



Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 01:53 PM EST

PDB ID : 6WMR
EMDB ID : EMD-21851
Title : F. tularensis RNAPs70-(MglA-SspA)-iglA DNA complex
Authors : Travis, B.A.; Brennan, R.G.; Schumacher, M.A.
Deposited on : 2020-04-21
Resolution : 3.46 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

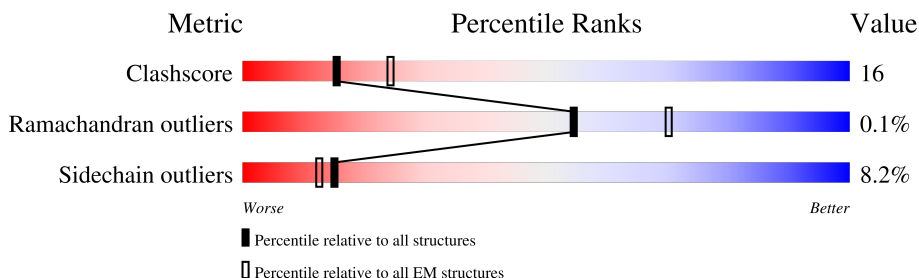
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.46 Å.

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



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

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	G	35	
2	H	24	
3	X	11	
4	J	11	
5	S	210	
6	M	205	
7	Z	577	
8	A	323	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	B	317	<div><div></div><div>6%</div><div>44%</div><div>26%</div><div>•</div><div>27%</div></div>
10	C	1358	<div><div></div><div>14%</div><div>58%</div><div>28%</div><div>•</div><div>13%</div></div>
11	D	1417	<div><div></div><div>9%</div><div>55%</div><div>25%</div><div>•</div><div>18%</div></div>
12	E	72	<div><div></div><div>31%</div><div>62%</div><div>29%</div><div>8%</div></div>

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 30440 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 DNA chain called DNA NT-strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	35	Total	C	N	O	P	0	0
			720	347	118	220	35		

- Molecule 2 is a DNA chain called DNA T-strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	24	Total	C	N	O	P	0	0
			487	233	94	136	24		

- Molecule 3 is a DNA chain called DNA NT-strand downstream.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	X	11	Total	C	N	O	P	0	0
			225	106	41	67	11		

- Molecule 4 is a DNA chain called DNA T-strand downstream.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	11	Total	C	N	O	P	0	0
			226	106	44	65	11		

- Molecule 5 is a protein called Stringent starvation protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	202	Total	C	N	O	S	0	0
			1583	1024	265	287	7		

- Molecule 6 is a protein called Macrophage growth locus, subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	201	Total	C	N	O	S	0	0
			1598	1042	258	293	5		

- Molecule 7 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Z	470	Total	C	N	O	S	0	0
			3772	2392	666	698	16		

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit alpha 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	223	Total	C	N	O	S	0	0
			1688	1075	280	331	2		

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit alpha 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	230	Total	C	N	O	S	0	0
			1769	1116	289	358	6		

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	1186	Total	C	N	O	S	0	0
			8922	5616	1560	1709	37		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	1159	Total	C	N	O	S	0	0
			8880	5589	1568	1681	42		

- Molecule 12 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	72	Total	C	N	O	S	0	0
			567	349	98	116	4		

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
13	D	1	Total	Mg	0
			1	1	

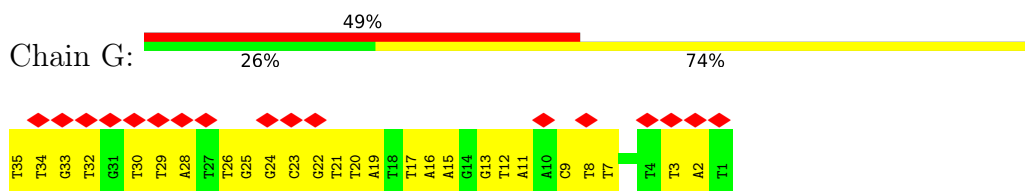
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
14	D	2	Total	Zn	0
			2	2	

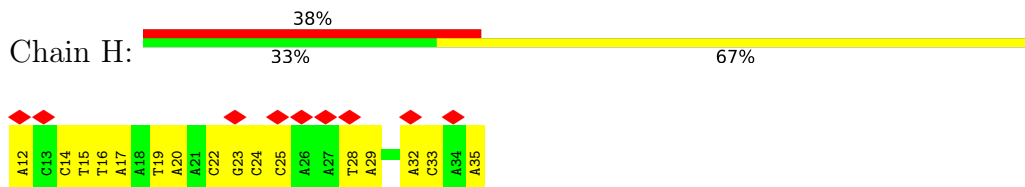
3 Residue-property plots [i](#)

