:ARG:NH2	2.27	0.48
1:A:1179:MET:HE2	1:A:1179:MET:HA	1.95	0.48
2:B:640:HIS:HE1	2:B:642:SER:HB2	1.77	0.48
5:E:158:GLU:O	5:E:162:ARG:HG2	2.14	0.48
11:K:53:VAL:HG21	11:K:98:LEU:HD13	1.96	0.48
1:A:627:GLU:HG3	1:A:631:ARG:NE	2.28	0.48
7:G:17:ILE:O	7:G:69:PHE:HB2	2.14	0.48
8:H:83:VAL:HG22	8:H:93:VAL:HG22	1.95	0.48
1:A:720:GLU:OE1	11:K:68:PRO:HG3	2.14	0.48
1:A:906:ASP:OD1	1:A:907:ALA:N	2.46	0.48
1:A:1123:PRO:HG3	5:E:202:ARG:NH1	2.28	0.48
2:B:274:LYS:HG3	2:B:275:ASP:HB3	1.96	0.48
6:F:89:LEU:HG	7:G:68:PRO:HB3	1.95	0.48
7:G:15:LEU:HD22	7:G:32:HIS:CE1	2.48	0.48
8:H:88:ASP:OD1	8:H:89:GLU:N	2.47	0.48
13:U:29:DT:H2'	13:U:30:DA:C8	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:653:GLU:HB3	2:B:657:MET:SD	2.54	0.48
2:B:1131:ILE:HB	2:B:1139:LYS:HD2	1.96	0.48
1:A:604:ILE:O	1:A:605:LEU:HD23	2.14	0.48
1:A:604:ILE:HD13	2:B:1072:LEU:HD21	1.96	0.48
1:A:1016:ARG:HH12	2:B:495:LYS:HG3	1.78	0.48
1:A:1024:VAL:HG21	2:B:494:ARG:HH21	1.79	0.48
3:C:342:LEU:HD13	11:K:91:LEU:HD23	1.95	0.48
8:H:11:PHE:HA	8:H:31:SER:CB	2.44	0.48
11:K:37:PHE:CD2	11:K:91:LEU:HD22	2.49	0.48
1:A:205:THR:HG23	1:A:206:LEU:H	1.79	0.47
1:A:910:LYS:NZ	1:A:964:GLU:OE1	2.41	0.47
2:B:261:GLU:HB3	2:B:300:GLN:HE21	1.79	0.47
2:B:267:ILE:O	2:B:271:ILE:HG13	2.13	0.47
2:B:1134:ASP:N	2:B:1138:LYS:O	2.46	0.47
3:C:84:LEU:HD11	3:C:119:PHE:CE2	2.49	0.47
3:C:179:GLN:H	3:C:182:GLN:NE2	2.11	0.47
1:A:14:VAL:HA	2:B:1171:LEU:HA	1.96	0.47
1:A:786:PHE:HB3	1:A:791:LEU:HA	1.96	0.47
1:A:921:ILE:HG13	1:A:925:ILE:HG21	1.95	0.47
1:A:1025:LYS:HD2	1:A:1025:LYS:C	2.40	0.47
1:A:1235:ILE:HD11	1:A:1608:ILE:HG21	1.94	0.47
2:B:694:PHE:CD2	2:B:949:ILE:HG13	2.49	0.47
2:B:900:ASP:OD1	2:B:1024:MET:HB3	2.14	0.47
3:C:291:ARG:HH21	3:C:292:HIS:CE1	2.32	0.47
8:H:43:ASN:CG	8:H:46:ILE:HG22	2.39	0.47
1:A:952:ASN:OD1	2:B:943:MET:HE2	2.14	0.47
2:B:30:LYS:O	2:B:34:ASP:HB2	2.14	0.47
2:B:313:VAL:HG23	2:B:314:VAL:HG23	1.96	0.47
2:B:375:GLN:NE2	2:B:481:ARG:HE	2.12	0.47
3:C:182:GLN:HA	3:C:185:ARG:HB2	1.97	0.47
4:D:17:LEU:HB2	7:G:8:LYS:HB2	1.95	0.47
8:H:97:PHE:HB2	8:H:100:LEU:HB2	1.96	0.47
13:U:27:DA:H1'	13:U:28:DG:H5'	1.95	0.47
1:A:58:LEU:O	1:A:59:LYS:HB2	2.13	0.47
1:A:427:PHE:O	1:A:431:ILE:HG12	2.15	0.47
1:A:1189:ASP:CG	6:F:76:THR:HB	2.40	0.47
2:B:1081:SER:OG	2:B:1082:ASP:N	2.48	0.47
3:C:140:VAL:HG12	3:C:214:HIS:ND1	2.30	0.47
8:H:42:ILE:HD13	8:H:49:LEU:HD12	1.95	0.47
1:A:79:HIS:HD2	1:A:364:ASN:HD21	1.61	0.47
1:A:1274:GLU:HB3	9:I:56:ALA:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:335:VAL:HG13	2:B:336:LEU:H	1.80	0.47
2:B:379:LEU:HD21	2:B:527:ILE:HG21	1.97	0.47
2:B:542:LEU:HA	2:B:546:VAL:O	2.14	0.47
2:B:629:SER:O	2:B:629:SER:OG	2.29	0.47
2:B:983:GLU:O	2:B:987:LYS:HG2	2.15	0.47
5:E:89:THR:HG23	5:E:90:PHE:CD1	2.49	0.47
9:I:10:CYS:SG	9:I:12:GLU:N	2.87	0.47
14:T:8:DA:H2"	14:T:9:DG:H8	1.80	0.47
1:A:71:ARG:HD2	1:A:72:TYR:CZ	2.50	0.47
1:A:362:LEU:HD12	1:A:362:LEU:O	2.15	0.47
1:A:542:SER:N	1:A:594:TYR:O	2.26	0.47
1:A:692:MET:HE3	1:A:692:MET:HB3	1.72	0.47
1:A:760:PRO:HG2	1:A:1087:LYS:HB3	1.95	0.47
1:A:893:GLU:HA	1:A:985:TYR:HE1	1.79	0.47
1:A:1038:LYS:HG2	1:A:1626:ILE:HG12	1.96	0.47
1:A:1053:ASP:OD1	1:A:1054:SER:N	2.48	0.47
1:A:1069:ASP:N	1:A:1188:VAL:HG22	2.30	0.47
2:B:58:PHE:HB3	2:B:74:LYS:HA	1.96	0.47
2:B:123:TRP:HE3	2:B:131:GLN:O	1.98	0.47
2:B:251:PRO:HG2	2:B:254:MET:HB2	1.97	0.47
2:B:549:PRO:HD3	2:B:570:TRP:CD1	2.50	0.47
2:B:643:THR:HG22	2:B:644:GLY:N	2.30	0.47
2:B:925:GLU:OE1	2:B:997:PRO:HB2	2.15	0.47
3:C:204:ARG:HG3	10:J:60:LEU:HB3	1.96	0.47
5:E:128:GLU:OE1	5:E:184:GLY:HA2	2.15	0.47
7:G:36:MET:HB2	7:G:36:MET:HE3	1.68	0.47
9:I:23:GLN:HG3	9:I:24:TRP:H	1.80	0.47
13:U:32:DT:H3	14:T:8:DA:H61	1.62	0.47
1:A:252:SER:OG	1:A:255:ASN:OD1	2.32	0.47
1:A:489:ARG:NH2	1:A:648:GLU:OE2	2.48	0.47
1:A:698:CYS:O	1:A:701:THR:HG22	2.14	0.47
1:A:1588:GLU:O	1:A:1592:VAL:HG23	2.15	0.47
5:E:138:ASN:HD22	5:E:141:HIS:CE1	2.32	0.47
1:A:1051:VAL:HG12	1:A:1060:GLN:O	2.15	0.47
1:A:1263:PHE:O	1:A:1267:VAL:HG12	2.15	0.47
2:B:56:CYS:SG	2:B:57:ALA:N	2.88	0.47
7:G:14:TYR:CZ	7:G:71:PHE:HB3	2.50	0.47
1:A:113:LYS:O	1:A:116:VAL:HG12	2.14	0.47
1:A:1064:GLY:C	1:A:1066:ASP:H	2.23	0.47
1:A:1337:LYS:O	1:A:1337:LYS:HD3	2.15	0.47
1:A:1643:HIS:O	1:A:1646:THR:HG22	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:479:VAL:O	2:B:518:LEU:HB2	2.15	0.47
2:B:767:ASP:N	2:B:767:ASP:OD1	2.48	0.47
3:C:94:ASN:H	12:L:53:ARG:HH11	1.62	0.47
4:D:32:THR:HG22	4:D:33:ILE:HG12	1.96	0.47
1:A:543:HIS:CB	1:A:553:SER:HA	2.45	0.46
1:A:744:LYS:HB3	1:A:791:LEU:HB3	1.96	0.46
1:A:847:ASP:OD2	1:A:938:MET:N	2.48	0.46
1:A:1297:TYR:CE2	1:A:1494:LEU:HD12	2.49	0.46
1:A:1634:ALA:O	1:A:1638:PHE:HD1	1.98	0.46
1:A:1643:HIS:O	1:A:1647:GLU:HG2	2.15	0.46
2:B:468:ASN:OD1	2:B:469:PHE:N	2.49	0.46
2:B:1028:LYS:HG3	2:B:1029:PHE:HD2	1.80	0.46
3:C:246:ILE:HG22	3:C:298:LYS:HD3	1.96	0.46
5:E:103:ILE:HA	5:E:128:GLU:O	2.15	0.46
7:G:62:LYS:O	7:G:71:PHE:N	2.44	0.46
1:A:384:GLU:H	1:A:384:GLU:HG2	1.49	0.46
1:A:1068:LEU:HD12	1:A:1186:SER:C	2.40	0.46
2:B:391:LYS:NZ	2:B:436:LYS:HB3	2.30	0.46
2:B:881:SER:OG	2:B:882:GLU:N	2.49	0.46
10:J:51:THR:O	10:J:51:THR:OG1	2.29	0.46
1:A:3:ILE:HD13	6:F:89:LEU:HD11	1.97	0.46
1:A:23:ASP:HA	1:A:26:LYS:HB2	1.97	0.46
1:A:895:VAL:HG12	1:A:902:LEU:CD2	2.46	0.46
1:A:1003:ILE:HD11	1:A:1008:TYR:CD2	2.50	0.46
1:A:1016:ARG:NH1	2:B:496:LEU:H	2.13	0.46
1:A:1025:LYS:HG3	1:A:1210:THR:OG1	2.15	0.46
1:A:1045:VAL:HG12	1:A:1051:VAL:HB	1.96	0.46
1:A:1070:VAL:HA	1:A:1073:GLN:HG2	1.98	0.46
1:A:1113:LYS:HE3	1:A:1121:TYR:CE1	2.50	0.46
1:A:1325:SER:OG	1:A:1326:ASN:N	2.48	0.46
2:B:1088:VAL:HG21	2:B:1171:LEU:HD11	1.97	0.46
3:C:126:LEU:HB2	3:C:127:PRO:HD2	1.97	0.46
5:E:173:ILE:N	5:E:208:ILE:O	2.48	0.46
12:L:51:LYS:HG2	12:L:52:MET:N	2.29	0.46
1:A:243:PHE:HB3	1:A:439:HIS:HE1	1.81	0.46
1:A:465:LYS:HG2	1:A:466:GLN:NE2	2.31	0.46
2:B:532:SER:OG	2:B:533:ASP:N	2.48	0.46
5:E:87:MET:HB3	5:E:118:ILE:HG12	1.98	0.46
1:A:85:PRO:HB3	1:A:362:LEU:O	2.14	0.46
1:A:965:LEU:HD12	1:A:965:LEU:O	2.16	0.46
1:A:977:LYS:HB3	1:A:984:PRO:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:640:HIS:HA	2:B:673:HIS:CD2	2.51	0.46
2:B:735:PRO:HG3	2:B:1017:TYR:CE1	2.50	0.46
2:B:779:HIS:CE1	2:B:915:LYS:HD2	2.50	0.46
3:C:130:GLU:CD	3:C:130:GLU:H	2.23	0.46
3:C:171:SER:N	3:C:198:ILE:O	2.49	0.46
10:J:67:LYS:NZ	12:L:29:ALA:HA	2.30	0.46
1:A:1:MET:HG2	1:A:2:ASN:N	2.31	0.46
1:A:386:ILE:HD13	1:A:462:PRO:HD2	1.98	0.46
1:A:917:THR:O	1:A:921:ILE:HG22	2.15	0.46
2:B:571:CYS:SG	2:B:576:ALA:HB2	2.55	0.46
2:B:921:MET:HE1	2:B:933:ILE:HG13	1.95	0.46
5:E:130:PHE:HA	5:E:181:ARG:HH21	1.80	0.46
1:A:685:LEU:HD22	1:A:689:HIS:ND1	2.31	0.46
1:A:759:ARG:NH2	1:A:1088:SER:O	2.49	0.46
1:A:1641:THR:OG1	1:A:1642:CYS:N	2.49	0.46
2:B:205:GLY:HA3	2:B:208:TYR:CD2	2.51	0.46
2:B:248:TYR:OH	2:B:314:VAL:HG21	2.16	0.46
2:B:1021:LEU:HD23	2:B:1021:LEU:HA	1.76	0.46
2:B:1043:GLN:NE2	2:B:1154:VAL:HG21	2.31	0.46
8:H:80:VAL:HG12	8:H:117:ASP:O	2.16	0.46
14:T:16:DA:H2'	14:T:17:DG:C8	2.51	0.46
1:A:533:ASN:ND2	1:A:539:PRO:HD2	2.30	0.46
1:A:1281:VAL:HG21	1:A:1505:MET:HG2	1.97	0.46
1:A:1659:ASN:OD1	1:A:1659:ASN:N	2.48	0.46
2:B:108:GLU:OE2	12:L:50:TYR:OH	2.28	0.46
2:B:1107:VAL:HG23	2:B:1108:GLY:H	1.81	0.46
5:E:106:TYR:H	5:E:132:GLU:H	1.63	0.46
1:A:77:PHE:CD2	2:B:1096:ILE:HG21	2.50	0.46
1:A:228:CYS:HB3	1:A:231:CYS:H	1.81	0.46
1:A:445:ILE:HG22	1:A:446:ASP:OD2	2.16	0.46
1:A:634:TYR:OH	2:B:766:TYR:O	2.33	0.46
1:A:1659:ASN:OD1	1:A:1662:SER:HB3	2.16	0.46
2:B:208:TYR:CD1	2:B:232:LEU:HB3	2.51	0.46
2:B:241:PHE:CD1	2:B:334:VAL:HG11	2.51	0.46