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

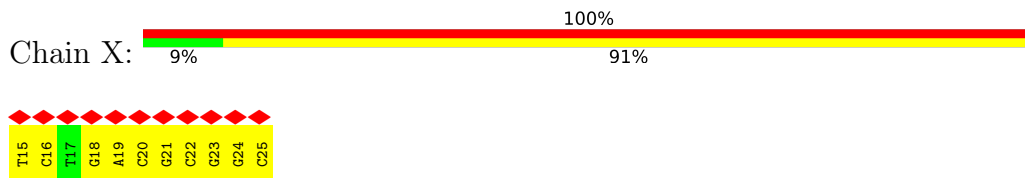
- Molecule 1: DNA NT-strand



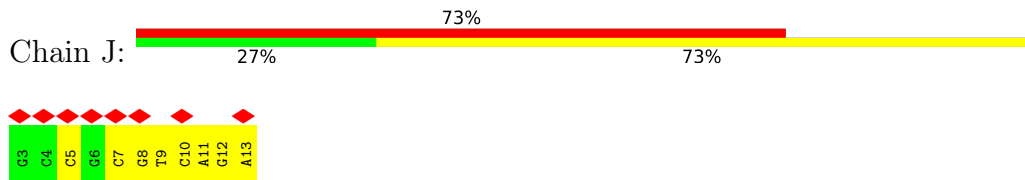
- Molecule 2: DNA T-strand



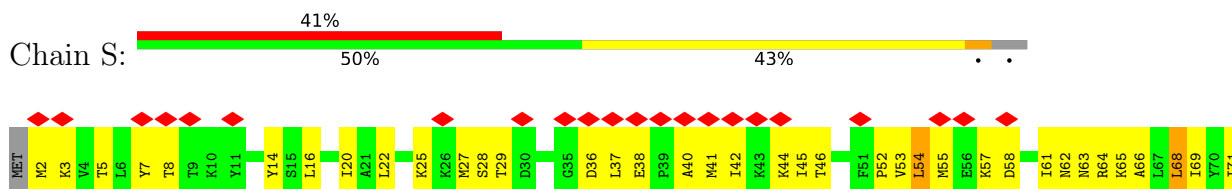
- Molecule 3: DNA NT-strand downstream

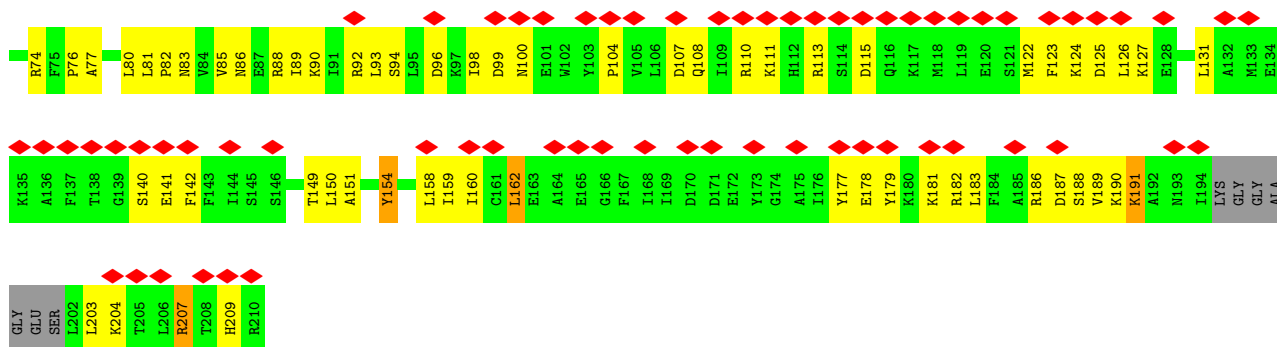


- Molecule 4: DNA T-strand downstream

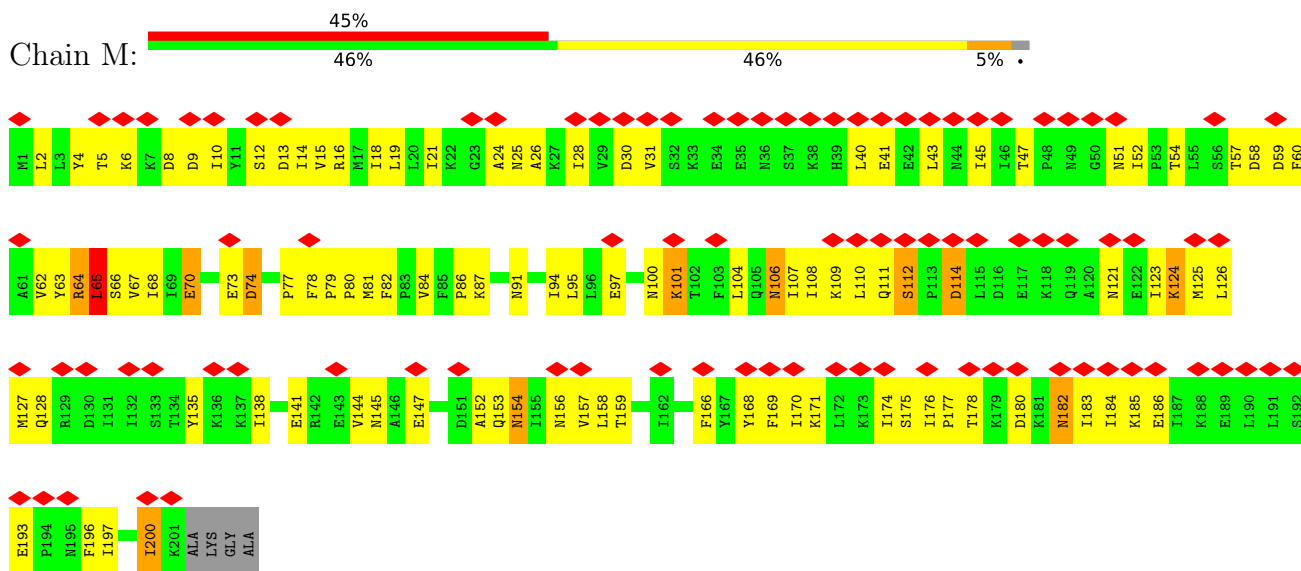


- Molecule 5: Stringent starvation protein A

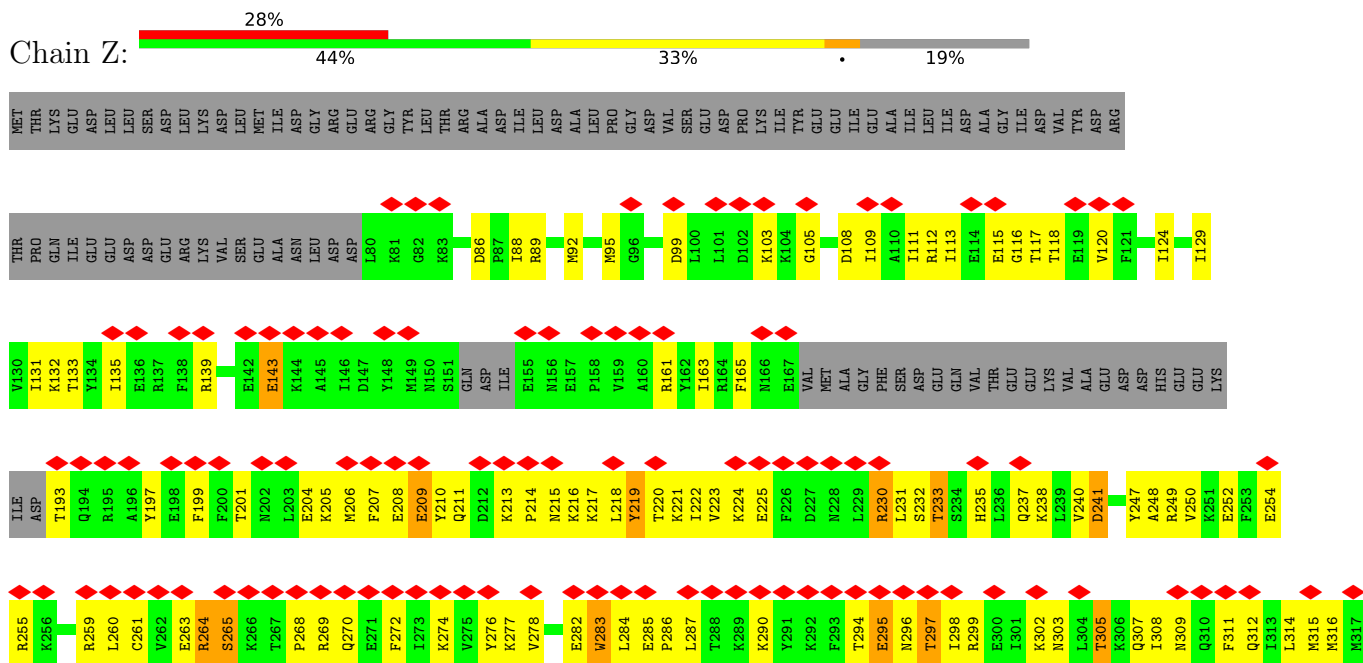


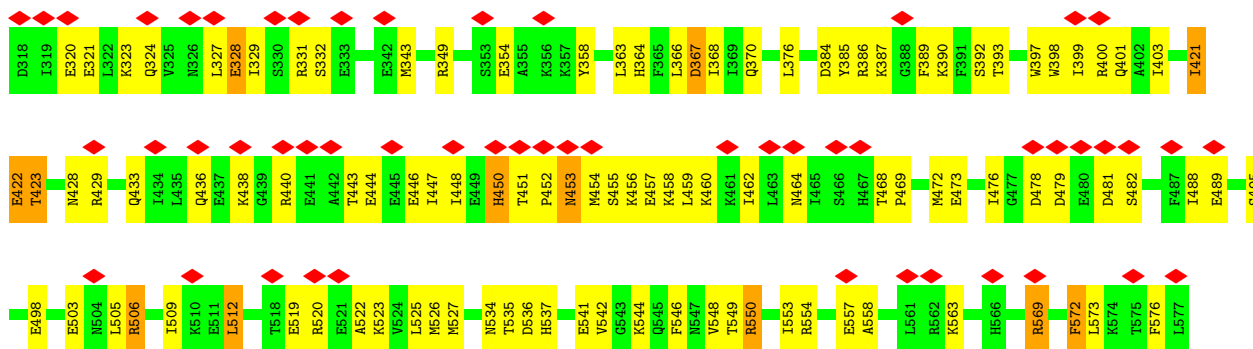


• Molecule 6: Macrophage growth locus, subunit A

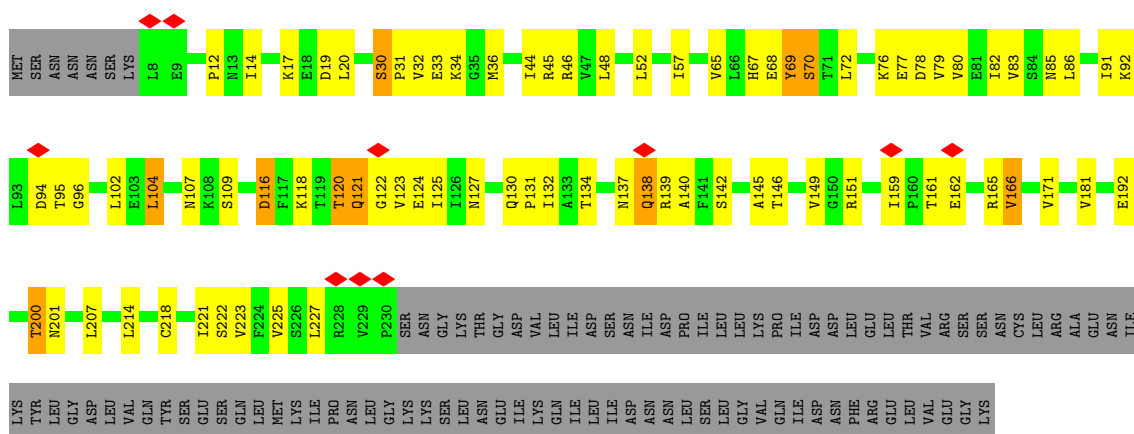


• Molecule 7: RNA polymerase sigma factor RpoD

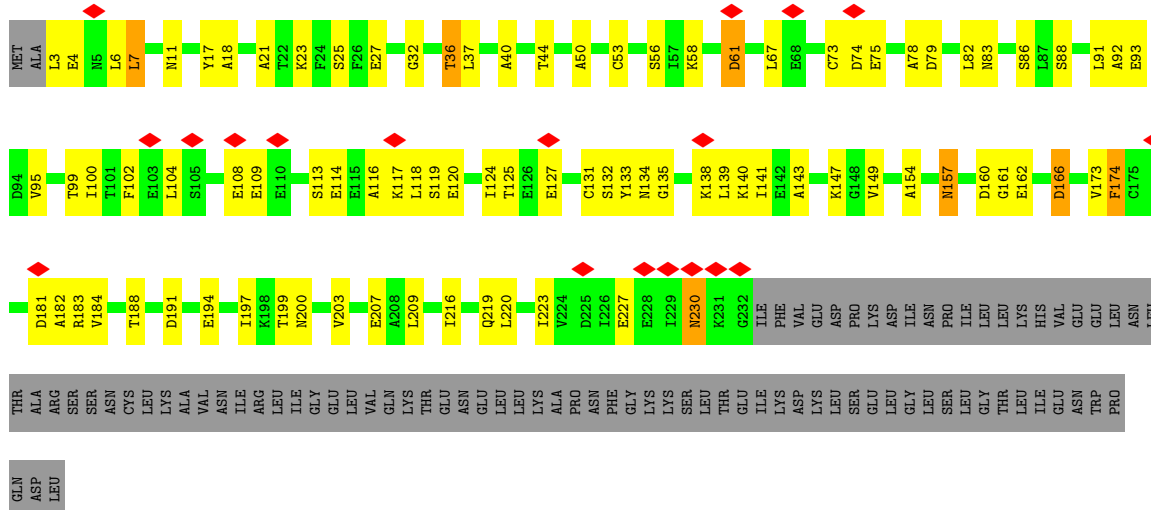
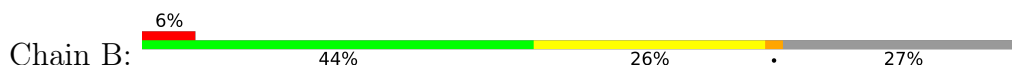




• Molecule 8: DNA-directed RNA polymerase subunit alpha 1

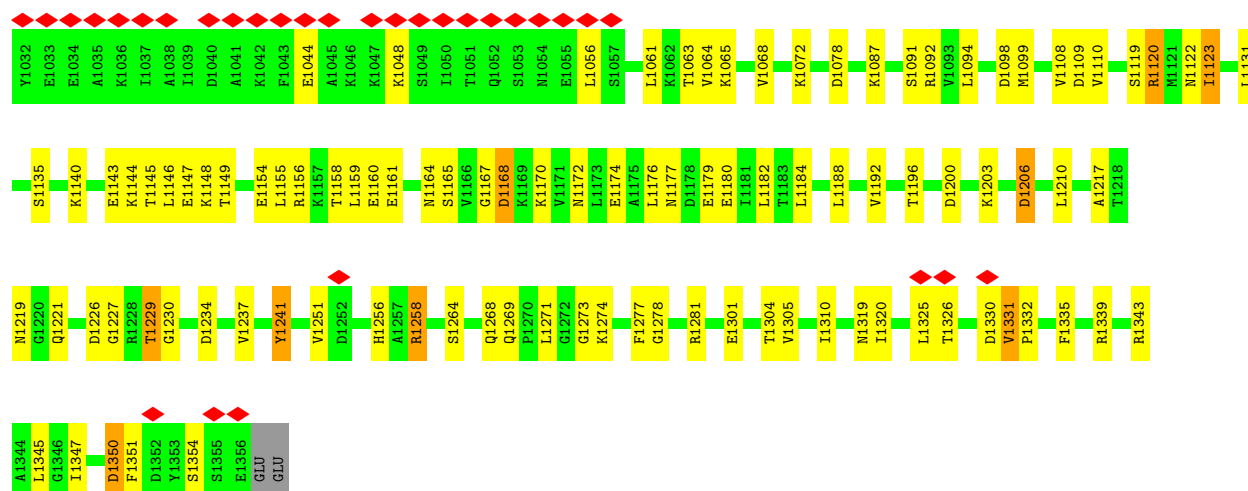


• Molecule 9: DNA-directed RNA polymerase subunit alpha 2

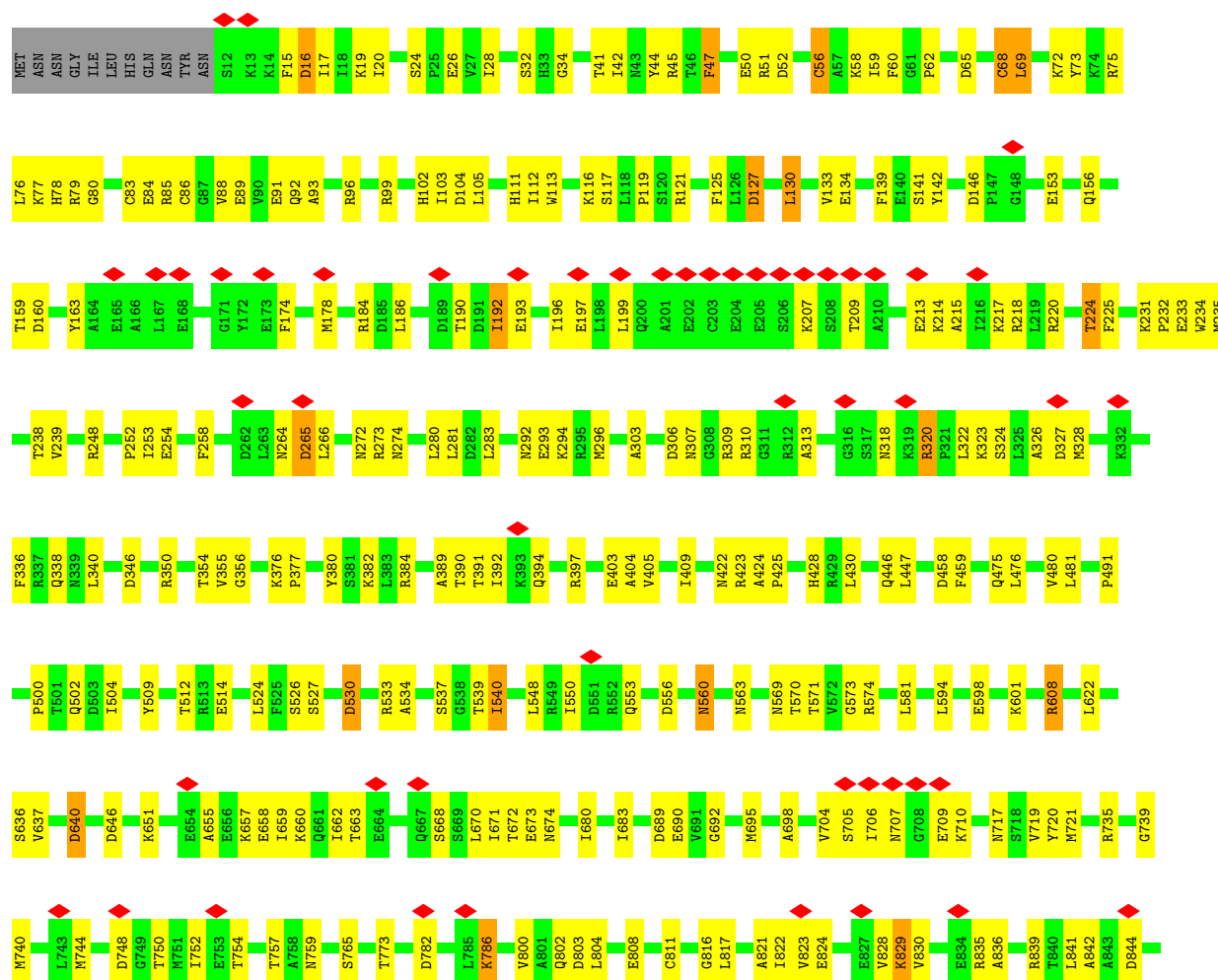


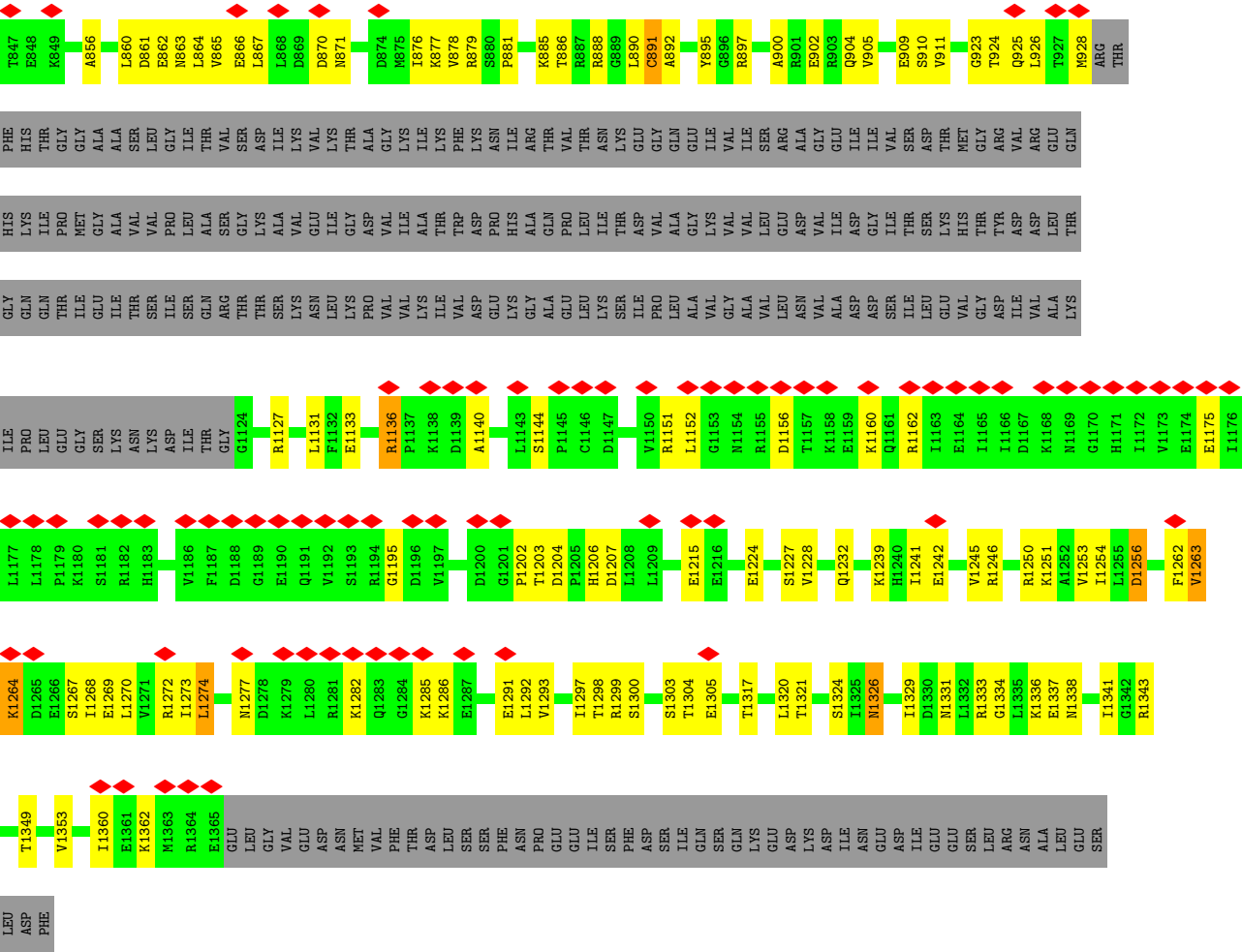
• Molecule 10: DNA-directed RNA polymerase subunit beta





• Molecule 11: DNA-directed RNA polymerase subunit beta'





• Molecule 12: DNA-directed RNA polymerase subunit omega



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21457	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	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	36.668	Depositor
Minimum map value	-21.358	Depositor
Average map value	0.006	Depositor
Map value standard deviation	1.641	Depositor
Recommended contour level	6.5	Depositor
Map size (\AA)	379.47998, 379.47998, 379.47998	wwPDB
Map dimensions	358, 358, 358	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	G	0.70	0/804	1.07	0/1241
2	H	0.72	0/547	0.89	0/839
3	X	0.66	0/251	0.96	0/385
4	J	0.65	0/253	0.81	0/388
5	S	0.34	0/1611	0.47	0/2173
6	M	0.34	0/1626	0.46	0/2208
7	Z	0.33	0/3825	0.47	0/5138
8	A	0.43	0/1708	0.53	0/2318
9	B	0.39	0/1789	0.49	0/2414
10	C	0.47	0/9064	0.51	0/12264
11	D	0.46	1/9000 (0.0%)	0.51	0/12149
12	E	0.35	0/568	0.49	0/760
All	All	0.45	1/31046 (0.0%)	0.55	0/42277

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
7	Z	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	47	PHE	C-N	-5.02	1.22	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	Z	213	LYS	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	G	720	0	403	26	0
2	H	487	0	269	15	0
3	X	225	0	124	13	0
4	J	226	0	123	9	0
5	S	1583	0	1600	79	0
6	M	1598	0	1650	78	0
7	Z	3772	0	3813	166	0
8	A	1688	0	1726	60	0
9	B	1769	0	1767	57	0
10	C	8922	0	8667	263	0
11	D	8880	0	8947	274	0
12	E	567	0	581	23	0
13	D	1	0	0	0	0
14	D	2	0	0	0	0
All	All	30440	0	29670	983	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (983) 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)
8:A:12:PRO:HA	8:A:31:PRO:HD2	1.52	0.92
6:M:81:MET:HB3	6:M:157:VAL:HB	1.55	0.87
10:C:447:ASP:O	10:C:453:ASN:ND2	2.14	0.80
7:Z:109:ILE:HA	7:Z:112:ARG:HD3	1.65	0.79
10:C:94:THR:HG22	10:C:144:ASN:H	1.47	0.78
5:S:179:TYR:HA	5:S:182:ARG:HB2	1.65	0.78
11:D:146:ASP:HB2	11:D:174:PHE:HA	1.66	0.78
11:D:273:ARG:HD3	11:D:296:MET:HB3	1.65	0.78
4:J:13:DA:N1	10:C:545:ARG:NH1	2.32	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:287:LEU:HA	7:Z:290:LYS:HB2	1.65	0.77
1:G:11:DA:H61	7:Z:384:ASP:H	1.32	0.76
7:Z:447:ILE:O	7:Z:451:THR:OG1	2.04	0.74
8:A:76:LYS:NZ	10:C:773:VAL:O	2.17	0.74
9:B:102:PHE:HB2	9:B:141:ILE:HB	1.70	0.74
11:D:318:ASN:O	11:D:320:ARG:NH1	2.20	0.74
7:Z:315:MET:HG3	7:Z:316:MET:HG2	1.68	0.73
9:B:58:LYS:HB2	9:B:162:GLU:HG2	1.67	0.73
10:C:1148:LYS:HG2	10:C:1149:THR:HG23	1.70	0.73
6:M:128:GLN:NE2	6:M:175:SER:OG	2.22	0.73
10:C:585:ASN:HD21	10:C:589:PHE:HB2	1.54	0.73
11:D:844:ASP:OD1	11:D:856:ALA:N	2.22	0.73
6:M:152:ALA:O	6:M:153:GLN:NE2	2.21	0.73
6:M:57:THR:HG23	6:M:59:ASP:H	1.53	0.72
11:D:184:ARG:NH1	11:D:233:GLU:O	2.23	0.72
10:C:519:ASP:O	10:C:525:SER:OG	2.08	0.72
12:E:14:GLU:HG2	12:E:15:THR:HG23	1.72	0.72
1:G:23:DC:H2'	1:G:22:DG:C8	2.24	0.72
7:Z:295:GLU:OE1	7:Z:299:ARG:NH2	2.23	0.71
2:H:12:DA:N6	7:Z:401:GLN:OE1	2.24	0.71
10:C:934:GLN:HB2	10:C:1065:LYS:HB2	1.73	0.71
11:D:608:ARG:NH1	11:D:862:GLU:OE1	2.23	0.71
7:Z:453:ASN:ND2	7:Z:455:SER:O	2.24	0.71
10:C:734:ARG:O	10:C:734:ARG:NH1	2.24	0.71
7:Z:294:THR:HB	7:Z:297:THR:HB	1.71	0.71
11:D:553:GLN:NE2	11:D:563:ASN:OD1	2.25	0.70
10:C:760:ARG:NH1	10:C:764:ASN:OD1	2.24	0.70
10:C:1161:GLU:O	10:C:1165:SER:OG	2.06	0.70
10:C:372:LEU:HD12	10:C:386:LEU:HD21	1.74	0.70
5:S:65:LYS:NZ	6:M:97:GLU:OE1	2.25	0.70
6:M:8:ASP:O	6:M:111:GLN:NE2	2.25	0.70
10:C:1167:GLY:O	10:C:1170:LYS:NZ	2.22	0.69
7:Z:250:VAL:HG23	7:Z:308:ILE:HD12	1.73	0.69
8:A:137:ASN:ND2	10:C:729:GLU:OE1	2.24	0.69
3:X:23:DG:H22	4:J:5:DC:H42	1.38	0.69
6:M:13:ASP:OD2	6:M:168:TYR:OH	2.11	0.68
11:D:83:CYS:SG	11:D:84:GLU:N	2.66	0.68
9:B:11:ASN:HB3	9:B:27:GLU:HB3	1.76	0.68
10:C:123:ARG:NH2	10:C:490:LEU:O	2.27	0.68
10:C:900:GLU:OE1	10:C:900:GLU:N	2.27	0.68
11:D:1250:ARG:NH2	11:D:1300:SER:O	2.27	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:80:PRO:O	6:M:154:ASN:ND2	2.27	0.68
7:Z:237:GLN:HA	7:Z:240:VAL:HG22	1.76	0.67
1:G:29:DT:H2''	1:G:28:DA:C8	2.29	0.67
10:C:1044:GLU:O	10:C:1048:LYS:N	2.27	0.67
7:Z:305:THR:O	7:Z:309:ASN:ND2	2.27	0.67
10:C:769:GLN:HA	10:C:788:GLY:HA2	1.76	0.67
5:S:3:LYS:O	5:S:57:LYS:NZ	2.22	0.67
9:B:154:ALA:H	9:B:166:ASP:HB3	1.58	0.67
9:B:100:ILE:HB	9:B:143:ALA:HB3	1.77	0.67
5:S:151:ALA:HA	5:S:154:TYR:HB2	1.77	0.67
7:Z:208:GLU:OE1	7:Z:211:GLN:NE2	2.27	0.67
8:A:36:MET:HE1	9:B:216:ILE:HG12	1.77	0.66
11:D:213:GLU:O	11:D:217:LYS:NZ	2.28	0.66
9:B:75:GLU:HB3	9:B:79:ASP:HB3	1.77	0.66
10:C:593:PRO:HB2	10:C:658:VAL:HG21	1.78	0.66
5:S:63:ASN:HD22	6:M:94:ILE:HD13	1.60	0.66
9:B:183:ARG:HB3	9:B:188:THR:HG22	1.77	0.66
11:D:527:SER:N	11:D:530:ASP:OD2	2.26	0.66
4:J:8:DG:H2'	4:J:9:DT:H71	1.76	0.66
11:D:864:LEU:HA	11:D:867:LEU:HD12	1.78	0.66
11:D:119:PRO:O	11:D:121:ARG:NH1	2.28	0.66
11:D:928:MET:O	11:D:1232:GLN:NE2	2.28	0.66
10:C:731:ASP:OD1	10:C:734:ARG:NH1	2.29	0.66
10:C:1354:SER:HB2	11:D:17:ILE:HD13	1.78	0.66
7:Z:299:ARG:HA	7:Z:302:LYS:HE3	1.78	0.66
8:A:19:ASP:OD1	8:A:20:LEU:N	2.29	0.66
11:D:403:GLU:OE1	11:D:405:VAL:N	2.23	0.66
5:S:25:LYS:NZ	5:S:77:ALA:O	2.30	0.65
7:Z:550:ARG:O	7:Z:550:ARG:NH1	2.26	0.65
10:C:1256:HIS:NE2	10:C:1278:GLY:HA3	2.11	0.65
11:D:1250:ARG:NH2	11:D:1300:SER:OG	2.28	0.65
10:C:699:GLU:OE2	10:C:801:ASN:ND2	2.19	0.65
12:E:15:THR:OG1	12:E:18:ASP:OD1	2.14	0.65
1:G:12:DT:O4	7:Z:401:GLN:NE2	2.29	0.65
9:B:3:LEU:N	9:B:4:GLU:OE2	2.30	0.65
5:S:186:ARG:HB2	5:S:189:VAL:HG22	1.79	0.65
11:D:141:SER:OG	11:D:142:TYR:N	2.30	0.65
5:S:104:PRO:HA	5:S:108:GLN:HG3	1.79	0.64
10:C:1226:ASP:OD1	10:C:1227:GLY:N	2.30	0.64
10:C:1268:GLN:HE21	10:C:1310:ILE:HD11	1.61	0.64
11:D:800:VAL:HG21	11:D:1297:ILE:HB	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:89:ARG:NH2	10:C:374:PRO:O	2.31	0.64
5:S:20:ILE:HD12	5:S:189:VAL:HA	1.79	0.64
10:C:1160:GLU:OE1	10:C:1164:ASN:ND2	2.30	0.64
11:D:1136:ARG:NH1	11:D:1136:ARG:O	2.31	0.64
5:S:92:ARG:NH1	6:M:70:GLU:OE1	2.30	0.64
8:A:65:VAL:HG12	8:A:72:LEU:HD21	1.80	0.64
10:C:843:ARG:N	10:C:850:GLU:OE2	2.18	0.64
11:D:822:ILE:HD11	11:D:835:ARG:HD2	1.80	0.64
12:E:2:ALA:O	12:E:3:ARG:NH1	2.30	0.64
8:A:78:ASP:OD2	8:A:79:VAL:N	2.31	0.63
11:D:116:LYS:O	11:D:309:ARG:NH2	2.30	0.63
10:C:719:ILE:HD12	10:C:786:ALA:HB3	1.79	0.63
7:Z:328:GLU:HA	7:Z:331:ARG:HD2	1.81	0.63
10:C:408:ASN:O	10:C:412:GLY:N	2.31	0.63
11:D:265:ASP:N	11:D:265:ASP:OD1	2.29	0.63
8:A:107:ASN:O	8:A:138:GLN:NE2	2.24	0.63
10:C:730:VAL:HG12	10:C:735:ILE:HG23	1.80	0.63
11:D:26:GLU:OE1	11:D:26:GLU:N	2.32	0.63
7:Z:230:ARG:HH22	7:Z:232:SER:HB3	1.64	0.63
11:D:220:ARG:O	11:D:224:THR:OG1	2.17	0.63
7:Z:460:LYS:O	7:Z:464:ASN:ND2	2.32	0.62
11:D:17:ILE:HB	11:D:1329:ILE:HD11	1.79	0.62
11:D:186:LEU:O	11:D:190:THR:OG1	2.15	0.62
5:S:37:LEU:HD22	5:S:45:ILE:HD11	1.80	0.62
5:S:83:ASN:HA	5:S:88:ARG:HH21	1.63	0.62
6:M:123:ILE:O	6:M:127:MET:HG2	1.99	0.62
5:S:58:ASP:N	5:S:58:ASP:OD1	2.30	0.62
11:D:384:ARG:NH1	11:D:392:ILE:HG12	2.15	0.62
8:A:44:ILE:O	8:A:48:LEU:HB2	1.98	0.62
11:D:125:PHE:O	11:D:218:ARG:NH2	2.32	0.62
11:D:822:ILE:HD11	11:D:835:ARG:HH11	1.65	0.62
10:C:50:SER:N	10:C:53:GLU:OE1	2.32	0.62
11:D:306:ASP:HB3	11:D:326:ALA:HB3	1.81	0.62
11:D:1140:ALA:HA	11:D:1202:PRO:HD2	1.82	0.62
10:C:901:GLU:O	10:C:905:ARG:HG2	1.99	0.62
6:M:41:GLU:O	6:M:45:ILE:HG12	2.00	0.62
11:D:105:LEU:HA	11:D:274:ASN:HD21	1.64	0.62
11:D:382:LYS:NZ	12:E:42:GLU:OE1	2.33	0.62
10:C:897:LEU:HD23	10:C:897:LEU:H	1.64	0.61
10:C:929:THR:OG1	10:C:930:VAL:N	2.32	0.61
10:C:1319:ASN:HD21	10:C:1326:THR:HB	1.64	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:74:VAL:HB	10:C:102:LYS:HB3	1.83	0.61
5:S:74:ARG:NH1	11:D:80:GLY:O	2.34	0.61
7:Z:489:GLU:OE1	7:Z:489:GLU:N	2.33	0.61
2:H:19:DT:H2''	2:H:20:DA:C8	2.35	0.61
11:D:514:GLU:OE2	11:D:574:ARG:NH2	2.34	0.61
1:G:13:DG:H2''	1:G:12:DT:H5''	1.82	0.61
11:D:1273:ILE:O	11:D:1277:ASN:ND2	2.33	0.61
5:S:57:LYS:H	5:S:57:LYS:HD2	1.66	0.61
8:A:46:ARG:NH1	9:B:32:GLY:O	2.33	0.61
11:D:1152:LEU:HD12	11:D:1160:LYS:HE2	1.81	0.61
1:G:33:DG:H2'	1:G:32:DT:C6	2.36	0.61
6:M:30:ASP:OD1	6:M:31:VAL:N	2.28	0.61
10:C:13:LYS:NZ	10:C:14:GLU:O	2.33	0.61
5:S:66:ALA:HA	5:S:69:ILE:HD13	1.82	0.60
10:C:1177:ASN:ND2	10:C:1179:GLU:OE1	2.34	0.60
11:D:895:TYR:CD2	11:D:905:VAL:HG21	2.36	0.60
7:Z:456:LYS:O	7:Z:460:LYS:NZ	2.26	0.60
8:A:109:SER:O	8:A:109:SER:OG	2.17	0.60
10:C:178:PRO:HB3	10:C:397:TYR:CZ	2.36	0.60
10:C:698:SER:HB2	10:C:792:ASP:HB2	1.83	0.60
7:Z:443:THR:O	7:Z:446:GLU:N	2.33	0.60
7:Z:451:THR:HG22	7:Z:453:ASN:H	1.67	0.60
10:C:65:LYS:HE2	10:C:66:ASN:HD21	1.66	0.60
10:C:621:GLN:HE22	11:D:765:SER:HB2	1.66	0.60
5:S:86:ASN:HA	5:S:89:ILE:HD12	1.83	0.60
8:A:139:ARG:NH2	8:A:140:ALA:O	2.35	0.60
3:X:18:DG:H2''	3:X:19:DA:C8	2.36	0.60
7:Z:163:ILE:O	7:Z:235:HIS:ND1	2.35	0.60
10:C:851:GLU:HG3	10:C:853:THR:H	1.67	0.60
5:S:123:PHE:HD1	5:S:126:LEU:HD12	1.67	0.59
10:C:585:ASN:OD1	10:C:589:PHE:N	2.29	0.59
11:D:280:LEU:HD12	11:D:293:GLU:HG3	1.84	0.59
2:H:12:DA:H3'	7:Z:429:ARG:HH12	1.67	0.59
6:M:13:ASP:OD1	6:M:16:ARG:NH2	2.35	0.59
10:C:205:CYS:SG	10:C:207:THR:OG1	2.46	0.59
10:C:399:LEU:HB3	10:C:403:GLY:HA3	1.84	0.59
11:D:1133:GLU:OE2	11:D:1297:ILE:N	2.35	0.59
11:D:1256:ASP:OD1	11:D:1286:LYS:NZ	2.31	0.59
10:C:1156:ARG:NH1	10:C:1176:LEU:O	2.36	0.59
6:M:77:PRO:HG3	7:Z:541:GLU:HG3	1.83	0.59
7:Z:563:LYS:O	7:Z:569:ARG:NH2	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:227:GLU:O	9:B:230:ASN:ND2	2.35	0.59
11:D:695:MET:HA	11:D:698:ALA:HB3	1.85	0.59
8:A:77:GLU:OE1	8:A:134:THR:N	2.34	0.59
10:C:585:ASN:ND2	10:C:589:PHE:HB2	2.17	0.59
11:D:895:TYR:HD2	11:D:905:VAL:HG21	1.67	0.59
9:B:40:ALA:O	9:B:44:THR:HG22	2.03	0.58
1:G:11:DA:N6	7:Z:384:ASP:OD1	2.35	0.58
2:H:16:DT:H2''	2:H:17:DA:C8	2.38	0.58
9:B:83:ASN:O	9:B:86:SER:OG	2.21	0.58
10:C:1156:ARG:HH22	10:C:1174:GLU:HA	1.68	0.58
11:D:509:TYR:HE2	11:D:721:MET:HG2	1.68	0.58
8:A:92:LYS:HB3	8:A:124:GLU:HB3	1.86	0.58
11:D:76:LEU:HD23	11:D:79:ARG:HH21	1.67	0.58