2:B:610:GLU:O	2:B:610:GLU:HG2	2.15	0.46
5:E:69:LYS:C	5:E:100:LYS:HE3	2.41	0.46
5:E:107:ALA:HA	5:E:108:ASN:HA	1.56	0.46
7:G:124:PHE:HD1	7:G:136:TRP:HE3	1.62	0.46
8:H:9:GLU:HB2	8:H:11:PHE:CE2	2.50	0.46
10:J:56:ILE:HG12	10:J:60:LEU:HG	1.98	0.46
9:I:24:TRP:NE1	9:I:34:TYR:O	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:TYR:HE1	1:A:1194:VAL:HG11	1.80	0.45
2:B:640:HIS:HA	2:B:673:HIS:HD2	1.79	0.45
2:B:1016:VAL:HG12	2:B:1017:TYR:H	1.81	0.45
2:B:1158:LEU:O	2:B:1162:LEU:HB2	2.16	0.45
1:A:89:PRO:HB2	1:A:446:ASP:OD2	2.16	0.45
1:A:925:ILE:O	1:A:929:LEU:HD22	2.15	0.45
1:A:1327:ARG:NH2	1:A:1517:VAL:O	2.39	0.45
1:A:1493:GLU:C	1:A:1494:LEU:HD23	2.41	0.45
2:B:265:LYS:NZ	9:I:14:GLY:HA2	2.28	0.45
2:B:842:ASP:CG	2:B:843:PRO:HD2	2.41	0.45
2:B:898:ILE:HD12	2:B:898:ILE:H	1.81	0.45
2:B:984:GLN:O	2:B:987:LYS:HB2	2.16	0.45
1:A:100:ARG:HA	1:A:100:ARG:HD3	1.81	0.45
1:A:1680:PHE:HD2	7:G:60:SER:O	1.98	0.45
2:B:335:VAL:HG13	2:B:336:LEU:N	2.31	0.45
8:H:7:LEU:O	8:H:58:GLN:HA	2.15	0.45
1:A:687:GLN:HB3	2:B:937:HIS:CG	2.51	0.45
2:B:554:HIS:HE1	2:B:570:TRP:CZ3	2.34	0.45
2:B:932:ILE:HD12	2:B:1018:TYR:HD2	1.81	0.45
2:B:1006:GLU:CD	3:C:303:ARG:HH11	2.25	0.45
8:H:63:LEU:HD12	8:H:63:LEU:HA	1.83	0.45
1:A:3:ILE:HB	1:A:592:LYS:HE3	1.98	0.45
1:A:619:HIS:HE1	1:A:636:ASN:ND2	2.14	0.45
1:A:973:MET:SD	2:B:655:VAL:HG12	2.56	0.45
1:A:1066:ASP:C	1:A:1603:ARG:HE	2.23	0.45
1:A:1302:ASP:OD2	1:A:1303:LEU:N	2.50	0.45
2:B:56:CYS:SG	2:B:74:LYS:HG3	2.56	0.45
2:B:123:TRP:O	2:B:130:ARG:HA	2.16	0.45
2:B:354:ARG:NH1	2:B:358:ALA:HB2	2.31	0.45
2:B:1062:ASP:HA	2:B:1065:ILE:HG12	1.97	0.45
7:G:15:LEU:HD13	7:G:32:HIS:ND1	2.32	0.45
8:H:108:HIS:O	8:H:108:HIS:ND1	2.50	0.45
14:T:12:DC:H1'	14:T:13:DT:C4	2.52	0.45
1:A:102:THR:O	1:A:110:LYS:HE2	2.17	0.45
1:A:902:LEU:HD22	1:A:902:LEU:HA	1.61	0.45
1:A:1069:ASP:O	1:A:1071:THR:N	2.49	0.45
2:B:881:SER:O	12:L:38:VAL:HA	2.16	0.45
2:B:1032:ARG:CZ	2:B:1044:PRO:HB3	2.46	0.45
12:L:20:MET:O	12:L:32:THR:HA	2.16	0.45
1:A:1297:TYR:CB	1:A:1494:LEU:O	2.49	0.45
2:B:1028:LYS:HG3	2:B:1029:PHE:N	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:PHE:C	2:B:1076:ARG:HH22	2.25	0.45
1:A:727:ILE:N	11:K:80:GLN:OE1	2.50	0.45
1:A:1204:GLU:HB3	1:A:1205:PRO:HD3	1.98	0.45
1:A:1255:VAL:HG21	1:A:1557:ASN:HB3	1.99	0.45
2:B:17:LYS:HG2	2:B:157:ALA:HB2	1.98	0.45
2:B:231:TYR:HB2	2:B:356:LEU:HD21	1.99	0.45
1:A:133:GLU:OE1	1:A:133:GLU:N	2.34	0.45
1:A:465:LYS:NZ	1:A:469:GLU:OE1	2.48	0.45
1:A:880:SER:O	1:A:883:SER:OG	2.22	0.45
2:B:699:ARG:HH21	2:B:942:ARG:HG2	1.82	0.45
2:B:825:LYS:HG3	2:B:842:ASP:OD2	2.16	0.45
2:B:1024:MET:C	2:B:1028:LYS:HZ2	2.23	0.45
7:G:135:ARG:HD2	7:G:137:LYS:HD3	1.99	0.45
1:A:120:PHE:CZ	1:A:124:LYS:HD2	2.52	0.45
1:A:474:LEU:HD11	2:B:1157:TYR:CE2	2.52	0.45
2:B:723:ASP:HB3	2:B:726:LEU:HD21	1.99	0.45
2:B:762:SER:O	2:B:762:SER:OG	2.30	0.45
2:B:1016:VAL:HG12	2:B:1017:TYR:N	2.32	0.45
3:C:37:TRP:HB2	11:K:56:LYS:HB3	1.98	0.45
5:E:70:GLY:N	5:E:100:LYS:HE3	2.32	0.45
11:K:84:SER:OG	11:K:85:THR:HG23	2.16	0.45
14:T:18:DC:C2	14:T:19:DC:C5	3.05	0.45
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.65	0.44
1:A:775:TRP:CZ3	8:H:21:TYR:HE2	2.35	0.44
1:A:1065:GLU:HB2	5:E:200:SER:OG	2.18	0.44
14:T:22:DG:H2''	14:T:23:DT:H5'	1.98	0.44
1:A:481:GLY:CA	2:B:1057:GLY:HA3	2.46	0.44
1:A:604:ILE:HD11	2:B:1072:LEU:HD11	1.98	0.44
1:A:728:LYS:O	1:A:753:ASN:ND2	2.50	0.44
1:A:825:LEU:HD12	1:A:825:LEU:HA	1.81	0.44
1:A:1046:GLN:HB3	6:F:129:PRO:HD3	1.99	0.44
1:A:1189:ASP:OD2	6:F:76:THR:HB	2.16	0.44
2:B:86:LYS:HB3	2:B:150:HIS:CE1	2.52	0.44
2:B:274:LYS:O	2:B:276:LEU:N	2.50	0.44
2:B:733:GLN:HE21	2:B:755:ASN:HB2	1.82	0.44
5:E:127:ILE:O	5:E:127:ILE:HG13	2.17	0.44
10:J:23:THR:HA	10:J:26:GLN:HB3	1.99	0.44
1:A:118:LEU:HB2	1:A:182:ARG:NH1	2.32	0.44
1:A:205:THR:HG23	1:A:206:LEU:N	2.32	0.44
1:A:508:VAL:HG23	1:A:509:PHE:HD2	1.81	0.44
1:A:792:LEU:HD13	8:H:81:TYR:HB3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1251:LEU:HD11	1:A:1255:VAL:O	2.18	0.44
1:A:1259:ARG:HA	1:A:1259:ARG:HD2	1.85	0.44
2:B:8:ARG:HD2	2:B:748:ASP:CB	2.47	0.44
2:B:734:THR:OG1	10:J:51:THR:OG1	2.11	0.44
2:B:831:LEU:HB2	12:L:51:LYS:NZ	2.33	0.44
3:C:130:GLU:HG2	3:C:131:ALA:N	2.32	0.44
3:C:207:GLN:H	3:C:207:GLN:HG2	1.62	0.44
1:A:759:ARG:HH22	1:A:1092:LYS:HB2	1.82	0.44
1:A:1066:ASP:O	1:A:1603:ARG:NE	2.37	0.44
1:A:1083:ALA:HB2	1:A:1175:PHE:CE1	2.53	0.44
2:B:833:PHE:CE2	12:L:56:ARG:HD3	2.51	0.44
2:B:1024:MET:HG2	2:B:1025:VAL:HG12	2.00	0.44
3:C:283:ASP:OD1	3:C:284:THR:N	2.51	0.44
4:D:16:LYS:HA	4:D:16:LYS:HD2	1.83	0.44
1:A:1:MET:HG2	1:A:2:ASN:O	2.18	0.44
2:B:85:ALA:O	2:B:115:SER:OG	2.25	0.44
2:B:123:TRP:CE2	2:B:422:LEU:HD22	2.52	0.44
2:B:842:ASP:N	2:B:859:THR:OG1	2.51	0.44
2:B:891:ARG:NH1	3:C:101:GLU:OE1	2.50	0.44
2:B:934:ILE:HG12	2:B:935:ASN:H	1.81	0.44
2:B:1075:ASP:HA	2:B:1079:ASN:HD22	1.81	0.44
8:H:76:MET:HE3	8:H:97:PHE:CG	2.52	0.44
1:A:494:PRO:HG3	1:A:644:PHE:HD1	1.80	0.44
1:A:1593:PHE:CD1	1:A:1600:VAL:HG21	2.53	0.44
2:B:891:ARG:HD2	3:C:99:GLN:HG3	1.98	0.44
3:C:124:HIS:CG	3:C:125:PRO:HD2	2.52	0.44
1:A:333:ARG:O	1:A:337:VAL:HG23	2.17	0.44
1:A:732:PRO:HA	1:A:741:TRP:CD1	2.53	0.44
1:A:744:LYS:HZ3	1:A:794:GLY:H	1.64	0.44
1:A:763:ASN:ND2	1:A:1084:LYS:HG3	2.33	0.44
1:A:1009:TYR:CE2	2:B:506:PRO:HB3	2.53	0.44
1:A:1158:ALA:HB1	1:A:1162:GLU:HB3	2.00	0.44
1:A:1602:PRO:HB2	5:E:199:THR:HG21	2.00	0.44
2:B:165:GLU:HA	10:J:62:TYR:OH	2.18	0.44
2:B:384:TYR:O	2:B:387:ILE:HG22	2.18	0.44
2:B:517:LEU:O	2:B:519:ASN:ND2	2.49	0.44
2:B:733:GLN:NE2	2:B:755:ASN:HB2	2.33	0.44
2:B:1134:ASP:OD1	2:B:1136:SER:N	2.39	0.44
3:C:315:THR:HG21	10:J:6:ARG:NH2	2.32	0.44
6:F:117:GLN:HB3	6:F:119:LYS:HE2	1.99	0.44
1:A:498:ILE:O	1:A:499:GLU:HG2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:971:PRO:HD2	1:A:1013:MET:HE1	2.00	0.44
1:A:1038:LYS:HD2	1:A:1038:LYS:O	2.18	0.44
1:A:1041:GLU:CG	1:A:1042:GLY:H	2.31	0.44
1:A:1163:SER:HA	1:A:1166:ASP:OD2	2.18	0.44
2:B:6:LEU:HD23	2:B:6:LEU:HA	1.79	0.44
2:B:505:CYS:HB2	2:B:683:SER:HB2	2.00	0.44
2:B:564:ASP:HB3	2:B:628:PHE:HA	2.00	0.44
2:B:573:TYR:HE1	2:B:623:PRO:HB2	1.83	0.44
2:B:828:ALA:HB3	12:L:20:MET:HE2	2.00	0.44
2:B:834:ILE:HG21	12:L:53:ARG:HB2	1.98	0.44
2:B:899:GLY:HA2	2:B:911:ILE:HG23	2.00	0.44
3:C:91:ILE:HD13	3:C:100:ASP:CG	2.43	0.44
7:G:145:GLU:HB3	7:G:146:PRO:HD3	1.99	0.44
1:A:109:PHE:CE2	1:A:116:VAL:HG21	2.52	0.43
1:A:957:SER:O	1:A:998:ARG:HD2	2.18	0.43
1:A:1273:SER:HA	1:A:1276:VAL:HG12	1.99	0.43
2:B:22:PHE:CE2	2:B:746:GLY:HA3	2.53	0.43
2:B:733:GLN:HE21	2:B:755:ASN:N	2.15	0.43
1:A:1038:LYS:NZ	1:A:1629:ASN:HD22	2.16	0.43
2:B:304:LEU:HD23	2:B:304:LEU:HA	1.83	0.43
7:G:92:LYS:HD2	7:G:148:LYS:HB3	2.00	0.43
1:A:1058:ILE:HG21	1:A:1061:PHE:CZ	2.53	0.43
2:B:23:PRO:HA	2:B:26:GLN:NE2	2.33	0.43
2:B:45:LEU:O	2:B:49:VAL:HG22	2.18	0.43
2:B:985:LEU:HD23	2:B:985:LEU:HA	1.83	0.43
3:C:218:GLY:HA3	3:C:226:PHE:CD1	2.53	0.43
3:C:285:VAL:O	3:C:287:ARG:N	2.50	0.43
5:E:139:ILE:HG13	5:E:140:THR:N	2.33	0.43
7:G:125:ILE:HG21	7:G:135:ARG:NH2	2.33	0.43
8:H:75:ILE:HG12	8:H:122:LEU:HD22	2.01	0.43
1:A:119:PHE:CE1	1:A:218:PHE:HB2	2.54	0.43
1:A:1636:MET:CE	1:A:1645:LEU:HD12	2.48	0.43
4:D:50:LEU:HA	4:D:53:VAL:HG12	2.00	0.43
14:T:16:DA:H2'	14:T:17:DG:H8	1.83	0.43
1:A:1047:TYR:OH	6:F:79:GLU:OE2	2.29	0.43
2:B:79:VAL:HG23	2:B:396:LEU:HD21	2.00	0.43
2:B:213:LEU:HD22	2:B:352:MET:SD	2.58	0.43
2:B:951:SER:OG	2:B:1014:GLY:HA3	2.19	0.43
3:C:29:TYR:HD1	11:K:61:GLU:HG3	1.83	0.43
4:D:21:ALA:O	4:D:24:LYS:HG3	2.18	0.43
5:E:97:HIS:HB3	5:E:99:HIS:ND1	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:82:ARG:HH22	7:G:65:TYR:HD2	1.67	0.43
8:H:58:GLN:HE21	8:H:124:ARG:HH21	1.67	0.43
9:I:25:THR:HG21	9:I:39:PHE:CE2	2.53	0.43
14:T:18:DC:H2'	14:T:19:DC:C6	2.54	0.43
1:A:763:ASN:OD1	1:A:1085:ASN:HB3	2.19	0.43
1:A:1330:LYS:HA	1:A:1330:LYS:HD3	1.76	0.43
2:B:261:GLU:O	2:B:261:GLU:HG2	2.18	0.43
2:B:468:ASN:HD21	2:B:752:ASN:HD21	1.65	0.43
2:B:508:HIS:CE1	2:B:520:HIS:CD2	3.06	0.43
10:J:7:CYS:HB2	10:J:48:MET:HG3	2.01	0.43
1:A:218:PHE:O	1:A:222:ILE:HG12	2.19	0.43
1:A:1582:ARG:CZ	5:E:195:ARG:HD2	2.49	0.43
2:B:21:SER:O	2:B:23:PRO:HD3	2.18	0.43
2:B:321:LEU:HD23	2:B:321:LEU:HA	1.88	0.43
2:B:523:ARG:N	2:B:682:LEU:O	2.48	0.43
2:B:590:TYR:CE1	2:B:603:ALA:HA	2.54	0.43
2:B:1045:VAL:HG22	2:B:1046:LYS:N	2.33	0.43
3:C:116:PRO:O	3:C:217:LEU:HD11	2.19	0.43
7:G:49:LEU:HD21	7:G:109:PHE:HZ	1.84	0.43
8:H:17:ASP:HA	8:H:18:LYS:CB	2.41	0.43
1:A:476:ARG:HH22	1:A:1034:ARG:NH1	2.17	0.43
1:A:1028:ARG:C	1:A:1030:GLY:H	2.27	0.43
2:B:178:ILE:O	2:B:178:ILE:HG13	2.18	0.43
2:B:692:SER:HB3	2:B:968:PRO:HG3	2.01	0.43
4:D:45:SER:O	4:D:48:SER:OG	2.23	0.43
5:E:142:HIS:HD2	5:E:144:LEU:HB2	1.84	0.43
8:H:115:SER:OG	8:H:116:LEU:N	2.52	0.43
1:A:488:ALA:HB2	2:B:1031:VAL:HG23	2.01	0.43
1:A:632:MET:CE	1:A:636:ASN:HB2	2.48	0.43
1:A:1038:LYS:HD3	1:A:1638:PHE:CE1	2.54	0.43
1:A:1272:LEU:HD21	1:A:1324:PHE:HD1	1.84	0.43
1:A:1550:LYS:HA	1:A:1553:TRP:CD1	2.54	0.43
1:A:1664:LEU:HD12	2:B:1073:MET:SD	2.59	0.43
2:B:372:PRO:HA	2:B:375:GLN:HB2	2.00	0.43
2:B:480:HIS:CE1	2:B:482:GLY:H	2.36	0.43
2:B:1045:VAL:HG22	2:B:1046:LYS:H	1.84	0.43
2:B:1048:ARG:H	2:B:1052:GLY:H	1.66	0.43
3:C:204:ARG:HB2	10:J:63:ASN:HD21	1.84	0.43
5:E:70:GLY:H	5:E:100:LYS:HB2	1.84	0.43
7:G:90:GLU:HB3	7:G:151:GLU:OE1	2.18	0.43
1:A:77:PHE:CE1	1:A:368:PRO:HA	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:HIS:O	2:B:1043:GLN:NE2	2.40	0.43
1:A:674:LEU:HD12	1:A:1071:THR:O	2.19	0.43
1:A:787:ASP:OD1	1:A:788:ASP:N	2.52	0.43
1:A:903:GLN:HA	1:A:906:ASP:OD2	2.18	0.43
1:A:1511:LYS:HE3	1:A:1511:LYS:HB3	1.82	0.43
1:A:1511:LYS:HE3	1:A:1515:GLU:OE2	2.19	0.43
1:A:1567:ASN:HB3	1:A:1588:GLU:HG3	1.99	0.43
2:B:151:LEU:HD11	2:B:164:GLU:OE1	2.19	0.43
2:B:536:GLN:OE1	2:B:604:LYS:HD3	2.19	0.43
2:B:692:SER:O	2:B:700:ASN:ND2	2.52	0.43
2:B:826:LEU:HA	2:B:832:PRO:HA	2.01	0.43
3:C:76:ILE:HD11	3:C:331:LEU:HD13	2.00	0.43
3:C:195:ASN:HB3	3:C:198:ILE:HG13	1.99	0.43
5:E:4:GLU:HB2	5:E:5:GLU:H	1.68	0.43
1:A:377:LYS:HD3	1:A:382:VAL:HG22	2.00	0.42
1:A:694:VAL:HG13	1:A:795:ILE:HD12	2.01	0.42
2:B:75:ILE:HA	2:B:124:SER:O	2.19	0.42
2:B:245:LYS:O	2:B:245:LYS:HG3	2.18	0.42
2:B:338:HIS:CD2	2:B:339:LEU:HG	2.53	0.42
2:B:772:MET:O	2:B:913:SER:HB3	2.17	0.42
2:B:790:LYS:NZ	2:B:792:GLU:OE1	2.45	0.42
2:B:900:ASP:OD2	2:B:1020:ARG:NE	2.52	0.42
3:C:262:VAL:HG23	3:C:263:ILE:HG12	2.01	0.42
6:F:96:PRO:HG3	7:G:23:ARG:HD3	2.00	0.42
7:G:75:ARG:HE	7:G:75:ARG:HB2	1.57	0.42
1:A:842:THR:HB	2:B:1011:ILE:HG23	2.01	0.42
2:B:163:LYS:HG2	2:B:720:TYR:CD2	2.54	0.42
2:B:1089:CYS:HA	2:B:1145:ASN:O	2.19	0.42
1:A:852:GLU:HA	1:A:855:ASP:OD2	2.19	0.42
2:B:40:THR:HG21	2:B:147:ASN:HB3	2.00	0.42
2:B:216:ARG:HA	2:B:226:THR:HG22	2.00	0.42
2:B:503:PHE:CE1	2:B:636:ARG:HD3	2.54	0.42
3:C:305:ARG:HD3	3:C:305:ARG:HA	1.87	0.42
5:E:46:CYS:SG	5:E:47:GLY:N	2.92	0.42
8:H:59:ILE:HD11	8:H:114:LEU:HD21	2.01	0.42
13:U:34:DG:H2"	13:U:35:DA:C8	2.54	0.42
1:A:1572:ILE:O	1:A:1576:TYR:N	2.51	0.42
2:B:39:LEU:HD21	2:B:385:GLY:HA3	2.01	0.42
2:B:218:VAL:CG2	2:B:222:GLN:HA	2.49	0.42
2:B:290:ARG:NH2	9:I:18:GLU:OE1	2.40	0.42
2:B:877:ASP:HB3	2:B:878:VAL:H	1.69	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:ARG:HA	1:A:741:TRP:CZ3	2.54	0.42
1:A:739:ILE:HD13	3:C:32:ASP:HB2	2.02	0.42
1:A:814:GLU:HG3	1:A:1075:HIS:CE1	2.53	0.42
2:B:537:ILE:HG21	2:B:563:LEU:HD13	2.01	0.42
5:E:186:LYS:HB2	5:E:189:GLU:OE2	2.19	0.42
7:G:138:THR:HG23	7:G:141:GLY:H	1.84	0.42
10:J:9:SER:HB2	10:J:44:CYS:SG	2.59	0.42
14:T:20:DT:H2'	14:T:21:DG:H5''	2.01	0.42
1:A:203:LEU:HG	1:A:204:THR:H	1.84	0.42
1:A:867:SER:O	1:A:868:PHE:C	2.62	0.42
1:A:897:ARG:HB3	2:B:619:ASN:HD22	1.84	0.42
2:B:40:THR:HG23	2:B:41:ASN:H	1.85	0.42
2:B:109:ARG:HA	2:B:874:LEU:HG	2.01	0.42
2:B:501:TRP:HZ2	2:B:661:CYS:SG	2.42	0.42
2:B:979:ASP:OD1	2:B:992:TYR:OH	2.36	0.42
2:B:1098:ILE:O	2:B:1098:ILE:HG13	2.17	0.42
3:C:94:ASN:H	12:L:53:ARG:NH1	2.17	0.42
5:E:14:ALA:HA	5:E:17:THR:HG22	2.00	0.42
7:G:59:LYS:HD3	7:G:73:TRP:HD1	1.85	0.42
1:A:20:ASP:O	1:A:24:VAL:HG13	2.19	0.42
1:A:79:HIS:HD2	1:A:81:VAL:HG22	1.85	0.42
1:A:119:PHE:CZ	1:A:218:PHE:HB2	2.55	0.42
1:A:657:THR:HA	1:A:660:ARG:HG2	2.02	0.42
1:A:920:ILE:HD11	1:A:959:LEU:HD22	2.02	0.42
1:A:1028:ARG:HA	1:A:1028:ARG:HD3	1.71	0.42
1:A:1143:ARG:O	1:A:1147:GLU:HG2	2.20	0.42
1:A:1255:VAL:HG13	1:A:1259:ARG:HB3	2.01	0.42
1:A:1605:LEU:HD12	1:A:1605:LEU:HA	1.82	0.42
1:A:1662:SER:O	1:A:1665:VAL:HG12	2.20	0.42
2:B:289:LEU:HD23	2:B:289:LEU:HA	1.74	0.42
2:B:1061:ARG:O	2:B:1065:ILE:HG12	2.20	0.42
3:C:243:LEU:HD12	3:C:297:ASP:O	2.19	0.42
1:A:495:ASP:O	1:A:633:HIS:HA	2.20	0.42
2:B:261:GLU:H	2:B:261:GLU:CD	2.28	0.42
2:B:666:ILE:HG23	2:B:671:SER:OG	2.19	0.42
2:B:936:PRO:C	2:B:938:ALA:H	2.27	0.42
5:E:86:GLU:HG3	5:E:90:PHE:CE1	2.55	0.42
13:U:39:DT:H6	13:U:39:DT:H2'	1.73	0.42
1:A:122:ARG:O	1:A:126:LEU:HD23	2.20	0.42
1:A:470:LYS:C	1:A:472:GLU:H	2.26	0.42
1:A:515:TYR:HB3	1:A:653:PHE:CE2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:815:LEU:HD21	1:A:1085:ASN:ND2	2.35	0.42
1:A:1231:LEU:HA	1:A:1231:LEU:HD12	1.88	0.42
1:A:1659:ASN:ND2	1:A:1661:SER:OG	2.53	0.42
2:B:63:GLN:HB2	2:B:67:GLY:H	1.84	0.42
2:B:106:ALA:HB2	2:B:113:TYR:HD1	1.84	0.42
2:B:274:LYS:HE2	2:B:275:ASP:HB3	2.01	0.42
2:B:350:LEU:HD23	2:B:350:LEU:HA	1.75	0.42
2:B:1038:HIS:HB2	2:B:1043:GLN:O	2.20	0.42
3:C:31:PHE:O	3:C:32:ASP:HB3	2.19	0.42
3:C:55:GLN:NE2	3:C:319:LYS:HE2	2.35	0.42
3:C:253:LYS:HB2	3:C:253:LYS:HE2	1.92	0.42
3:C:342:LEU:O	3:C:345:ILE:HG12	2.19	0.42
5:E:54:ARG:HB3	5:E:78:LYS:HD3	2.01	0.42
11:K:41:LYS:HE2	11:K:41:LYS:HB2	1.82	0.42
13:U:30:DA:N1	14:T:11:DA:N1	2.68	0.42
14:T:10:DT:C2	14:T:11:DA:C8	3.08	0.42
1:A:373:ARG:HB3	1:A:385:ASN:ND2	2.26	0.42
1:A:1193:SER:O	1:A:1197:LEU:HD23	2.19	0.42
1:A:1551:ALA:O	1:A:1555:PHE:HD2	2.03	0.42
2:B:145:ARG:NH2	2:B:159:LEU:HD11	2.34	0.42
1:A:172:ALA:HB3	1:A:175:ALA:HB3	2.02	0.41
1:A:390:LEU:O	1:A:390:LEU:HD23	2.19	0.41
1:A:595:ARG:CZ	1:A:598:ARG:HE	2.33	0.41
1:A:815:LEU:HD21	1:A:1085:ASN:HD22	1.84	0.41
1:A:1005:PRO:HG3	2:B:969:PHE:CG	2.54	0.41
2:B:306:TYR:O	2:B:310:LYS:HG2	2.19	0.41
2:B:773:ILE:HG22	2:B:774:LEU:N	2.33	0.41
2:B:1100:SER:HA	2:B:1113:VAL:HA	2.02	0.41
3:C:285:VAL:O	3:C:285:VAL:HG12	2.20	0.41
5:E:130:PHE:HZ	5:E:182:TYR:HA	1.85	0.41
7:G:49:LEU:HD12	7:G:79:LEU:O	2.20	0.41
1:A:1045:VAL:HG23	1:A:1191:GLY:N	2.34	0.41
1:A:1085:ASN:OD1	1:A:1085:ASN:N	2.46	0.41
2:B:492:THR:OG1	2:B:493:VAL:N	2.46	0.41
2:B:1112:GLU:HG2	2:B:1114:ARG:HH12	1.85	0.41
3:C:160:PRO:HB2	3:C:164:TYR:CD2	2.54	0.41
6:F:66:LYS:HG3	6:F:69:ARG:NH2	2.35	0.41
8:H:27:ILE:HD12	8:H:55:PHE:HZ	1.85	0.41
1:A:474:LEU:C	1:A:476:ARG:H	2.29	0.41
1:A:960:LEU:HB2	1:A:995:ILE:HG13	2.02	0.41
1:A:1050:THR:O	1:A:1052:ARG:HG3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:441:LEU:HD23	2:B:441:LEU:HA	1.76	0.41
2:B:507:VAL:HG13	2:B:508:HIS:N	2.35	0.41
2:B:534:VAL:O	2:B:537:ILE:HB	2.20	0.41
2:B:536:GLN:OE1	2:B:604:LYS:HA	2.21	0.41
2:B:822:TRP:CE2	2:B:857:ILE:HD12	2.56	0.41
3:C:107:ILE:O	3:C:110:VAL:HG22	2.21	0.41
6:F:108:LEU:HD23	6:F:112:MET:HE2	2.03	0.41
2:B:920:ASP:OD1	3:C:75:ARG:NH1	2.53	0.41
2:B:1042:ARG:HH21	2:B:1084:ALA:HB2	1.86	0.41
2:B:1078:MET:HE2	2:B:1083:TYR:HE2	1.85	0.41