11:D:534:ALA:HB1	11:D:540:ILE:HD11	1.86	0.58
11:D:69:LEU:HB2	11:D:88:VAL:HG21	1.85	0.58
5:S:3:LYS:HG2	5:S:57:LYS:HE3	1.84	0.58
8:A:120:THR:OG1	8:A:121:GLN:NE2	2.37	0.58
11:D:306:ASP:OD1	11:D:306:ASP:N	2.34	0.58
12:E:14:GLU:N	12:E:14:GLU:OE1	2.37	0.58
11:D:892:ALA:O	11:D:904:GLN:NE2	2.36	0.58
5:S:179:TYR:HB3	5:S:182:ARG:HH21	1.69	0.58
7:Z:294:THR:O	7:Z:298:ILE:N	2.36	0.58
9:B:50:ALA:HA	9:B:149:VAL:HG12	1.85	0.58
11:D:51:ARG:HE	11:D:58:LYS:HZ1	1.51	0.58
5:S:53:VAL:HG23	5:S:54:LEU:H	1.69	0.58
7:Z:354:GLU:OE2	7:Z:400:ARG:NH2	2.32	0.58
7:Z:458:LYS:O	7:Z:462:ILE:N	2.33	0.58
10:C:49:HIS:ND1	10:C:53:GLU:OE2	2.37	0.58
7:Z:284:LEU:O	7:Z:287:LEU:HB2	2.04	0.57
8:A:46:ARG:HE	9:B:36:THR:HG22	1.68	0.57
11:D:1204:ASP:OD2	11:D:1207:ASP:N	2.37	0.57
6:M:109:LYS:O	6:M:112:SER:OG	2.16	0.57
10:C:404:ARG:NH2	10:C:422:THR:O	2.36	0.57
11:D:1291:GLU:OE1	11:D:1292:LEU:N	2.37	0.57
7:Z:376:LEU:HB2	7:Z:399:ILE:HD11	1.86	0.57
10:C:1330:ASP:OD1	10:C:1331:VAL:N	2.36	0.57
5:S:107:ASP:OD1	5:S:110:ARG:NH2	2.38	0.57
7:Z:217:LYS:O	7:Z:220:THR:OG1	2.14	0.57
9:B:82:LEU:HD21	11:D:524:LEU:HG	1.86	0.57
11:D:428:HIS:CE1	11:D:430:LEU:HB2	2.40	0.57
6:M:114:ASP:OD1	6:M:114:ASP:N	2.31	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:199:LEU:HD11	11:D:215:ALA:HB1	1.87	0.57
5:S:187:ASP:OD1	5:S:188:SER:N	2.37	0.57
10:C:210:LEU:HA	10:C:213:LEU:HD12	1.87	0.57
7:Z:422:GLU:OE1	7:Z:423:THR:N	2.38	0.56
11:D:16:ASP:N	11:D:16:ASP:OD1	2.37	0.56
11:D:816:GLY:H	11:D:877:LYS:HE2	1.69	0.56
9:B:7:LEU:HD23	9:B:7:LEU:H	1.70	0.56
5:S:76:PRO:HG2	11:D:73:TYR:HE1	1.69	0.56
5:S:140:SER:O	5:S:182:ARG:NH2	2.38	0.56
7:Z:469:PRO:HB3	11:D:258:PHE:HB2	1.87	0.56
8:A:67:HIS:O	8:A:70:SER:OG	2.20	0.56
10:C:586:ASP:N	10:C:586:ASP:OD1	2.38	0.56
10:C:389:GLY:HA2	10:C:393:ILE:HG13	1.87	0.56
10:C:610:SER:OG	10:C:611:ALA:N	2.38	0.56
10:C:648:THR:HG21	10:C:652:ARG:HH21	1.70	0.56
11:D:491:PRO:HA	11:D:900:ALA:HB2	1.88	0.56
7:Z:197:TYR:O	7:Z:201:THR:HG23	2.05	0.56
7:Z:459:LEU:HA	7:Z:462:ILE:HG22	1.88	0.56
10:C:80:GLU:OE1	10:C:81:PRO:HD2	2.05	0.56
11:D:139:PHE:HZ	11:D:294:LYS:HE3	1.70	0.56
10:C:52:LEU:HD11	10:C:99:LEU:HD11	1.88	0.56
10:C:1325:LEU:O	10:C:1326:THR:OG1	2.23	0.56
1:G:12:DT:H73	7:Z:397:TRP:HB3	1.87	0.56
3:X:18:DG:H2"	3:X:19:DA:H8	1.71	0.56
5:S:159:ILE:HG22	5:S:160:ILE:HD13	1.88	0.56
10:C:787:ASP:OD2	10:C:793:PHE:N	2.39	0.56
10:C:1229:THR:OG1	10:C:1230:GLY:N	2.39	0.56
11:D:1334:GLY:O	11:D:1338:ASN:ND2	2.38	0.56
10:C:675:GLU:OE1	10:C:675:GLU:N	2.19	0.55
10:C:713:ARG:NH2	10:C:782:GLY:O	2.32	0.55
11:D:51:ARG:HH21	11:D:58:LYS:HZ3	1.54	0.55
7:Z:367:ASP:OD1	7:Z:367:ASP:N	2.39	0.55
10:C:519:ASP:N	10:C:519:ASP:OD2	2.37	0.55
11:D:571:THR:HG22	11:D:573:GLY:H	1.71	0.55
9:B:160:ASP:OD1	9:B:160:ASP:N	2.34	0.55
10:C:439:ARG:O	10:C:439:ARG:NH2	2.40	0.55
9:B:173:VAL:HG13	11:D:533:ARG:NH1	2.22	0.55
10:C:62:VAL:HG23	10:C:71:LEU:HD13	1.88	0.55
10:C:1258:ARG:NE	11:D:346:ASP:OD1	2.34	0.55
7:Z:509:ILE:HA	7:Z:512:LEU:HB3	1.87	0.55
9:B:166:ASP:OD1	9:B:166:ASP:N	2.35	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:389:ALA:HB1	11:D:394:GLN:HB3	1.87	0.55
11:D:1144:SER:O	11:D:1195:GLY:N	2.39	0.55
6:M:31:VAL:HG13	6:M:40:LEU:HD13	1.89	0.55
10:C:552:ASP:OD1	10:C:553:VAL:N	2.40	0.55
10:C:576:ASN:N	10:C:576:ASN:OD1	2.38	0.55
9:B:109:GLU:H	9:B:133:TYR:HB3	1.72	0.54
8:A:78:ASP:OD2	8:A:80:VAL:N	2.35	0.54
10:C:358:THR:HG23	10:C:363:GLU:HB3	1.88	0.54
11:D:817:LEU:O	11:D:877:LYS:HA	2.07	0.54
12:E:43:LYS:HB2	12:E:44:LYS:HZ2	1.73	0.54
9:B:181:ASP:OD1	9:B:182:ALA:N	2.38	0.54
10:C:596:LYS:HG2	10:C:655:TYR:CE1	2.42	0.54
1:G:9:DC:H5''	7:Z:390:LYS:HB2	1.89	0.54
5:S:122:MET:O	5:S:126:LEU:HG	2.08	0.54
6:M:110:LEU:HD21	6:M:123:ILE:HD12	1.89	0.54
7:Z:129:ILE:HG23	7:Z:132:LYS:HD3	1.90	0.54
8:A:130:GLN:NE2	8:A:131:PRO:O	2.33	0.54
10:C:34:SER:O	10:C:34:SER:OG	2.22	0.54
10:C:1219:ASN:HB3	10:C:1221:GLN:H	1.72	0.54
11:D:658:GLU:O	11:D:662:ILE:HG12	2.07	0.54
5:S:22:LEU:HD21	5:S:71:ILE:HD12	1.88	0.54
7:Z:109:ILE:O	7:Z:113:ILE:HG23	2.08	0.54
7:Z:537:HIS:H	7:Z:537:HIS:CD2	2.25	0.54
8:A:102:LEU:HD21	8:A:123:VAL:HG11	1.90	0.54
8:A:214:LEU:HD12	9:B:220:LEU:HD21	1.90	0.54
11:D:88:VAL:HG12	11:D:89:GLU:O	2.07	0.54
5:S:179:TYR:O	5:S:183:LEU:N	2.41	0.54
6:M:106:ASN:OD1	6:M:106:ASN:N	2.40	0.54
7:Z:86:ASP:OD1	7:Z:86:ASP:N	2.39	0.54
10:C:1177:ASN:OD1	10:C:1180:GLU:N	2.27	0.54
11:D:338:GLN:O	11:D:338:GLN:NE2	2.41	0.54
11:D:526:SER:OG	11:D:530:ASP:OD2	2.20	0.54
7:Z:131:ILE:HD12	7:Z:131:ILE:H	1.73	0.54
7:Z:328:GLU:OE1	7:Z:331:ARG:NH1	2.41	0.54
10:C:507:GLU:OE1	10:C:511:SER:OG	2.26	0.54
11:D:659:ILE:HD12	11:D:680:ILE:HG12	1.90	0.54
2:H:15:DT:H2''	2:H:16:DT:H5''	1.89	0.54
7:Z:105:GLY:O	7:Z:109:ILE:HG12	2.08	0.54
10:C:856:ILE:HD12	10:C:857:PRO:HD2	1.88	0.54
11:D:252:PRO:HB3	11:D:258:PHE:CE2	2.43	0.54
1:G:7:DT:O2	7:Z:349:ARG:HB2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:813:ASN:HA	10:C:817:SER:HB2	1.90	0.54
11:D:1207:ASP:N	11:D:1207:ASP:OD1	2.41	0.54
10:C:108:TYR:CB	10:C:118:ILE:H	2.21	0.53
10:C:379:ALA:HB3	10:C:382:SER:HB3	1.89	0.53
11:D:740:MET:HE3	11:D:757:THR:HA	1.91	0.53
7:Z:320:GLU:O	7:Z:324:GLN:NE2	2.42	0.53
10:C:173:SER:OG	10:C:174:ALA:N	2.42	0.53
11:D:42:ILE:N	11:D:50:GLU:OE1	2.41	0.53
11:D:52:ASP:OD1	11:D:52:ASP:N	2.38	0.53
5:S:37:LEU:HB2	5:S:42:ILE:HG12	1.90	0.53
5:S:158:LEU:O	5:S:162:LEU:HB2	2.08	0.53
6:M:6:LYS:HB2	6:M:52:ILE:HG21	1.91	0.53
7:Z:312:GLN:O	7:Z:316:MET:N	2.40	0.53
9:B:32:GLY:N	9:B:191:ASP:OD2	2.41	0.53
5:S:177:TYR:CZ	5:S:181:LYS:HG3	2.44	0.53
7:Z:450:HIS:O	7:Z:450:HIS:ND1	2.36	0.53
8:A:138:GLN:OE1	8:A:139:ARG:N	2.41	0.53
5:S:36:ASP:HB2	7:Z:259:ARG:HH22	1.74	0.53
10:C:1350:ASP:OD1	10:C:1350:ASP:N	2.40	0.53
11:D:1304:THR:OG1	11:D:1305:GLU:N	2.41	0.53
7:Z:287:LEU:HD22	7:Z:290:LYS:HE3	1.90	0.53
7:Z:323:LYS:O	7:Z:327:LEU:HG	2.08	0.53
3:X:23:DG:H1	4:J:5:DC:H42	1.57	0.53
10:C:632:PHE:HE2	10:C:653:VAL:HG21	1.74	0.53
10:C:79:GLY:HA3	10:C:98:PRO:HG2	1.89	0.52
10:C:148:ARG:NH1	10:C:515:SER:O	2.43	0.52
11:D:193:GLU:OE2	11:D:193:GLU:N	2.32	0.52
5:S:2:MET:N	5:S:57:LYS:HZ3	2.07	0.52
6:M:73:GLU:OE1	6:M:81:MET:N	2.39	0.52
11:D:306:ASP:HA	11:D:324:SER:OG	2.09	0.52
11:D:659:ILE:O	11:D:663:THR:HG23	2.09	0.52
5:S:177:TYR:OH	5:S:181:LYS:NZ	2.33	0.52
7:Z:263:GLU:O	7:Z:264:ARG:NH1	2.40	0.52
10:C:635:ASP:OD1	10:C:636:ILE:N	2.42	0.52
10:C:1172:ASN:HD21	10:C:1174:GLU:HG2	1.74	0.52
11:D:193:GLU:HA	11:D:196:ILE:HD12	1.91	0.52
1:G:30:DT:H2'	1:G:29:DT:C6	2.45	0.52
8:A:159:ILE:HG22	8:A:161:THR:H	1.74	0.52
8:A:200:THR:OG1	8:A:201:ASN:N	2.42	0.52
10:C:136:THR:OG1	10:C:137:THR:N	2.42	0.52
10:C:425:ASN:OD1	10:C:426:SER:N	2.41	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:253:ILE:HG12	11:D:254:GLU:H	1.73	0.52
11:D:1224:GLU:O	11:D:1227:SER:OG	2.19	0.52
6:M:182:ASN:O	6:M:186:GLU:HG3	2.09	0.52
7:Z:453:ASN:ND2	7:Z:455:SER:H	2.07	0.52
10:C:695:THR:OG1	10:C:696:LEU:N	2.43	0.52
11:D:72:LYS:HD2	11:D:85:ARG:CZ	2.39	0.52
11:D:103:ILE:O	11:D:239:VAL:HG23	2.10	0.52
11:D:403:GLU:OE1	11:D:404:ALA:N	2.43	0.52
7:Z:364:HIS:CD2	7:Z:364:HIS:H	2.27	0.52
10:C:351:ASP:OD1	10:C:351:ASP:N	2.42	0.52
10:C:597:VAL:HG12	10:C:602:VAL:HA	1.90	0.52
11:D:640:ASP:OD1	11:D:640:ASP:N	2.43	0.52
7:Z:572:PHE:HD2	7:Z:573:LEU:HD12	1.75	0.52
10:C:27:LEU:O	10:C:531:ARG:NH1	2.42	0.52
10:C:160:ALA:HA	10:C:175:ARG:O	2.09	0.52
10:C:408:ASN:ND2	10:C:418:LYS:HG2	2.25	0.52
10:C:621:GLN:HA	10:C:657:ASP:OD1	2.09	0.52
10:C:135:MET:HG2	10:C:136:THR:O	2.09	0.52
10:C:627:ASP:O	10:C:629:ASN:N	2.43	0.52
8:A:227:LEU:HD21	9:B:209:LEU:HD22	1.91	0.52
10:C:10:ARG:NH2	10:C:700:LYS:HG2	2.25	0.52
11:D:112:ILE:HD11	11:D:309:ARG:HB2	1.92	0.52
7:Z:209:GLU:O	7:Z:214:PRO:HD3	2.11	0.51
10:C:121:ASP:HA	10:C:123:ARG:HH12	1.75	0.51
11:D:111:HIS:HD2	11:D:113:TRP:H	1.58	0.51
11:D:116:LYS:HE2	11:D:310:ARG:HB3	1.92	0.51
11:D:475:GLN:HE21	12:E:48:THR:HG21	1.75	0.51
11:D:636:SER:OG	11:D:637:VAL:N	2.42	0.51
7:Z:129:ILE:O	7:Z:133:THR:HG23	2.10	0.51
7:Z:448:ILE:HG21	7:Z:456:LYS:HG2	1.92	0.51
10:C:1351:PHE:HB3	11:D:15:PHE:CG	2.46	0.51
5:S:68:LEU:HD12	5:S:150:LEU:HD21	1.92	0.51
5:S:88:ARG:O	5:S:92:ARG:HG3	2.11	0.51
6:M:9:ASP:OD2	6:M:12:SER:N	2.34	0.51
7:Z:103:LYS:HB2	7:Z:390:LYS:HE3	1.92	0.51
8:A:45:ARG:HA	8:A:181:VAL:HG11	1.91	0.51
10:C:70:GLU:H	10:C:105:LEU:HD12	1.76	0.51
10:C:613:ASP:N	10:C:613:ASP:OD1	2.43	0.51
10:C:1320:ILE:HG21	11:D:377:PRO:HB2	1.91	0.51
11:D:56:CYS:SG	11:D:58:LYS:HB3	2.51	0.51
3:X:23:DG:H1	4:J:5:DC:N4	2.08	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:64:ARG:O	6:M:66:SER:N	2.44	0.51
6:M:95:LEU:HD21	6:M:138:ILE:HG12	1.92	0.51
10:C:155:HIS:ND1	10:C:156:ARG:O	2.42	0.51
11:D:717:ASN:OD1	11:D:720:TYR:N	2.34	0.51
11:D:651:LYS:NZ	11:D:690:GLU:OE1	2.29	0.51
11:D:836:ALA:O	11:D:860:LEU:HD12	2.09	0.51
10:C:1264:SER:N	10:C:1269:GLN:O	2.42	0.51
11:D:1268:ILE:O	11:D:1272:ARG:HB2	2.11	0.51
10:C:63:GLU:HG3	10:C:69:TYR:O	2.11	0.51
11:D:910:SER:O	11:D:910:SER:OG	2.25	0.51
5:S:178:GLU:O	5:S:182:ARG:NE	2.44	0.51