4:D:26:LEU:O	4:D:30:ILE:HG13	2.20	0.41
5:E:152:SER:N	5:E:155:GLU:HB2	2.36	0.41
7:G:77:ASP:OD1	7:G:77:ASP:N	2.44	0.41
12:L:24:CYS:SG	12:L:27:CYS:N	2.90	0.41
1:A:18:ILE:HD13	1:A:359:MET:HG2	2.03	0.41
1:A:220:HIS:O	1:A:224:SER:OG	2.37	0.41
1:A:511:THR:O	1:A:596:HIS:NE2	2.54	0.41
1:A:636:ASN:OD1	1:A:683:ARG:NH1	2.52	0.41
1:A:903:GLN:HE21	1:A:968:ARG:HH21	1.67	0.41
1:A:1312:GLU:HB2	9:I:57:LEU:CD2	2.41	0.41
2:B:123:TRP:CE3	2:B:131:GLN:HG2	2.56	0.41
2:B:783:PHE:O	2:B:784:GLY:C	2.63	0.41
2:B:897:ILE:HD12	2:B:897:ILE:HA	1.86	0.41
2:B:1011:ILE:HG22	2:B:1012:TYR:N	2.34	0.41
3:C:323:LEU:HD13	3:C:323:LEU:HA	1.81	0.41
4:D:17:LEU:HB3	7:G:7:TYR:HA	2.02	0.41
5:E:53:ASP:HB2	5:E:54:ARG:HH11	1.84	0.41
7:G:122:TRP:CD1	7:G:122:TRP:N	2.88	0.41
8:H:63:LEU:HG	8:H:68:LEU:HD12	2.02	0.41
8:H:77:TYR:HE1	8:H:120:TYR:CZ	2.39	0.41
11:K:63:CYS:SG	11:K:79:ILE:HG12	2.60	0.41
1:A:204:THR:HB	1:A:207:LEU:HD13	2.02	0.41
1:A:248:GLU:HG2	1:A:249:ILE:HG12	2.02	0.41
1:A:519:VAL:HG22	1:A:527:MET:HG3	2.02	0.41
1:A:726:ARG:HA	11:K:78:ARG:NH2	2.33	0.41
1:A:742:THR:HG21	8:H:98:GLY:O	2.20	0.41
1:A:1005:PRO:HG3	2:B:969:PHE:CD1	2.55	0.41
1:A:1242:ILE:HD13	1:A:1567:ASN:OD1	2.20	0.41
2:B:609:LEU:HD23	2:B:610:GLU:N	2.35	0.41
2:B:733:GLN:HB2	10:J:51:THR:O	2.21	0.41
2:B:829:ASP:HB3	2:B:831:LEU:HG	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:928:MET:HE3	2:B:928:MET:HB3	1.96	0.41
2:B:945:ILE:HD12	2:B:948:PHE:HD2	1.86	0.41
7:G:122:TRP:HZ3	7:G:144:LEU:HD21	1.85	0.41
1:A:88:HIS:HB3	1:A:91:PHE:HD2	1.85	0.41
1:A:122:ARG:HB3	1:A:122:ARG:HH21	1.86	0.41
1:A:602:MET:HG3	1:A:618:ALA:HB1	2.03	0.41
1:A:815:LEU:HB3	1:A:816:TYR:CD1	2.56	0.41
1:A:1140:LYS:H	5:E:201:GLY:CA	2.33	0.41
1:A:1255:VAL:HG13	1:A:1259:ARG:HG3	2.03	0.41
1:A:1539:VAL:O	1:A:1541:LYS:HG3	2.20	0.41
1:A:1592:VAL:O	1:A:1595:VAL:HG22	2.20	0.41
2:B:183:ARG:HH12	2:B:480:HIS:CG	2.39	0.41
2:B:208:TYR:HA	2:B:232:LEU:HA	2.03	0.41
2:B:305:GLN:NE2	2:B:324:VAL:HG22	2.36	0.41
2:B:775:ASN:HD22	2:B:921:MET:HG3	1.85	0.41
2:B:1061:ARG:O	2:B:1065:ILE:HG23	2.21	0.41
3:C:144:ASN:HA	3:C:209:ILE:O	2.21	0.41
3:C:218:GLY:HA3	3:C:226:PHE:CE1	2.56	0.41
5:E:47:GLY:HA3	5:E:52:LEU:HB3	2.02	0.41
5:E:165:LEU:HD23	5:E:165:LEU:HA	1.89	0.41
6:F:77:LYS:HE3	6:F:77:LYS:HB2	1.76	0.41
8:H:107:SER:C	8:H:109:ARG:H	2.29	0.41
1:A:487:ALA:CB	2:B:1054:ILE:HD11	2.51	0.41
1:A:503:ILE:HG12	1:A:504:GLY:O	2.21	0.41
1:A:606:ASN:HD22	1:A:616:MET:HB2	1.86	0.41
1:A:717:LYS:HZ1	11:K:68:PRO:HA	1.86	0.41
1:A:936:ASN:OD1	1:A:938:MET:N	2.53	0.41
1:A:936:ASN:O	1:A:940:THR:OG1	2.34	0.41
1:A:1049:HIS:CE1	1:A:1187:LEU:HD12	2.56	0.41
2:B:701:MET:HE3	2:B:701:MET:HB2	1.69	0.41
7:G:25:PRO:O	7:G:29:ILE:N	2.48	0.41
10:J:67:LYS:HD3	10:J:67:LYS:HA	1.75	0.41
1:A:247:PHE:HD1	1:A:247:PHE:HA	1.66	0.41
1:A:697:THR:HB	1:A:795:ILE:HA	2.03	0.41
1:A:715:ALA:CB	1:A:831:LEU:HB2	2.50	0.41
1:A:1024:VAL:HG21	2:B:494:ARG:NH2	2.35	0.41
1:A:1331:ILE:O	1:A:1335:ILE:HG12	2.21	0.41
1:A:1591:SER:O	1:A:1595:VAL:HG13	2.21	0.41
2:B:232:LEU:HG	2:B:236:VAL:O	2.21	0.41
2:B:283:ASP:OD1	2:B:284:ARG:N	2.53	0.41
2:B:604:LYS:HE2	2:B:604:LYS:HB2	1.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:694:PHE:CE2	2:B:949:ILE:HG13	2.56	0.41
2:B:1155:PHE:HE1	2:B:1169:MET:HE2	1.85	0.41
2:B:1165:MET:O	2:B:1166:ASN:HB3	2.21	0.41
3:C:110:VAL:HA	3:C:111:PRO:HD3	1.93	0.41
4:D:46:VAL:O	4:D:50:LEU:HG	2.21	0.41
5:E:25:ARG:NH2	5:E:128:GLU:OE1	2.54	0.41
5:E:156:LYS:HE3	5:E:190:VAL:HG23	2.03	0.41
7:G:41:LEU:HA	7:G:42:PRO:HD3	1.90	0.41
7:G:61:ALA:HB1	7:G:71:PHE:O	2.21	0.41
11:K:113:LEU:H	11:K:113:LEU:HD23	1.86	0.41
1:A:715:ALA:HB2	1:A:831:LEU:HD13	2.02	0.41
1:A:763:ASN:HB3	1:A:787:ASP:OD1	2.20	0.41
1:A:964:GLU:HB2	1:A:967:GLY:O	2.20	0.41
1:A:1650:LEU:HD23	1:A:1650:LEU:HA	1.86	0.41
2:B:649:LEU:HD12	2:B:653:GLU:HB2	2.02	0.41
2:B:822:TRP:CZ2	2:B:857:ILE:HB	2.56	0.41
2:B:836:ILE:HD13	12:L:56:ARG:HE	1.85	0.41
2:B:908:GLN:HE22	2:B:942:ARG:HD2	1.86	0.41
3:C:120:LYS:O	3:C:217:LEU:HD12	2.20	0.41
3:C:134:THR:HG23	3:C:137:ASP:HB2	2.02	0.41
1:A:141:SER:O	1:A:142:LEU:HD12	2.21	0.40
1:A:687:GLN:H	1:A:687:GLN:HG3	1.44	0.40
1:A:744:LYS:HZ3	1:A:794:GLY:N	2.19	0.40
1:A:862:LEU:HA	1:A:862:LEU:HD23	1.72	0.40
1:A:1137:VAL:HG12	1:A:1183:TYR:CG	2.56	0.40
2:B:143:MET:HE3	2:B:143:MET:HB2	1.92	0.40
2:B:223:SER:HA	2:B:386:GLN:NE2	2.36	0.40
2:B:307:LEU:HD12	2:B:307:LEU:HA	1.95	0.40
2:B:499:GLU:N	2:B:499:GLU:OE2	2.54	0.40
2:B:1018:TYR:HD1	2:B:1018:TYR:HA	1.69	0.40
2:B:1112:GLU:CG	2:B:1114:ARG:HH12	2.34	0.40
10:J:21:TYR:HB2	10:J:38:LEU:HD21	2.03	0.40
1:A:30:LYS:HG3	1:A:31:GLN:H	1.86	0.40
1:A:84:ILE:HD11	1:A:401:ILE:HG21	2.02	0.40
1:A:502:GLU:OE1	1:A:622:ARG:HB2	2.21	0.40
1:A:658:ASN:O	1:A:661:SER:OG	2.35	0.40
1:A:941:MET:HE3	2:B:937:HIS:HA	2.02	0.40
1:A:1603:ARG:HH12	5:E:199:THR:HB	1.86	0.40
1:A:1621:PHE:HD1	1:A:1621:PHE:HA	1.76	0.40
1:A:1664:LEU:HD12	2:B:1073:MET:HE3	2.03	0.40
2:B:255:ILE:HD11	2:B:335:VAL:HB	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:341:GLU:O	2:B:345:LYS:HG3	2.21	0.40
2:B:563:LEU:HD12	2:B:627:LEU:O	2.21	0.40
2:B:609:LEU:HG	2:B:628:PHE:O	2.21	0.40
2:B:708:LYS:HB3	2:B:708:LYS:HE2	1.90	0.40
2:B:851:SER:OG	2:B:852:THR:N	2.54	0.40
2:B:921:MET:HE3	2:B:921:MET:HB3	1.84	0.40
2:B:1024:MET:HG2	2:B:1025:VAL:N	2.36	0.40
5:E:36:LEU:HD22	5:E:40:GLN:HG2	2.02	0.40
1:A:240:LYS:HA	1:A:246:ILE:HA	2.02	0.40
1:A:362:LEU:HD13	1:A:365:ILE:HG23	2.03	0.40
1:A:489:ARG:O	2:B:1029:PHE:HA	2.21	0.40
1:A:694:VAL:HG21	1:A:944:SER:OG	2.21	0.40
1:A:952:ASN:HA	2:B:943:MET:HE1	2.03	0.40
1:A:1170:LEU:HD23	1:A:1170:LEU:HA	1.84	0.40
1:A:1277:ARG:HG3	1:A:1304:TYR:OH	2.22	0.40
2:B:148:ARG:HD3	2:B:148:ARG:HA	1.82	0.40
2:B:283:ASP:OD1	2:B:284:ARG:HG2	2.21	0.40
2:B:822:TRP:CZ2	2:B:857:ILE:HD12	2.56	0.40
3:C:237:LEU:HD12	3:C:238:PRO:HD2	2.03	0.40
3:C:318:MET:HB2	3:C:323:LEU:HD21	2.03	0.40
5:E:178:PRO:HA	5:E:181:ARG:HD3	2.02	0.40
1:A:634:TYR:CE1	2:B:768:MET:HB2	2.57	0.40
1:A:949:SER:OG	1:A:950:ASN:N	2.54	0.40
2:B:699:ARG:HA	2:B:699:ARG:HD3	1.83	0.40
2:B:1085:GLN:HB3	2:B:1148:LEU:HD21	2.02	0.40
3:C:97:ILE:HG13	10:J:60:LEU:HD23	2.03	0.40
4:D:26:LEU:HD12	4:D:26:LEU:HA	1.96	0.40
5:E:23:HIS:N	5:E:24:ASP:HB2	2.36	0.40
8:H:42:ILE:CD1	8:H:49:LEU:HB2	2.51	0.40
8:H:63:LEU:HG	8:H:68:LEU:CD1	2.51	0.40
1:A:55:GLY:HA2	1:A:56:PRO:HD3	1.97	0.40
1:A:695:TRP:HZ2	1:A:934:PRO:O	2.05	0.40
1:A:715:ALA:HB2	1:A:831:LEU:HB2	2.03	0.40
1:A:742:THR:HG23	1:A:745:GLN:HB2	2.04	0.40
1:A:838:MET:HE2	1:A:838:MET:HB3	1.84	0.40
1:A:851:ASP:OD2	1:A:852:GLU:N	2.54	0.40
1:A:857:TRP:O	1:A:861:LEU:HG	2.22	0.40
1:A:960:LEU:HD13	1:A:997:SER:O	2.21	0.40
1:A:1171:ASN:HB3	1:A:1174:LYS:CB	2.52	0.40
2:B:468:ASN:ND2	2:B:710:THR:HB	2.36	0.40
2:B:679:THR:C	2:B:681:VAL:H	2.30	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:706:MET:HE3	2:B:706:MET:HB3	1.96	0.40
8:H:38:LEU:HD21	8:H:40:LEU:HD22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1377/1689 (82%)	1229 (89%)	143 (10%)	5 (0%)	30	64
2	B	1172/1174 (100%)	1022 (87%)	145 (12%)	5 (0%)	30	64
3	C	315/348 (90%)	290 (92%)	24 (8%)	1 (0%)	36	69
4	D	35/147 (24%)	33 (94%)	2 (6%)	0	100	100
5	E	205/210 (98%)	178 (87%)	27 (13%)	0	100	100
6	F	80/142 (56%)	71 (89%)	9 (11%)	0	100	100
7	G	156/173 (90%)	143 (92%)	13 (8%)	0	100	100
8	H	121/125 (97%)	92 (76%)	28 (23%)	1 (1%)	16	50
9	I	55/119 (46%)	50 (91%)	5 (9%)	0	100	100
10	J	66/71 (93%)	46 (70%)	20 (30%)	0	100	100
11	K	93/125 (74%)	88 (95%)	5 (5%)	0	100	100
12	L	43/63 (68%)	41 (95%)	2 (5%)	0	100	100
All	All	3718/4386 (85%)	3283 (88%)	423 (11%)	12 (0%)	37	69

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1067	SER
2	B	493	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	206	THR
1	A	782	GLY
3	C	286	SER
2	B	492	THR
1	A	1068	LEU
1	A	1568	ASP
2	B	409	ARG
2	B	827	ASP
1	A	85	PRO
8	H	24	VAL

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	1239/1484 (84%)	1231 (99%)	8 (1%)	78	80
2	B	1013/1013 (100%)	1008 (100%)	5 (0%)	81	82
3	C	281/308 (91%)	279 (99%)	2 (1%)	76	78
4	D	37/134 (28%)	37 (100%)	0	100	100
5	E	182/184 (99%)	181 (100%)	1 (0%)	81	82
6	F	70/121 (58%)	70 (100%)	0	100	100
7	G	143/154 (93%)	143 (100%)	0	100	100
8	H	112/114 (98%)	112 (100%)	0	100	100
9	I	51/105 (49%)	51 (100%)	0	100	100
10	J	63/66 (96%)	61 (97%)	2 (3%)	34	56
11	K	86/111 (78%)	85 (99%)	1 (1%)	63	72
12	L	39/53 (74%)	39 (100%)	0	100	100
All	All	3316/3847 (86%)	3297 (99%)	19 (1%)	76	80

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	PHE
1	A	346	LEU
1	A	362	LEU
1	A	616	MET
1	A	724	TYR
1	A	868	PHE
1	A	902	LEU
1	A	1605	LEU
2	B	215	ILE
2	B	652	PHE
2	B	1006	GLU
2	B	1018	TYR
2	B	1096	ILE
3	C	240	ILE
3	C	342	LEU
5	E	126	THR
10	J	50	LEU
10	J	65	LEU
11	K	22	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	107	HIS
1	A	108	HIS
1	A	132	ASN
1	A	232	GLN
1	A	257	GLN
1	A	330	ASN
1	A	331	HIS
1	A	364	ASN
1	A	439	HIS
1	A	450	ASN
1	A	466	GLN
1	A	497	ASN
1	A	543	HIS
1	A	545	GLN
1	A	606	ASN
1	A	608	GLN
1	A	612	HIS
1	A	652	HIS
1	A	710	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	735	GLN
1	A	860	GLN
1	A	963	GLN
1	A	1062	HIS
1	A	1075	HIS
1	A	1078	GLN
1	A	1152	ASN
1	A	1180	GLN
1	A	1252	ASN
1	A	1345	GLN
1	A	1486	ASN
1	A	1499	ASN
1	A	1557	ASN
1	A	1562	ASN
1	A	1629	ASN
2	B	26	GLN
2	B	32	HIS
2	B	83	GLN
2	B	126	ASN
2	B	150	HIS
2	B	192	HIS
2	B	203	ASN
2	B	227	ASN
2	B	300	GLN
2	B	305	GLN
2	B	374	HIS
2	B	386	GLN
2	B	468	ASN
2	B	508	HIS
2	B	520	HIS
2	B	554	HIS
2	B	562	GLN
2	B	640	HIS
2	B	673	HIS
2	B	687	ASN
2	B	695	ASN
2	B	700	ASN
2	B	703	GLN
2	B	733	GLN
2	B	742	HIS
2	B	861	HIS
2	B	876	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	908	GLN
2	B	1005	GLN
2	B	1038	HIS
2	B	1039	ASN
2	B	1043	GLN
2	B	1145	ASN
3	C	99	GLN
3	C	124	HIS
3	C	150	ASN
3	C	182	GLN
3	C	207	GLN
3	C	223	HIS
3	C	292	HIS
4	D	27	ASN
5	E	7	ASN
5	E	65	ASN
5	E	99	HIS
5	E	138	ASN
5	E	142	HIS
7	G	9	GLN
8	H	45	GLN
8	H	58	GLN
8	H	118	HIS
9	I	15	ASN
10	J	63	ASN
11	K	48	ASN
11	K	76	ASN
11	K	112	GLN
12	L	31	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	R	6/20 (30%)	2 (33%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	R	15	C
15	R	17	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