11:D:130:LEU:O	11:D:133:VAL:N	2.44	0.51
11:D:888:ARG:HH12	11:D:1333:ARG:HH11	1.58	0.51
6:M:86:PRO:HD2	11:D:80:GLY:HA3	1.93	0.50
8:A:116:ASP:OD1	8:A:116:ASP:N	2.41	0.50
10:C:102:LYS:HD2	10:C:126:TYR:CZ	2.46	0.50
6:M:84:VAL:HG13	7:Z:534:ASN:HB3	1.92	0.50
7:Z:261:CYS:O	7:Z:265:SER:OG	2.22	0.50
7:Z:457:GLU:HA	7:Z:460:LYS:HD2	1.94	0.50
10:C:860:SER:OG	10:C:862:SER:OG	2.21	0.50
1:G:16:DA:H1'	1:G:15:DA:H5'	1.93	0.50
5:S:41:MET:O	5:S:45:ILE:HG13	2.11	0.50
7:Z:88:ILE:HD12	7:Z:88:ILE:H	1.76	0.50
11:D:422:ASN:OD1	11:D:423:ARG:N	2.45	0.50
11:D:34:GLY:HA3	11:D:59:ILE:HG23	1.93	0.50
7:Z:495:SER:N	7:Z:498:GLU:OE1	2.39	0.50
11:D:841:LEU:HD21	11:D:876:ILE:HD12	1.93	0.50
6:M:100:ASN:HA	6:M:104:LEU:HG	1.94	0.50
7:Z:111:ILE:HG22	7:Z:385:TYR:CZ	2.47	0.50
7:Z:161:ARG:NH1	7:Z:193:THR:OG1	2.38	0.50
10:C:16:GLY:HA2	10:C:1200:ASP:O	2.12	0.50
10:C:51:GLY:O	10:C:55:VAL:HG23	2.12	0.50
11:D:217:LYS:H	11:D:217:LYS:HD2	1.76	0.50
7:Z:366:LEU:HB3	11:D:296:MET:SD	2.52	0.50
10:C:659:SER:OG	10:C:660:ALA:N	2.43	0.50
6:M:5:THR:O	6:M:31:VAL:HG23	2.12	0.50
10:C:404:ARG:NH2	10:C:420:ILE:O	2.41	0.50
11:D:32:SER:OG	11:D:34:GLY:O	2.30	0.50
6:M:128:GLN:HB3	6:M:177:PRO:HG3	1.94	0.49
7:Z:208:GLU:HA	7:Z:211:GLN:NE2	2.27	0.49
10:C:153:GLN:NE2	10:C:536:LEU:O	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:197:ARG:HD3	10:C:203:LYS:HG2	1.92	0.49
11:D:458:ASP:N	11:D:458:ASP:OD1	2.45	0.49
12:E:18:ASP:OD1	12:E:18:ASP:N	2.45	0.49
6:M:10:ILE:HD11	6:M:104:LEU:HB3	1.94	0.49
7:Z:557:GLU:HG3	7:Z:558:ALA:N	2.25	0.49
11:D:266:LEU:HD21	11:D:322:LEU:HD12	1.95	0.49
12:E:43:LYS:HB2	12:E:44:LYS:NZ	2.27	0.49
7:Z:503:GLU:OE1	7:Z:503:GLU:N	2.44	0.49
11:D:509:TYR:CE2	11:D:721:MET:HG2	2.47	0.49
11:D:706:ILE:HG12	11:D:707:ASN:H	1.76	0.49
12:E:62:SER:HA	12:E:65:ILE:HG13	1.94	0.49
1:G:20:DT:H2''	1:G:19:DA:N7	2.27	0.49
1:G:8:DT:H3'	1:G:7:DT:H73	1.95	0.49
3:X:15:DT:H1'	3:X:16:DC:H5'	1.95	0.49
5:S:127:LYS:O	5:S:131:LEU:HG	2.12	0.49
10:C:187:GLU:N	10:C:187:GLU:OE1	2.45	0.49
10:C:1140:LYS:O	10:C:1144:LYS:HG2	2.12	0.49
7:Z:448:ILE:HD13	7:Z:456:LYS:HG2	1.94	0.49
9:B:25:SER:HB2	9:B:194:GLU:HG2	1.93	0.49
10:C:432:ILE:O	10:C:436:ILE:HG12	2.12	0.49
10:C:478:ILE:HD11	10:C:496:VAL:HA	1.95	0.49
10:C:756:THR:O	10:C:756:THR:OG1	2.25	0.49
10:C:768:ASN:OD1	10:C:768:ASN:N	2.45	0.49
10:C:840:CYS:HB2	10:C:920:LEU:HD22	1.95	0.49
5:S:179:TYR:HA	5:S:182:ARG:HE	1.78	0.49
9:B:18:ALA:HB3	9:B:21:ALA:HB3	1.95	0.49
2:H:22:DC:H2''	2:H:23:DG:C8	2.47	0.49
2:H:33:DC:OP2	7:Z:554:ARG:NH2	2.46	0.49
10:C:4:SER:OG	10:C:5:TYR:N	2.46	0.49
3:X:20:DC:H2''	3:X:21:DG:H5''	1.94	0.49
9:B:104:LEU:HD21	9:B:139:LEU:HB3	1.95	0.49
10:C:694:PRO:HB3	10:C:790:ALA:HB2	1.95	0.49
1:G:30:DT:H2''	1:G:29:DT:H5'	1.95	0.49
7:Z:260:LEU:HD12	7:Z:297:THR:HG23	1.95	0.49
8:A:44:ILE:HG12	8:A:214:LEU:HD21	1.95	0.49
9:B:58:LYS:HD3	9:B:61:ASP:HA	1.95	0.49
9:B:119:SER:OG	9:B:120:GLU:N	2.46	0.49
10:C:186:PHE:CE2	10:C:428:ILE:HD11	2.48	0.49
10:C:937:GLU:HG3	10:C:938:ASN:H	1.76	0.49
11:D:307:ASN:ND2	11:D:313:ALA:HB1	2.28	0.49
11:D:1274:LEU:HA	11:D:1277:ASN:OD1	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:53:VAL:O	5:S:54:LEU:HB2	2.13	0.48
10:C:4:SER:O	10:C:8:LYS:HE3	2.13	0.48
11:D:657:LYS:NZ	11:D:660:LYS:HD2	2.27	0.48
11:D:888:ARG:HH22	11:D:1333:ARG:CZ	2.26	0.48
9:B:74:ASP:OD2	9:B:132:SER:OG	2.23	0.48
10:C:166:ASP:OD1	10:C:166:ASP:N	2.40	0.48
11:D:127:ASP:OD1	11:D:218:ARG:NH1	2.46	0.48
7:Z:249:ARG:HA	7:Z:252:GLU:CD	2.34	0.48
11:D:68:CYS:HB2	11:D:88:VAL:HB	1.94	0.48
11:D:861:ASP:O	11:D:865:VAL:HG23	2.14	0.48
5:S:27:MET:HG2	5:S:28:SER:H	1.77	0.48
8:A:201:ASN:N	8:A:201:ASN:OD1	2.45	0.48
10:C:178:PRO:HD3	10:C:183:TRP:HB3	1.95	0.48
10:C:715:SER:OG	10:C:717:ASN:ND2	2.46	0.48
10:C:821:SER:O	10:C:823:ARG:N	2.47	0.48
11:D:1326:ASN:N	11:D:1326:ASN:OD1	2.46	0.48
10:C:1325:LEU:HD21	12:E:32:LYS:HG3	1.95	0.48
11:D:355:VAL:HG13	11:D:356:GLY:H	1.79	0.48
5:S:100:ASN:ND2	6:M:64:ARG:HE	2.12	0.48
11:D:480:VAL:HG11	12:E:19:LEU:HD23	1.96	0.48
7:Z:248:ALA:O	7:Z:252:GLU:HG3	2.13	0.48
11:D:1241:ILE:O	11:D:1245:VAL:HG23	2.13	0.48
3:X:24:DG:H2''	3:X:25:DC:H5'	1.95	0.48
10:C:1274:LYS:O	10:C:1274:LYS:HG2	2.14	0.48
5:S:141:GLU:HG3	5:S:142:PHE:CD2	2.49	0.48
7:Z:113:ILE:O	7:Z:117:THR:HG23	2.13	0.48
10:C:391:PHE:HB2	10:C:392:PHE:CE2	2.49	0.48
11:D:105:LEU:HB2	11:D:238:THR:O	2.14	0.48
11:D:689:ASP:HA	11:D:735:ARG:HH22	1.79	0.48
11:D:816:GLY:HA3	11:D:878:VAL:O	2.14	0.48
11:D:881:PRO:O	11:D:1246:ARG:NH1	2.47	0.48
7:Z:108:ASP:O	7:Z:111:ILE:HG12	2.13	0.48
12:E:5:THR:OG1	12:E:6:VAL:N	2.47	0.48
12:E:15:THR:C	12:E:17:PHE:H	2.18	0.48
10:C:596:LYS:HG2	10:C:655:TYR:HE1	1.77	0.47
10:C:1109:ASP:N	10:C:1109:ASP:OD1	2.45	0.47
10:C:1172:ASN:ND2	10:C:1174:GLU:HG2	2.29	0.47
11:D:811:CYS:HB3	11:D:891:CYS:HB3	1.96	0.47
3:X:22:DC:H1'	3:X:23:DG:C8	2.49	0.47
7:Z:201:THR:O	7:Z:205:LYS:HG2	2.14	0.47
7:Z:215:ASN:HB3	7:Z:216:LYS:HD3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:272:PHE:HB2	7:Z:276:TYR:CE1	2.48	0.47
10:C:758:PHE:H	10:C:768:ASN:HB3	1.78	0.47
10:C:1123:ILE:HD13	10:C:1123:ILE:HA	1.69	0.47
9:B:56:SER:OG	9:B:162:GLU:OE1	2.24	0.47
10:C:1339:ARG:CZ	10:C:1343:ARG:HH12	2.27	0.47
10:C:1168:ASP:OD1	10:C:1168:ASP:N	2.46	0.47
10:C:22:LEU:HD23	10:C:658:VAL:HG11	1.96	0.47
11:D:811:CYS:SG	11:D:879:ARG:NH2	2.87	0.47
6:M:57:THR:OG1	6:M:58:ASP:N	2.48	0.47
6:M:193:GLU:HB3	6:M:196:PHE:HB3	1.96	0.47
10:C:11:ILE:HG13	10:C:1184:LEU:HD11	1.96	0.47
3:X:15:DT:O4	10:C:545:ARG:NH1	2.45	0.47
3:X:23:DG:N2	4:J:5:DC:H42	2.09	0.47
7:Z:222:ILE:HA	7:Z:225:GLU:HG3	1.97	0.47
8:A:94:ASP:OD2	8:A:122:GLY:HA2	2.14	0.47
9:B:138:LYS:HB3	9:B:138:LYS:HE3	1.70	0.47
10:C:427:ASP:OD1	10:C:427:ASP:N	2.46	0.47
10:C:648:THR:HG22	10:C:649:GLU:H	1.80	0.47
10:C:889:ILE:HA	10:C:917:ASP:HA	1.97	0.47
10:C:1335:PHE:HE2	10:C:1351:PHE:HE1	1.63	0.47
11:D:231:LYS:HB2	11:D:234:TRP:CE2	2.50	0.47
11:D:842:ALA:N	11:D:877:LYS:O	2.39	0.47
11:D:1337:GLU:N	11:D:1337:GLU:OE1	2.47	0.47
12:E:15:THR:O	12:E:17:PHE:N	2.47	0.47
12:E:40:GLU:O	12:E:44:LYS:NZ	2.44	0.47
6:M:126:LEU:HD23	6:M:126:LEU:HA	1.71	0.47
7:Z:523:LYS:O	7:Z:527:MET:HG2	2.14	0.47
11:D:689:ASP:HA	11:D:735:ARG:NH2	2.29	0.47
5:S:22:LEU:HD23	5:S:22:LEU:HA	1.72	0.47
7:Z:120:VAL:HG23	7:Z:329:ILE:HD12	1.95	0.47
10:C:603:THR:HG21	10:C:605:GLU:HG2	1.97	0.47
10:C:1170:LYS:HD3	10:C:1170:LYS:HA	1.62	0.47
2:H:32:DA:H3'	7:Z:554:ARG:NH2	2.30	0.47
6:M:18:ILE:O	6:M:21:ILE:HB	2.14	0.47
6:M:26:ALA:O	6:M:28:ILE:N	2.48	0.47
7:Z:89:ARG:HH21	10:C:376:ASP:HB2	1.79	0.47
7:Z:208:GLU:O	7:Z:211:GLN:HG2	2.15	0.47
10:C:1273:GLY:H	10:C:1278:GLY:HA2	1.79	0.46
11:D:44:TYR:CG	11:D:45:ARG:N	2.83	0.46
12:E:8:ASP:N	12:E:8:ASP:OD1	2.48	0.46
2:H:14:DC:H2'	2:H:15:DT:H72	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:165:PHE:O	7:Z:230:ARG:HD3	2.16	0.46
10:C:1135:SER:OG	10:C:1192:VAL:O	2.30	0.46
10:C:1159:LEU:HD23	10:C:1159:LEU:HA	1.77	0.46
11:D:1254:ILE:O	11:D:1263:VAL:HG12	2.15	0.46
12:E:29:LYS:HA	12:E:29:LYS:HD3	1.80	0.46
7:Z:231:LEU:HD12	7:Z:235:HIS:HB3	1.97	0.46
10:C:522:ASN:HD22	10:C:798:LEU:HD22	1.80	0.46
10:C:649:GLU:HG3	10:C:651:SER:H	1.80	0.46
10:C:787:ASP:HB2	10:C:791:THR:OG1	2.15	0.46
5:S:141:GLU:HG3	5:S:142:PHE:HD2	1.80	0.46
5:S:190:LYS:O	5:S:191:LYS:NZ	2.38	0.46
6:M:10:ILE:HG22	6:M:168:TYR:CE1	2.50	0.46
7:Z:287:LEU:HD13	7:Z:290:LYS:HB3	1.96	0.46
11:D:42:ILE:HD11	11:D:47:PHE:HB3	1.97	0.46
11:D:233:GLU:OE1	11:D:233:GLU:N	2.30	0.46
5:S:16:LEU:O	5:S:20:ILE:HG12	2.16	0.46
7:Z:219:TYR:O	7:Z:223:VAL:HG13	2.15	0.46
7:Z:272:PHE:O	7:Z:276:TYR:HB2	2.14	0.46
10:C:731:ASP:O	10:C:733:ASN:N	2.49	0.46
1:G:26:DT:H2"	1:G:25:DG:C8	2.51	0.46
10:C:566:THR:O	10:C:687:ASN:ND2	2.34	0.46
10:C:585:ASN:HB3	10:C:591:GLU:OE2	2.15	0.46
10:C:593:PRO:HA	10:C:607:GLU:O	2.15	0.46
11:D:512:THR:HG21	11:D:594:LEU:HD12	1.98	0.46
6:M:78:PHE:CG	6:M:79:PRO:HD2	2.49	0.46
6:M:87:LYS:HB3	6:M:87:LYS:HE2	1.58	0.46
7:Z:519:GLU:OE2	7:Z:520:ARG:HG2	2.15	0.46
10:C:852:ILE:HG23	10:C:888:LYS:HG3	1.96	0.46
11:D:803:ASP:N	11:D:803:ASP:OD1	2.49	0.46
2:H:28:DT:H2"	2:H:29:DA:C8	2.51	0.46
10:C:65:LYS:O	10:C:67:GLY:N	2.48	0.46
12:E:13:VAL:HG22	12:E:14:GLU:H	1.81	0.46
7:Z:218:LEU:HA	7:Z:221:LYS:HG3	1.98	0.46
7:Z:422:GLU:H	7:Z:422:GLU:HG3	1.62	0.46
10:C:156:ARG:HH21	10:C:448:ILE:HD11	1.80	0.46
11:D:91:GLU:OE2	11:D:92:GLN:HG3	2.16	0.46
11:D:232:PRO:O	11:D:235:MET:HG3	2.16	0.46
11:D:705:SER:HA	11:D:710:LYS:HA	1.97	0.46
5:S:209:HIS:C	7:Z:249:ARG:HH12	2.19	0.46
7:Z:296:ASN:HA	7:Z:299:ARG:NE	2.31	0.46
10:C:347:ARG:HG2	10:C:351:ASP:OD1	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:404:ARG:HA	10:C:404:ARG:HD3	1.77	0.46
10:C:1241:TYR:HD1	10:C:1241:TYR:HA	1.53	0.46
11:D:207:LYS:O	11:D:209:THR:N	2.44	0.46
11:D:548:LEU:HD22	11:D:550:ILE:HG22	1.98	0.46
11:D:1127:ARG:O	11:D:1131:LEU:HG	2.15	0.46
8:A:30:SER:OG	8:A:31:PRO:HD3	2.15	0.45
10:C:55:VAL:HG21	10:C:464:GLU:HG3	1.98	0.45
10:C:827:ASP:N	10:C:827:ASP:OD1	2.49	0.45