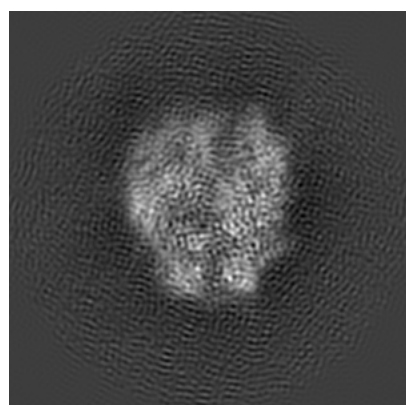
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11842. These allow visual inspection of the internal detail of the map and identification of artifacts.

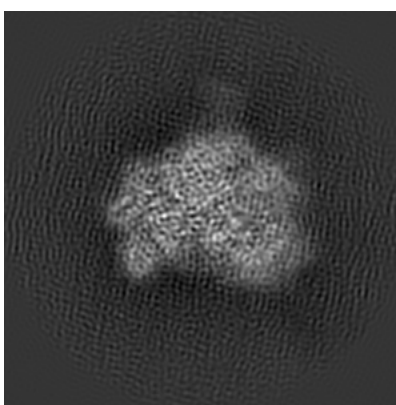
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

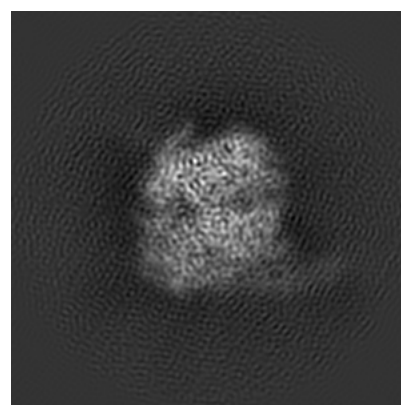
6.1.1 Primary map



X



Y

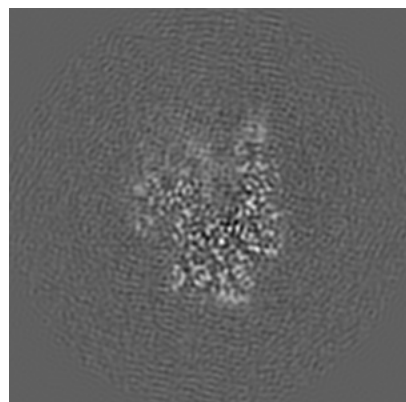


Z

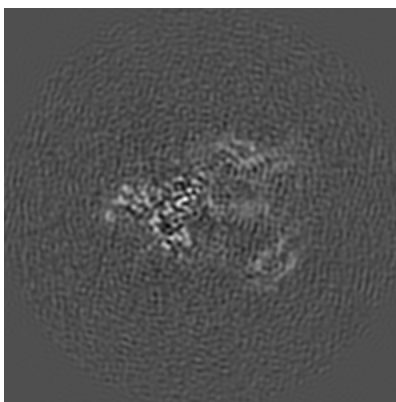
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

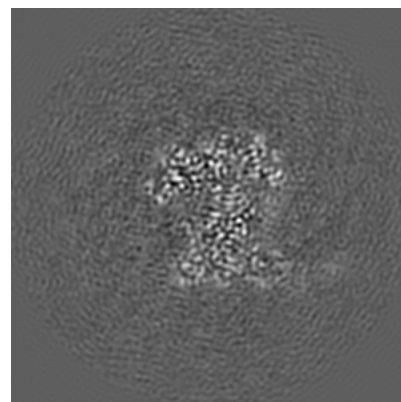
6.2.1 Primary map



X Index: 128



Y Index: 128

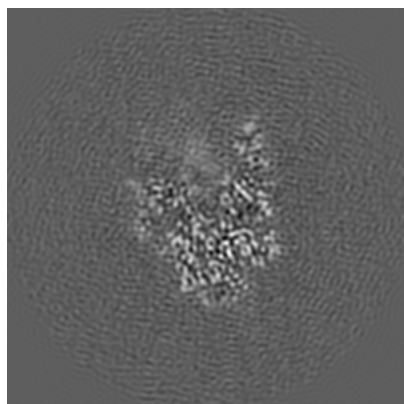


Z Index: 128

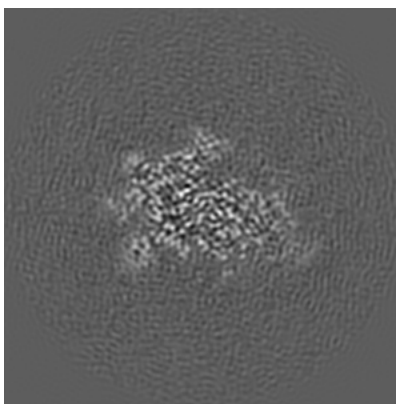
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

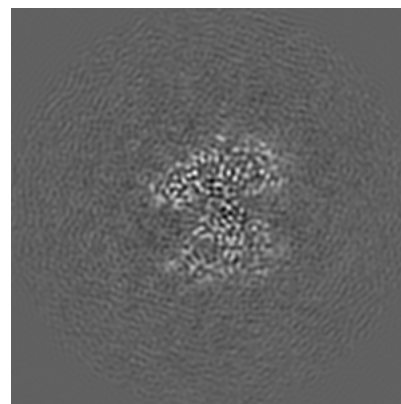
6.3.1 Primary map



X Index: 125



Y Index: 151

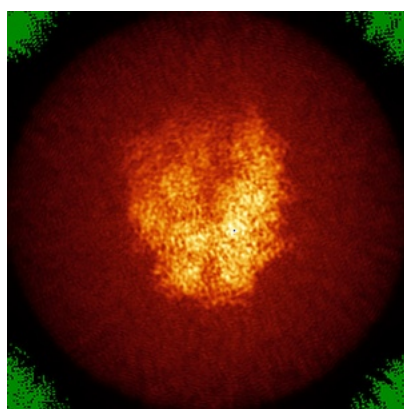


Z Index: 118

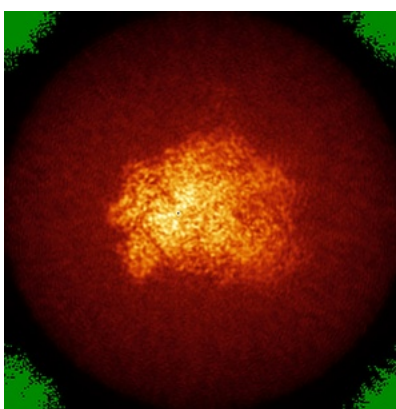
The images above show the largest variance slices of the map in three orthogonal directions.

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

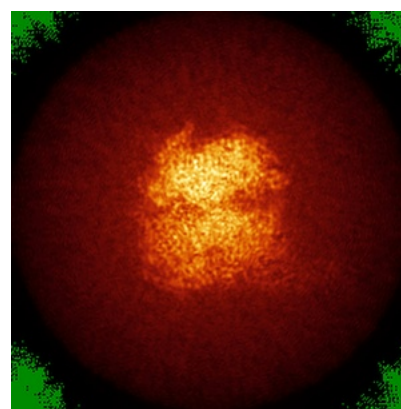
6.4.1 Primary map



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 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

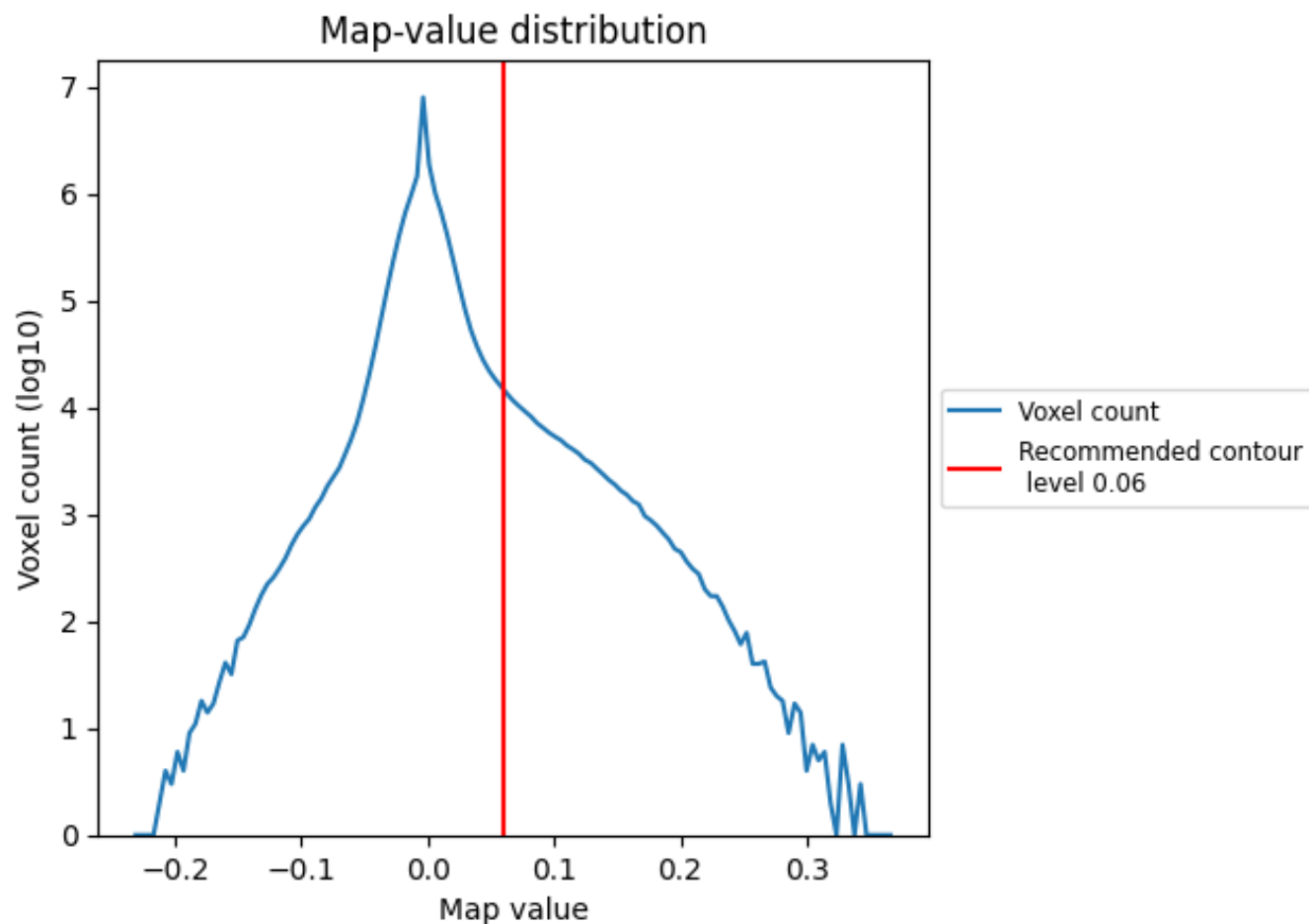
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

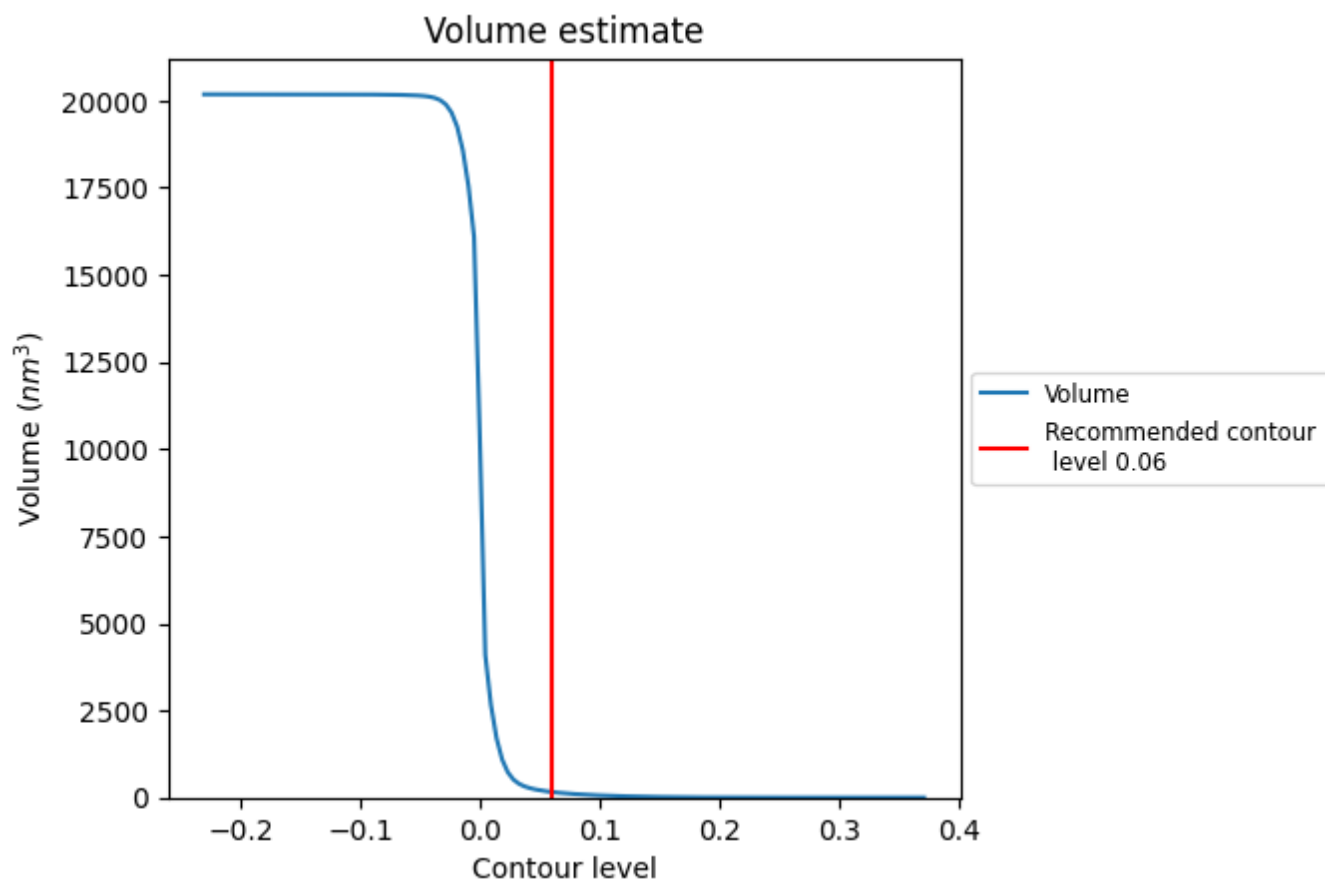
This section contains the results of statistical analysis of the map.