11:D:890:LEU:HD23	11:D:890:LEU:HA	1.80	0.45
1:G:25:DG:C6	1:G:24:DG:C6	3.04	0.45
7:Z:368:ILE:HG23	7:Z:403:ILE:HD11	1.98	0.45
7:Z:522:ALA:O	7:Z:526:MET:HG3	2.16	0.45
8:A:165:ARG:HG2	8:A:166:VAL:H	1.80	0.45
9:B:157:ASN:OD1	9:B:157:ASN:N	2.49	0.45
11:D:1341:ILE:HG13	11:D:1343:ARG:HG3	1.97	0.45
7:Z:120:VAL:HB	7:Z:332:SER:OG	2.17	0.45
8:A:227:LEU:HD13	8:A:227:LEU:HA	1.76	0.45
9:B:113:SER:OG	9:B:127:GLU:HA	2.16	0.45
9:B:114:GLU:HG3	9:B:127:GLU:OE1	2.16	0.45
10:C:1144:LYS:O	10:C:1147:GLU:HG2	2.15	0.45
6:M:14:ILE:O	6:M:18:ILE:HG12	2.17	0.45
8:A:86:LEU:HD23	8:A:132:ILE:HD12	1.97	0.45
10:C:10:ARG:CZ	10:C:700:LYS:HG2	2.45	0.45
10:C:96:ASP:OD2	10:C:97:ALA:N	2.48	0.45
10:C:1120:ARG:O	10:C:1122:ASN:N	2.48	0.45
11:D:51:ARG:HH21	11:D:58:LYS:NZ	2.15	0.45
7:Z:525:LEU:HD23	7:Z:525:LEU:HA	1.70	0.45
10:C:55:VAL:HG13	10:C:468:ARG:HE	1.82	0.45
10:C:65:LYS:HG3	10:C:66:ASN:ND2	2.32	0.45
11:D:104:ASP:O	11:D:274:ASN:ND2	2.49	0.45
7:Z:247:TYR:HA	7:Z:250:VAL:HG12	1.99	0.45
7:Z:421:ILE:HD12	7:Z:421:ILE:HA	1.73	0.45
10:C:854:ALA:HB2	10:C:871:GLY:HA2	1.98	0.45
11:D:105:LEU:HA	11:D:274:ASN:ND2	2.30	0.45
11:D:1239:LYS:HA	11:D:1242:GLU:HG2	1.99	0.45
1:G:34:DT:H2"	1:G:33:DG:C8	2.51	0.45
10:C:627:ASP:C	10:C:629:ASN:H	2.20	0.45
11:D:130:LEU:HD21	11:D:134:GLU:OE2	2.17	0.45
11:D:480:VAL:HG12	11:D:481:LEU:HD23	1.99	0.45
11:D:1133:GLU:OE1	11:D:1298:THR:OG1	2.30	0.45
4:J:7:DC:H2"	4:J:8:DG:H5"	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:52:ILE:HD13	6:M:52:ILE:HA	1.72	0.45
8:A:151:ARG:NH1	9:B:6:LEU:HD21	2.32	0.45
9:B:154:ALA:N	9:B:166:ASP:HB3	2.29	0.45
10:C:756:THR:O	10:C:768:ASN:HA	2.17	0.45
7:Z:135:ILE:O	7:Z:139:ARG:HG2	2.16	0.45
7:Z:495:SER:O	7:Z:498:GLU:N	2.50	0.45
7:Z:535:THR:HG23	11:D:77:LYS:HG3	1.98	0.45
7:Z:544:LYS:HA	7:Z:544:LYS:HD2	1.76	0.45
10:C:596:LYS:O	10:C:603:THR:HG22	2.17	0.45
11:D:86:CYS:HB2	11:D:88:VAL:HG23	1.98	0.45
11:D:1272:ARG:HD2	11:D:1272:ARG:HA	1.73	0.45
5:S:14:TYR:CE1	5:S:154:TYR:HE1	2.35	0.45
7:Z:283:TRP:O	7:Z:286:PRO:HD2	2.16	0.45
7:Z:303:ASN:OD1	7:Z:307:GLN:NE2	2.50	0.45
7:Z:370:GLN:HE22	11:D:292:ASN:HB3	1.81	0.45
10:C:821:SER:OG	10:C:1099:MET:HG3	2.17	0.45
11:D:24:SER:O	11:D:28:ILE:HG13	2.17	0.45
11:D:622:LEU:HD23	11:D:622:LEU:HA	1.76	0.45
11:D:1360:ILE:HD11	12:E:66:LEU:HB3	1.99	0.45
6:M:24:ALA:O	6:M:26:ALA:N	2.49	0.44
7:Z:232:SER:OG	7:Z:233:THR:N	2.50	0.44
7:Z:503:GLU:HA	7:Z:506:ARG:HB3	1.99	0.44
10:C:522:ASN:N	10:C:522:ASN:OD1	2.50	0.44
10:C:805:ALA:HB2	10:C:1108:VAL:HG11	1.99	0.44
11:D:76:LEU:H	11:D:76:LEU:HD12	1.82	0.44
6:M:121:ASN:O	6:M:125:MET:HG2	2.17	0.44
6:M:185:LYS:HG3	6:M:186:GLU:N	2.33	0.44
7:Z:436:GLN:NE2	10:C:497:ASN:OD1	2.44	0.44
10:C:194:ILE:H	10:C:352:THR:HG21	1.81	0.44
10:C:1094:LEU:HD23	10:C:1094:LEU:HA	1.69	0.44
11:D:65:ASP:OD1	11:D:93:ALA:N	2.30	0.44
11:D:598:GLU:OE1	11:D:598:GLU:N	2.50	0.44
11:D:804:LEU:HA	11:D:804:LEU:HD12	1.73	0.44
11:D:1151:ARG:NE	11:D:1152:LEU:O	2.44	0.44
5:S:80:LEU:O	5:S:150:LEU:HB2	2.17	0.44
5:S:124:LYS:HD3	5:S:124:LYS:HA	1.85	0.44
6:M:43:LEU:O	6:M:47:THR:HG22	2.18	0.44
7:Z:120:VAL:O	7:Z:124:ILE:HG12	2.17	0.44
7:Z:316:MET:SD	7:Z:321:GLU:HB3	2.56	0.44
8:A:120:THR:OG1	8:A:121:GLN:N	2.50	0.44
10:C:929:THR:O	10:C:1068:VAL:HG13	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:203:LEU:O	5:S:207:ARG:HB2	2.17	0.44
8:A:57:ILE:HG23	8:A:145:ALA:HB1	2.00	0.44
10:C:681:ARG:HG2	10:C:1122:ASN:HB3	1.99	0.44
5:S:5:THR:O	5:S:55:MET:N	2.51	0.44
5:S:76:PRO:HG2	11:D:73:TYR:CE1	2.52	0.44
7:Z:438:LYS:HE3	7:Z:438:LYS:HB3	1.70	0.44
10:C:103:LEU:HD12	10:C:104:ARG:N	2.33	0.44
10:C:567:PRO:HD3	10:C:575:ILE:HB	2.00	0.44
10:C:1237:VAL:HG13	11:D:636:SER:HB2	2.00	0.44
10:C:1331:VAL:HG22	10:C:1332:PRO:HD2	1.99	0.44
11:D:60:PHE:O	11:D:99:ARG:HD2	2.17	0.44
11:D:384:ARG:HH12	11:D:392:ILE:HA	1.82	0.44
11:D:923:GLY:HA2	11:D:926:LEU:HG	1.99	0.44
5:S:81:LEU:HD23	5:S:81:LEU:HA	1.82	0.44
6:M:65:LEU:HA	6:M:68:ILE:HD12	1.99	0.44
6:M:144:VAL:O	6:M:147:GLU:HG3	2.16	0.44
6:M:176:ILE:HG22	6:M:178:THR:HG22	2.00	0.44
7:Z:221:LYS:O	7:Z:224:LYS:HG2	2.18	0.44
7:Z:370:GLN:NE2	11:D:292:ASN:HB3	2.33	0.44
7:Z:476:ILE:HG12	7:Z:482:SER:O	2.17	0.44
9:B:113:SER:HB2	9:B:124:ILE:HG12	1.99	0.44
10:C:132:ILE:HD13	10:C:132:ILE:HA	1.88	0.44
10:C:821:SER:C	10:C:823:ARG:H	2.20	0.44
11:D:113:TRP:CE2	11:D:1317:THR:HG23	2.53	0.44
11:D:1317:THR:O	11:D:1321:THR:HG22	2.18	0.44
8:A:14:ILE:HB	9:B:223:ILE:HD13	1.98	0.44
8:A:120:THR:HG1	8:A:121:GLN:NE2	2.14	0.44
10:C:4:SER:O	10:C:8:LYS:HB2	2.17	0.44
10:C:726:GLU:OE1	10:C:726:GLU:N	2.50	0.44
10:C:815:GLU:HB2	11:D:459:PHE:HD2	1.82	0.44
11:D:153:GLU:O	11:D:156:GLN:HB3	2.18	0.44
11:D:885:LYS:HA	11:D:885:LYS:HD3	1.62	0.44
11:D:1204:ASP:OD2	11:D:1206:HIS:N	2.51	0.44
11:D:1251:LYS:HD3	11:D:1267:SER:HA	1.99	0.44
11:D:1267:SER:OG	11:D:1269:GLU:N	2.50	0.44
6:M:59:ASP:HB3	6:M:60:PHE:CD1	2.52	0.44
7:Z:238:LYS:HA	7:Z:241:ASP:OD2	2.16	0.44
7:Z:364:HIS:CE1	11:D:273:ARG:HH22	2.36	0.44
10:C:65:LYS:HA	10:C:65:LYS:HD2	1.74	0.44
11:D:139:PHE:HD1	11:D:178:MET:HG3	1.83	0.44
11:D:1215:GLU:OE1	11:D:1215:GLU:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:193:ILE:HG23	10:C:352:THR:HG22	1.99	0.44
11:D:692:GLY:O	11:D:695:MET:HG3	2.18	0.44
11:D:786:LYS:NZ	11:D:924:THR:OG1	2.49	0.44
7:Z:440:ARG:HD2	7:Z:440:ARG:HA	1.76	0.43
10:C:415:LYS:HD2	10:C:415:LYS:N	2.33	0.43
10:C:911:LYS:HB2	10:C:911:LYS:HE3	1.69	0.43
10:C:1304:THR:OG1	10:C:1305:VAL:N	2.51	0.43
5:S:45:ILE:HG22	5:S:46:THR:HG23	1.98	0.43
6:M:109:LYS:HA	6:M:109:LYS:HD3	1.72	0.43
7:Z:274:LYS:HA	7:Z:277:LYS:NZ	2.33	0.43
8:A:33:GLU:OE1	9:B:219:GLN:NE2	2.51	0.43
10:C:34:SER:O	10:C:460:GLY:HA3	2.18	0.43
10:C:111:ASP:O	10:C:113:LEU:N	2.51	0.43
10:C:1203:LYS:N	10:C:1206:ASP:OD2	2.51	0.43
11:D:744:MET:O	11:D:752:ILE:HG13	2.18	0.43
11:D:897:ARG:HD3	11:D:902:GLU:HA	2.00	0.43
6:M:171:LYS:HA	6:M:171:LYS:HD3	1.71	0.43
7:Z:210:TYR:O	7:Z:214:PRO:HD2	2.18	0.43
10:C:649:GLU:OE2	10:C:650:SER:N	2.52	0.43
10:C:1271:LEU:HD13	10:C:1271:LEU:HA	1.76	0.43
11:D:272:ASN:OD1	11:D:272:ASN:N	2.51	0.43
11:D:924:THR:HG23	11:D:925:GLN:HG3	1.99	0.43
11:D:1162:ARG:H	11:D:1175:GLU:CB	2.32	0.43
5:S:61:ILE:HD11	6:M:94:ILE:HD12	2.00	0.43
10:C:121:ASP:HA	10:C:123:ARG:NH1	2.34	0.43
10:C:1146:LEU:HD13	10:C:1155:LEU:HD11	2.00	0.43
11:D:62:PRO:O	11:D:96:ARG:HD2	2.18	0.43
6:M:101:LYS:HE3	6:M:101:LYS:HB3	1.56	0.43
7:Z:109:ILE:HD12	7:Z:343:MET:HB2	2.00	0.43
8:A:67:HIS:HD2	8:A:69:TYR:H	1.66	0.43
8:A:95:THR:OG1	8:A:96:GLY:N	2.51	0.43
9:B:88:SER:HB2	9:B:200:ASN:ND2	2.34	0.43
10:C:724:VAL:HG23	10:C:779:VAL:O	2.19	0.43
11:D:281:LEU:HD23	11:D:281:LEU:HA	1.76	0.43
1:G:24:DG:H2'	1:G:23:DC:H6	1.84	0.43
2:H:32:DA:H2''	2:H:33:DC:C6	2.53	0.43
5:S:62:ASN:OD1	5:S:63:ASN:N	2.51	0.43
5:S:107:ASP:HA	5:S:110:ARG:CZ	2.49	0.43
7:Z:363:LEU:HD23	7:Z:363:LEU:HA	1.83	0.43
7:Z:505:LEU:HB2	7:Z:576:PHE:CE1	2.54	0.43
1:G:9:DC:N3	1:G:8:DT:N3	2.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:83:ASN:O	5:S:88:ARG:NH2	2.52	0.43
5:S:94:SER:O	5:S:98:ILE:HG13	2.19	0.43
6:M:5:THR:HB	6:M:28:ILE:HD11	2.00	0.43
7:Z:124:ILE:HD13	7:Z:124:ILE:HA	1.89	0.43
7:Z:329:ILE:HD13	7:Z:329:ILE:HA	1.80	0.43
8:A:162:GLU:H	8:A:162:GLU:HG2	1.62	0.43
10:C:104:ARG:HE	10:C:104:ARG:HB3	1.69	0.43
10:C:1217:ALA:C	10:C:1219:ASN:H	2.22	0.43
10:C:1325:LEU:HD23	12:E:31:LEU:HB3	2.00	0.43
11:D:829:LYS:O	11:D:830:VAL:HG23	2.18	0.43
11:D:842:ALA:HB3	11:D:877:LYS:HB3	2.00	0.43
10:C:815:GLU:HB2	11:D:459:PHE:CD2	2.54	0.43
10:C:839:THR:OG1	10:C:1065:LYS:HG2	2.19	0.43
10:C:886:VAL:HG11	10:C:1064:VAL:HG21	2.00	0.43
11:D:139:PHE:CD1	11:D:178:MET:HG3	2.53	0.43
11:D:1303:SER:O	11:D:1303:SER:OG	2.29	0.43
1:G:17:DT:OP1	11:D:45:ARG:NH1	2.52	0.43
5:S:38:GLU:OE1	5:S:40:ALA:HB3	2.19	0.43
7:Z:546:PHE:O	7:Z:548:VAL:HG22	2.18	0.43
8:A:67:HIS:NE2	10:C:931:ILE:HG22	2.34	0.43
9:B:92:ALA:HB3	9:B:95:VAL:HG22	2.01	0.43
11:D:336:PHE:O	11:D:340:LEU:HB2	2.18	0.43
11:D:424:ALA:HB3	11:D:425:PRO:HD3	2.01	0.43
7:Z:115:GLU:O	7:Z:118:THR:HG22	2.19	0.43
7:Z:132:LYS:HB3	7:Z:207:PHE:CE2	2.53	0.43
9:B:91:LEU:HD23	9:B:147:LYS:HZ2	1.84	0.43
10:C:188:PHE:CE1	10:C:194:ILE:HG12	2.54	0.43
10:C:840:CYS:SG	10:C:888:LYS:HD3	2.59	0.43
11:D:384:ARG:NH2	11:D:390:THR:O	2.51	0.43
11:D:581:LEU:HD23	11:D:581:LEU:HA	1.86	0.43
6:M:25:ASN:ND2	6:M:25:ASN:O	2.52	0.42
10:C:708:GLU:OE1	10:C:708:GLU:N	2.35	0.42
10:C:815:GLU:OE2	11:D:502:GLN:NE2	2.52	0.42
10:C:856:ILE:HD12	10:C:857:PRO:CD	2.49	0.42
11:D:560:ASN:ND2	11:D:560:ASN:H	2.17	0.42
11:D:601:LYS:HE3	11:D:601:LYS:HB2	1.76	0.42
11:D:668:SER:HB2	11:D:670:LEU:HG	2.01	0.42
11:D:672:THR:OG1	11:D:673:GLU:N	2.52	0.42
11:D:871:ASN:OD1	11:D:871:ASN:N	2.51	0.42
6:M:10:ILE:HG21	6:M:107:ILE:HG21	2.02	0.42
7:Z:536:ASP:OD2	10:C:902:ARG:NH1	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:118:LYS:HA	8:A:118:LYS:HD3	1.83	0.42
10:C:609:LEU:HD23	10:C:610:SER:N	2.34	0.42
11:D:504:ILE:H	11:D:504:ILE:HG13	1.57	0.42
11:D:839:ARG:HE	11:D:839:ARG:HB3	1.64	0.42