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.

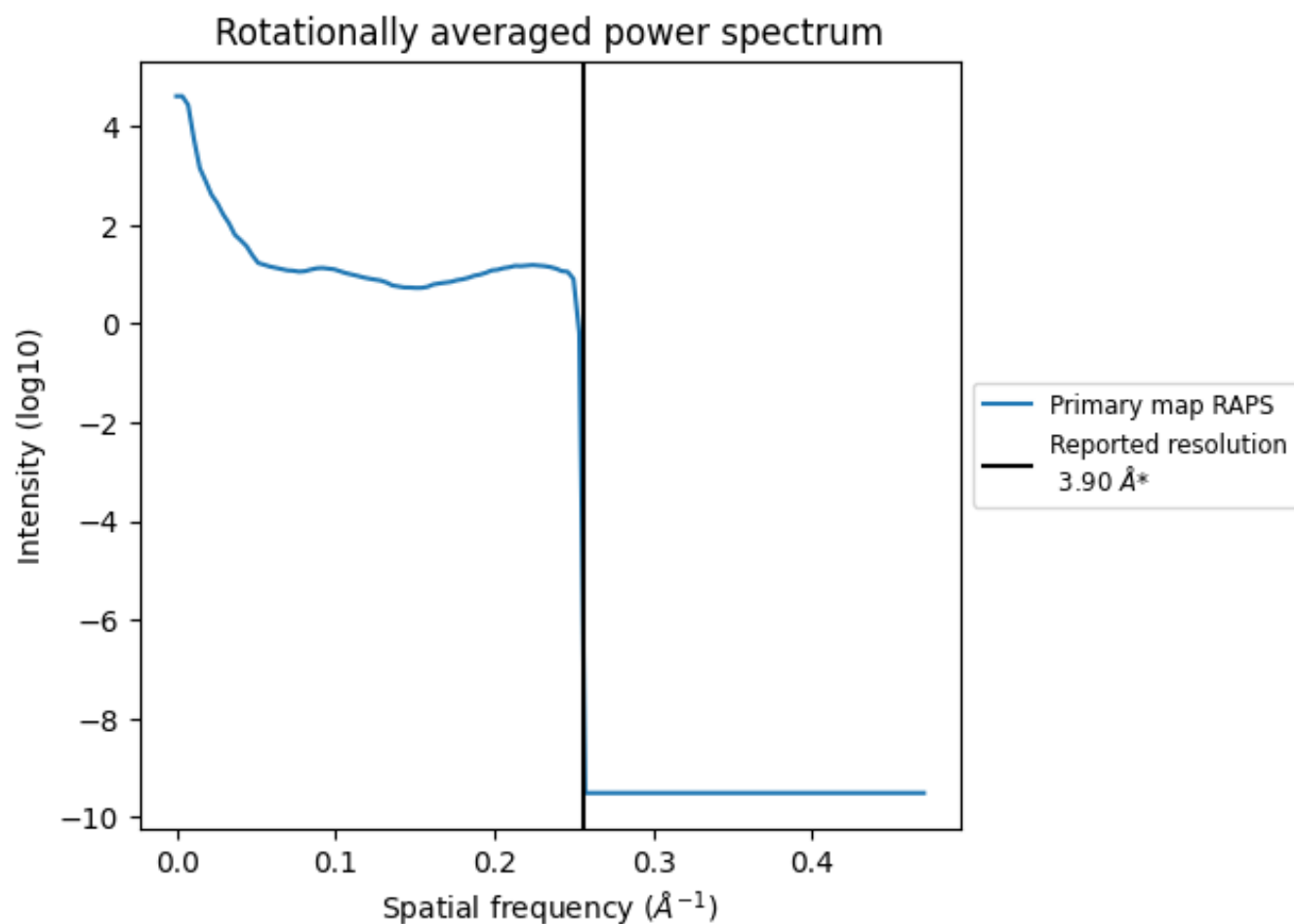
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 159 nm³; this corresponds to an approximate mass of 144 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 0.256 Å⁻¹

8 Fourier-Shell correlation

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

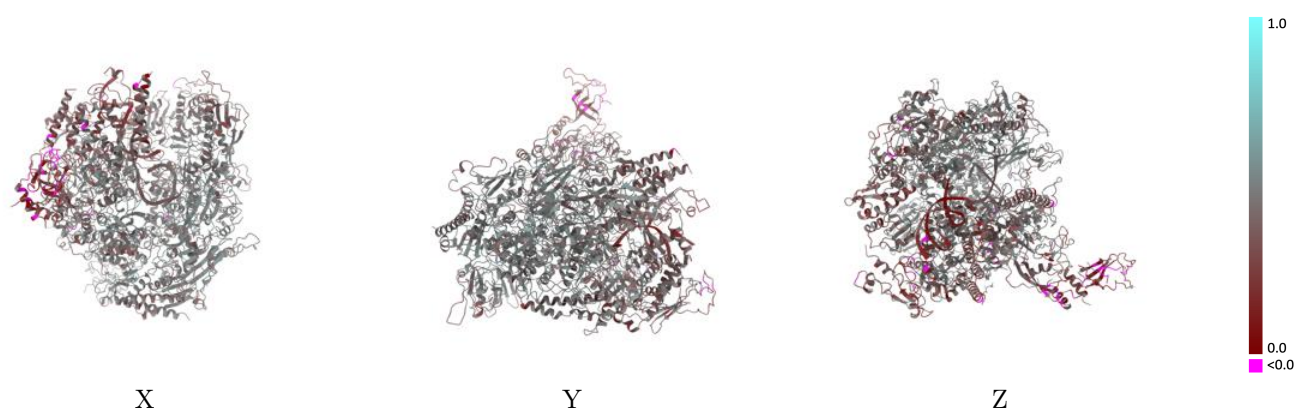
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11842 and PDB model 7AOE. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

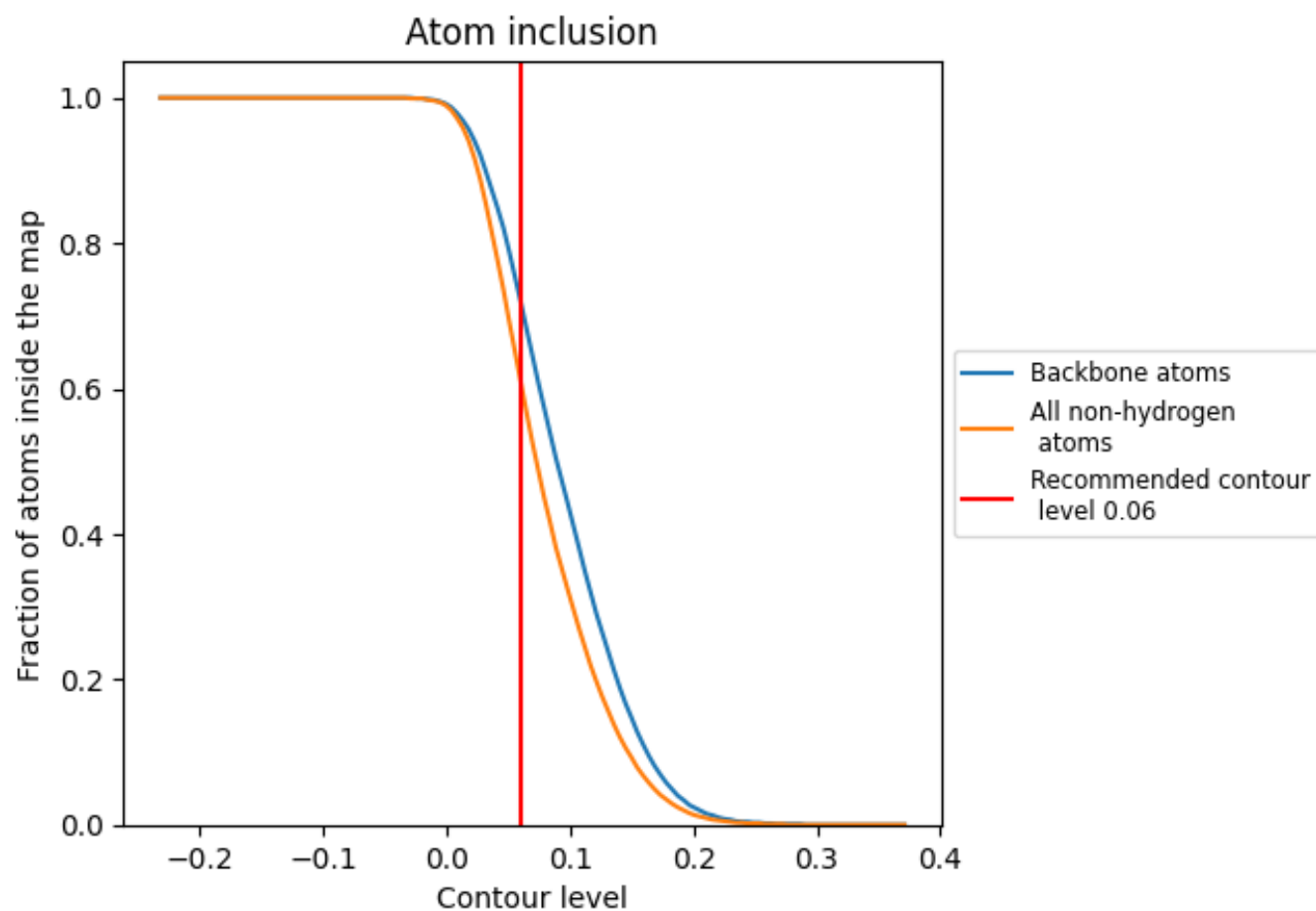


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 61% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6120	0.4220
A	0.5750	0.4190
B	0.7330	0.4630
C	0.7480	0.4580
D	0.0030	0.2100
E	0.3790	0.3490
F	0.6750	0.4550
G	0.1760	0.2540
H	0.7400	0.4640
I	0.2160	0.3490
J	0.8220	0.4870
K	0.7920	0.4730
L	0.7850	0.4680
R	0.8100	0.4310
T	0.4070	0.2750
U	0.0910	0.1450