4:J:11:DA:H2'	4:J:12:DG:C8	2.54	0.42
5:S:7:TYR:O	5:S:52:PRO:HA	2.19	0.42
6:M:193:GLU:O	6:M:197:ILE:HG13	2.19	0.42
7:Z:294:THR:HB	7:Z:297:THR:CB	2.44	0.42
7:Z:444:GLU:O	7:Z:448:ILE:HG13	2.20	0.42
7:Z:454:MET:N	7:Z:454:MET:SD	2.92	0.42
10:C:8:LYS:HE3	10:C:8:LYS:HB2	1.80	0.42
10:C:209:ILE:O	10:C:213:LEU:HG	2.20	0.42
10:C:728:ALA:HB3	10:C:736:VAL:HB	2.01	0.42
10:C:1155:LEU:HA	10:C:1158:THR:HG22	1.99	0.42
7:Z:509:ILE:HG22	7:Z:573:LEU:HD21	2.01	0.42
10:C:101:VAL:O	10:C:126:TYR:HA	2.18	0.42
11:D:52:ASP:HA	11:D:56:CYS:HB2	2.01	0.42
11:D:111:HIS:CD2	11:D:113:TRP:H	2.37	0.42
11:D:197:GLU:H	11:D:197:GLU:HG3	1.62	0.42
6:M:184:ILE:HG13	6:M:185:LYS:N	2.34	0.42
9:B:37:LEU:HD23	9:B:37:LEU:HA	1.76	0.42
11:D:717:ASN:OD1	11:D:719:VAL:N	2.53	0.42
4:J:9:DT:H2''	4:J:10:DC:H5'	2.02	0.42
6:M:108:ILE:HD13	6:M:108:ILE:HA	1.92	0.42
6:M:180:ASP:CG	6:M:183:ILE:H	2.23	0.42
7:Z:252:GLU:HA	7:Z:255:ARG:HH11	1.83	0.42
7:Z:387:LYS:HE2	7:Z:387:LYS:HB2	1.84	0.42
10:C:448:ILE:HG23	10:C:449:ASP:OD1	2.19	0.42
10:C:584:VAL:HG22	10:C:590:LEU:HD23	2.00	0.42
11:D:32:SER:OG	11:D:102:HIS:HD2	2.02	0.42
11:D:214:LYS:HA	11:D:217:LYS:HZ2	1.84	0.42
5:S:82:PRO:O	5:S:88:ARG:NE	2.38	0.42
5:S:113:ARG:HA	5:S:113:ARG:HD2	1.85	0.42
10:C:1210:LEU:HD23	10:C:1210:LEU:HA	1.91	0.42
11:D:192:ILE:O	11:D:196:ILE:HG13	2.19	0.42
11:D:1267:SER:HB3	11:D:1270:LEU:HG	2.02	0.42
11:D:1349:THR:O	11:D:1353:VAL:HG23	2.20	0.42
3:X:21:DG:H2'	3:X:22:DC:C5	2.54	0.42
6:M:51:ASN:O	6:M:54:THR:OG1	2.38	0.42
7:Z:314:LEU:HD23	7:Z:314:LEU:HA	1.91	0.42
8:A:78:ASP:CG	8:A:79:VAL:N	2.72	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:617:TYR:CG	10:C:655:TYR:HE2	2.38	0.42
11:D:19:LYS:HB3	11:D:1329:ILE:HD13	2.00	0.42
11:D:231:LYS:HB3	11:D:233:GLU:CD	2.40	0.42
11:D:303:ALA:HA	11:D:307:ASN:HB3	2.01	0.42
11:D:680:ILE:HA	11:D:683:ILE:HD12	2.02	0.42
11:D:1144:SER:O	11:D:1144:SER:OG	2.38	0.42
11:D:1262:PHE:O	11:D:1264:LYS:N	2.52	0.42
1:G:13:DG:H2'	7:Z:398:TRP:CH2	2.54	0.42
5:S:92:ARG:NH2	6:M:74:ASP:OD2	2.53	0.42
6:M:121:ASN:HA	6:M:124:LYS:HZ3	1.84	0.42
6:M:156:ASN:OD1	6:M:159:THR:HG23	2.20	0.42
8:A:104:LEU:O	8:A:142:SER:HA	2.20	0.42
9:B:102:PHE:CE1	9:B:116:ALA:HB2	2.54	0.42
9:B:140:LYS:HD2	9:B:141:ILE:H	1.84	0.42
10:C:64:SER:OG	10:C:65:LYS:N	2.52	0.42
10:C:541:LEU:HD23	10:C:546:ALA:HB2	2.01	0.42
11:D:318:ASN:OD1	11:D:318:ASN:N	2.53	0.42
1:G:8:DT:H71	7:Z:393:THR:HA	2.01	0.42
5:S:53:VAL:HG12	5:S:62:ASN:HB2	2.02	0.42
7:Z:206:MET:O	7:Z:218:LEU:HD21	2.20	0.42
10:C:473:ARG:HA	10:C:473:ARG:HD3	1.61	0.42
11:D:866:GLU:O	11:D:870:ASP:HB2	2.19	0.42
11:D:1262:PHE:CD2	11:D:1263:VAL:HG13	2.55	0.42
5:S:85:VAL:HG22	5:S:89:ILE:HD11	2.01	0.41
5:S:189:VAL:C	5:S:191:LYS:H	2.24	0.41
7:Z:135:ILE:HG23	7:Z:204:GLU:HG2	2.02	0.41
10:C:681:ARG:NH2	10:C:1120:ARG:HD3	2.35	0.41
11:D:909:GLU:O	11:D:911:VAL:HG23	2.20	0.41
5:S:90:LYS:NZ	6:M:59:ASP:OD2	2.53	0.41
8:A:82:ILE:HA	8:A:85:ASN:HD22	1.85	0.41
10:C:369:TYR:CE1	10:C:373:ARG:HD2	2.55	0.41
10:C:841:VAL:HG23	10:C:1063:THR:HB	2.01	0.41
11:D:354:THR:O	11:D:446:GLN:HA	2.21	0.41
11:D:537:SER:OG	11:D:539:THR:HG23	2.20	0.41
11:D:888:ARG:HH12	11:D:1333:ARG:NH1	2.17	0.41
11:D:1338:ASN:HB3	11:D:1343:ARG:HB2	2.02	0.41
6:M:19:LEU:HD13	6:M:19:LEU:HA	1.91	0.41
8:A:34:LYS:HA	8:A:192:GLU:CD	2.41	0.41
8:A:91:ILE:HG12	8:A:125:ILE:HD13	2.01	0.41
9:B:58:LYS:HG3	9:B:161:GLY:O	2.20	0.41
10:C:135:MET:SD	10:C:139:GLY:HA2	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:1188:LEU:HD23	10:C:1188:LEU:HA	1.81	0.41
11:D:323:LYS:NZ	11:D:328:MET:HG2	2.35	0.41
5:S:90:LYS:NZ	6:M:60:PHE:HB3	2.35	0.41
5:S:96:ASP:OD1	5:S:100:ASN:ND2	2.53	0.41
7:Z:295:GLU:OE1	7:Z:296:ASN:N	2.53	0.41
11:D:704:VAL:O	11:D:710:LYS:HA	2.20	0.41
11:D:1320:LEU:HD23	11:D:1320:LEU:HA	1.78	0.41
6:M:5:THR:OG1	6:M:6:LYS:N	2.53	0.41
7:Z:452:PRO:O	7:Z:454:MET:HG2	2.20	0.41
10:C:834:HIS:ND1	10:C:1072:LYS:HD2	2.35	0.41
11:D:20:ILE:HG23	11:D:1324:SER:HA	2.03	0.41
11:D:556:ASP:HB2	11:D:560:ASN:HB2	2.03	0.41
11:D:655:ALA:O	11:D:659:ILE:HG12	2.20	0.41
11:D:808:GLU:OE1	11:D:886:THR:OG1	2.29	0.41
11:D:861:ASP:O	11:D:864:LEU:N	2.53	0.41
1:G:35:DT:N3	2:H:35:DA:N1	2.68	0.41
5:S:178:GLU:H	5:S:178:GLU:CD	2.16	0.41
6:M:121:ASN:HA	6:M:124:LYS:NZ	2.36	0.41
7:Z:116:GLY:O	7:Z:120:VAL:HG12	2.20	0.41
7:Z:250:VAL:HG22	7:Z:254:GLU:OE2	2.21	0.41
8:A:52:LEU:HA	8:A:52:LEU:HD13	1.87	0.41
9:B:184:VAL:HG12	9:B:184:VAL:O	2.21	0.41
10:C:17:VAL:HG12	10:C:1200:ASP:OD2	2.21	0.41
10:C:392:PHE:HA	10:C:422:THR:CG2	2.50	0.41
10:C:845:THR:HG23	10:C:847:LEU:H	1.84	0.41
11:D:41:THR:OG1	11:D:42:ILE:HG22	2.19	0.41
11:D:280:LEU:HD23	11:D:280:LEU:HA	1.79	0.41
11:D:802:GLN:OE1	11:D:1336:LYS:HD3	2.20	0.41
2:H:32:DA:H3'	7:Z:554:ARG:HH21	1.86	0.41
7:Z:269:ARG:HB3	7:Z:270:GLN:NE2	2.35	0.41
9:B:91:LEU:HG	9:B:92:ALA:H	1.85	0.41
10:C:804:VAL:HG23	10:C:1110:VAL:HB	2.01	0.41
10:C:1131:LEU:HA	10:C:1131:LEU:HD12	1.78	0.41
11:D:119:PRO:HG2	11:D:121:ARG:HH12	1.85	0.41
11:D:659:ILE:HD13	11:D:659:ILE:HA	1.87	0.41
2:H:24:DC:H2''	2:H:25:DC:C6	2.56	0.41
5:S:37:LEU:HB2	5:S:42:ILE:CG1	2.50	0.41
9:B:117:LYS:H	9:B:117:LYS:NZ	2.19	0.41
11:D:500:PRO:HB3	11:D:504:ILE:HB	2.02	0.41
5:S:54:LEU:HD12	5:S:54:LEU:HA	1.77	0.41
6:M:66:SER:OG	6:M:67:VAL:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:218:LEU:HD12	7:Z:221:LYS:HB2	2.03	0.41
7:Z:478:ASP:O	7:Z:481:ASP:N	2.43	0.41
7:Z:488:ILE:HG22	11:D:253:ILE:HD12	2.03	0.41
7:Z:553:ILE:HD13	7:Z:553:ILE:HA	1.98	0.41
8:A:68:GLU:O	8:A:79:VAL:HB	2.20	0.41
8:A:83:VAL:HG13	8:A:171:VAL:HG22	2.03	0.41
10:C:700:LYS:H	10:C:700:LYS:HG3	1.54	0.41
10:C:1345:LEU:C	10:C:1347:ILE:H	2.24	0.41
10:C:1351:PHE:HB3	11:D:15:PHE:CD2	2.56	0.41
11:D:56:CYS:SG	11:D:59:ILE:HG13	2.60	0.41
11:D:127:ASP:HB2	11:D:218:ARG:CZ	2.51	0.41
11:D:671:ILE:HD12	11:D:671:ILE:HA	1.91	0.41
11:D:709:GLU:HG2	11:D:710:LYS:H	1.85	0.41
11:D:821:ALA:HB1	11:D:828:VAL:HG23	2.03	0.41
11:D:1136:ARG:HH11	11:D:1136:ARG:HB2	1.85	0.41
11:D:1262:PHE:CE2	11:D:1263:VAL:HG13	2.55	0.41
11:D:1282:LYS:HE3	11:D:1285:LYS:NZ	2.36	0.41
12:E:10:LEU:HD23	12:E:10:LEU:HA	1.68	0.41
7:Z:129:ILE:HA	7:Z:132:LYS:HG2	2.03	0.41
8:A:222:SER:O	8:A:225:VAL:HG12	2.22	0.41
10:C:372:LEU:HD23	10:C:372:LEU:HA	1.88	0.41
10:C:629:ASN:HB3	10:C:631:HIS:CE1	2.56	0.41
11:D:1331:ASN:ND2	11:D:1331:ASN:H	2.19	0.41
1:G:21:DT:H6	1:G:21:DT:H2'	1.73	0.40
6:M:10:ILE:HG22	6:M:168:TYR:CD1	2.56	0.40
7:Z:370:GLN:NE2	11:D:293:GLU:HG2	2.36	0.40
9:B:17:TYR:CE1	9:B:23:LYS:HG3	2.56	0.40
10:C:428:ILE:HD12	10:C:428:ILE:HA	1.82	0.40
10:C:471:LEU:HD12	10:C:471:LEU:HA	1.88	0.40
10:C:883:ASP:N	10:C:883:ASP:OD1	2.54	0.40
11:D:397:ARG:HD2	11:D:397:ARG:HA	1.76	0.40
11:D:739:GLY:O	11:D:759:ASN:ND2	2.53	0.40
3:X:21:DG:H2'	3:X:22:DC:C4	2.56	0.40
6:M:197:ILE:HA	6:M:200:ILE:HD11	2.03	0.40
7:Z:282:GLU:HA	7:Z:285:GLU:OE2	2.21	0.40
8:A:32:VAL:HG22	8:A:192:GLU:O	2.21	0.40
10:C:182:SER:O	10:C:397:TYR:HE1	2.04	0.40
10:C:353:LEU:HD23	10:C:353:LEU:HA	1.94	0.40
11:D:376:LYS:HD3	11:D:380:TYR:OH	2.21	0.40
11:D:1253:VAL:HG13	11:D:1293:VAL:HG21	2.04	0.40
6:M:141:GLU:OE1	6:M:145:ASN:ND2	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:76:LYS:HB3	8:A:134:THR:OG1	2.21	0.40
8:A:218:CYS:SG	9:B:220:LEU:HD13	2.61	0.40
8:A:221:ILE:O	8:A:223:VAL:N	2.54	0.40
9:B:108:GLU:HG3	9:B:134:ASN:C	2.42	0.40
10:C:867:LEU:HA	10:C:867:LEU:HD22	1.90	0.40
11:D:382:LYS:HB3	11:D:409:ILE:HD11	2.04	0.40
12:E:26:ARG:HE	12:E:30:ILE:HD11	1.86	0.40
2:H:22:DC:H2''	2:H:23:DG:H8	1.86	0.40
5:S:14:TYR:HB2	5:S:64:ARG:NH2	2.35	0.40
5:S:93:LEU:HD22	6:M:62:VAL:HG12	2.03	0.40
7:Z:458:LYS:HE3	7:Z:458:LYS:HB2	1.76	0.40
9:B:174:PHE:O	9:B:197:ILE:HA	2.22	0.40
10:C:157:SER:HA	10:C:158:PRO:HD3	1.95	0.40
10:C:425:ASN:O	10:C:428:ILE:HG22	2.21	0.40
10:C:809:TRP:CE3	10:C:810:ASN:HB2	2.57	0.40
10:C:1056:LEU:HD23	10:C:1056:LEU:HA	1.91	0.40
11:D:283:LEU:HD23	11:D:283:LEU:HA	1.86	0.40
11:D:1262:PHE:O	11:D:1264:LYS:HG2	2.21	0.40
1:G:3:DT:H1'	1:G:2:DA:C8	2.57	0.40
6:M:4:TYR:CG	6:M:43:LEU:HD12	2.56	0.40
6:M:12:SER:O	6:M:15:VAL:HG12	2.22	0.40
7:Z:131:ILE:HB	7:Z:207:PHE:CE1	2.56	0.40
7:Z:143:GLU:H	7:Z:143:GLU:HG3	1.68	0.40
7:Z:265:SER:O	7:Z:268:PRO:HD3	2.22	0.40
8:A:124:GLU:OE1	8:A:125:ILE:N	2.54	0.40
8:A:222:SER:O	8:A:222:SER:OG	2.37	0.40
9:B:67:LEU:HD12	9:B:78:ALA:HB2	2.04	0.40
9:B:108:GLU:OE2	9:B:135:GLY:HA3	2.22	0.40
10:C:932:ASN:OD1	10:C:933:VAL:N	2.55	0.40
11:D:248:ARG:HD2	11:D:264:ASN:ND2	2.36	0.40
11:D:881:PRO:CG	11:D:1242:GLU:HG3	2.52	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	
5	S	198/210 (94%)	164 (83%)	33 (17%)	1 (0%)	29	66
6	M	199/205 (97%)	176 (88%)	22 (11%)	1 (0%)	29	66
7	Z	464/577 (80%)	398 (86%)	65 (14%)	1 (0%)	47	80
8	A	221/323 (68%)	188 (85%)	33 (15%)	0	100	100
9	B	228/317 (72%)	199 (87%)	29 (13%)	0	100	100
10	C	1180/1358 (87%)	988 (84%)	192 (16%)	0	100	100
11	D	1155/1417 (82%)	996 (86%)	158 (14%)	1 (0%)	51	84
12	E	70/72 (97%)	56 (80%)	13 (19%)	1 (1%)	11	44
All	All	3715/4479 (83%)	3165 (85%)	545 (15%)	5 (0%)	54	84

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	M	65	LEU
12	E	62	SER
5	S	54	LEU
7	Z	479	ASP
11	D	1263	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	
5	S	165/184 (90%)	151 (92%)	14 (8%)	10	38
6	M	179/191 (94%)	157 (88%)	22 (12%)	4	22
7	Z	401/527 (76%)	360 (90%)	41 (10%)	7	30
8	A	189/287 (66%)	173 (92%)	16 (8%)	10	38
9	B	194/276 (70%)	177 (91%)	17 (9%)	10	36
10	C	911/1169 (78%)	831 (91%)	80 (9%)	10	36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	D	937/1219 (77%)	885 (94%)	52 (6%)	21	53
12	E	63/64 (98%)	56 (89%)	7 (11%)	6	26
All	All	3039/3917 (78%)	2790 (92%)	249 (8%)	15	39

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	S	8	THR
5	S	29	THR
5	S	44	LYS
5	S	68	LEU
5	S	99	ASP
5	S	111	LYS
5	S	115	ASP
5	S	125	ASP
5	S	149	THR
5	S	154	TYR
5	S	162	LEU
5	S	191	LYS
5	S	204	LYS
5	S	207	ARG
6	M	2	LEU
6	M	63	TYR
6	M	64	ARG
6	M	65	LEU
6	M	70	GLU
6	M	74	ASP
6	M	82	PHE
6	M	91	ASN
6	M	101	LYS
6	M	106	ASN
6	M	112	SER
6	M	114	ASP
6	M	124	LYS
6	M	135	TYR
6	M	154	ASN
6	M	158	LEU
6	M	166	PHE
6	M	169	PHE
6	M	170	ILE
6	M	174	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	M	182	ASN
6	M	200	ILE
7	Z	92	MET
7	Z	95	MET
7	Z	99	ASP
7	Z	143	GLU
7	Z	199	PHE
7	Z	209	GLU
7	Z	219	TYR
7	Z	230	ARG
7	Z	233	THR
7	Z	241	ASP
7	Z	264	ARG
7	Z	265	SER
7	Z	278	VAL
7	Z	283	TRP
7	Z	295	GLU
7	Z	297	THR
7	Z	305	THR
7	Z	311	PHE
7	Z	328	GLU
7	Z	358	TYR
7	Z	367	ASP
7	Z	386	ARG
7	Z	389	PHE
7	Z	392	SER
7	Z	421	ILE
7	Z	422	GLU
7	Z	423	THR
7	Z	428	ASN
7	Z	433	GLN
7	Z	450	HIS
7	Z	453	ASN
7	Z	468	THR
7	Z	472	MET
7	Z	473	GLU
7	Z	506	ARG
7	Z	512	LEU
7	Z	542	VAL
7	Z	549	THR
7	Z	550	ARG
7	Z	569	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	Z	572	PHE
8	A	17	LYS
8	A	30	SER
8	A	69	TYR
8	A	70	SER
8	A	104	LEU
8	A	116	ASP
8	A	120	THR
8	A	121	GLN
8	A	127	ASN
8	A	138	GLN
8	A	146	THR
8	A	149	VAL
8	A	166	VAL
8	A	193	THR
8	A	200	THR
8	A	207	LEU
9	B	7	LEU
9	B	36	THR
9	B	53	CYS
9	B	61	ASP
9	B	73	CYS
9	B	93	GLU
9	B	99	THR
9	B	118	LEU
9	B	125	THR
9	B	131	CYS
9	B	157	ASN
9	B	166	ASP
9	B	174	PHE
9	B	199	THR
9	B	203	VAL
9	B	207	GLU
9	B	230	ASN
10	C	2	SER
10	C	3	TYR
10	C	35	TYR
10	C	37	LYS
10	C	40	THR
10	C	42	ASP
10	C	60	PHE
10	C	66	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	C	73	TYR
10	C	77	GLN
10	C	86	THR
10	C	95	TYR
10	C	136	THR
10	C	140	THR
10	C	188	PHE
10	C	199	ASP
10	C	205	CYS
10	C	213	LEU
10	C	351	ASP
10	C	366	VAL
10	C	394	GLU
10	C	419	ASP
10	C	472	TYR
10	C	516	GLN
10	C	548	PHE
10	C	556	THR
10	C	560	ARG
10	C	562	CYS
10	C	576	ASN
10	C	580	SER
10	C	586	ASP
10	C	604	ASP
10	C	607	GLU
10	C	613	ASP
10	C	616	ASN
10	C	648	THR
10	C	652	ARG
10	C	680	ASN
10	C	698	SER
10	C	700	LYS
10	C	714	ASP
10	C	734	ARG
10	C	748	ASN
10	C	754	SER
10	C	756	THR
10	C	766	CYS
10	C	827	ASP
10	C	832	SER
10	C	841	VAL
10	C	856	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	C	864	LEU
10	C	897	LEU
10	C	927	SER
10	C	929	THR
10	C	1061	LEU
10	C	1078	ASP
10	C	1087	LYS
10	C	1091	SER
10	C	1092	ARG
10	C	1098	ASP
10	C	1119	SER
10	C	1120	ARG
10	C	1123	ILE
10	C	1143	GLU
10	C	1145	THR
10	C	1154	GLU
10	C	1168	ASP
10	C	1182	LEU
10	C	1196	THR
10	C	1206	ASP
10	C	1229	THR
10	C	1234	ASP
10	C	1241	TYR
10	C	1251	VAL
10	C	1258	ARG
10	C	1277	PHE
10	C	1281	ARG
10	C	1301	GLU
10	C	1331	VAL
10	C	1350	ASP
11	D	16	ASP
11	D	56	CYS
11	D	68	CYS
11	D	69	LEU
11	D	75	ARG
11	D	78	HIS
11	D	117	SER
11	D	127	ASP
11	D	130	LEU
11	D	159	THR
11	D	160	ASP
11	D	163	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	D	192	ILE
11	D	224	THR
11	D	225	PHE
11	D	265	ASP
11	D	320	ARG
11	D	327	ASP
11	D	350	ARG
11	D	391	THR
11	D	447	LEU
11	D	476	LEU
11	D	530	ASP
11	D	540	ILE
11	D	560	ASN
11	D	569	ASN
11	D	570	THR
11	D	608	ARG
11	D	640	ASP
11	D	646	ASP
11	D	674	ASN
11	D	748	ASP
11	D	750	THR
11	D	754	THR
11	D	773	THR
11	D	782	ASP
11	D	786	LYS
11	D	823	VAL
11	D	824	GLU
11	D	829	LYS
11	D	863	ASN
11	D	891	CYS
11	D	1136	ARG
11	D	1156	ASP
11	D	1203	THR
11	D	1228	VAL
11	D	1256	ASP
11	D	1264	LYS
11	D	1274	LEU
11	D	1299	ARG
11	D	1326	ASN
11	D	1362	LYS
12	E	5	THR
12	E	8	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	E	18	ASP
12	E	31	LEU
12	E	35	TYR
12	E	44	LYS
12	E	64	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
5	S	63	ASN
5	S	100	ASN
5	S	112	HIS
6	M	88	GLN
6	M	105	GLN
6	M	128	GLN
6	M	154	ASN
7	Z	309	ASN
7	Z	324	GLN
7	Z	347	ASN
7	Z	364	HIS
7	Z	453	ASN
7	Z	464	ASN
7	Z	467	HIS
7	Z	537	HIS
8	A	85	ASN
8	A	121	GLN
9	B	230	ASN
10	C	31	GLN
10	C	66	ASN
10	C	72	HIS
10	C	144	ASN
10	C	631	HIS
10	C	717	ASN
10	C	810	ASN
10	C	1130	HIS
10	C	1172	ASN
10	C	1268	GLN
10	C	1319	ASN
10	C	1336	ASN
11	D	102	HIS
11	D	111	HIS
11	D	362	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	D	388	HIS
11	D	428	HIS
11	D	433	GLN
11	D	475	GLN
11	D	487	ASN
11	D	543	HIS
11	D	553	GLN
11	D	560	ASN
11	D	563	ASN
11	D	679	ASN
11	D	774	HIS
11	D	1277	ASN
11	D	1331	ASN
11	D	1338	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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.

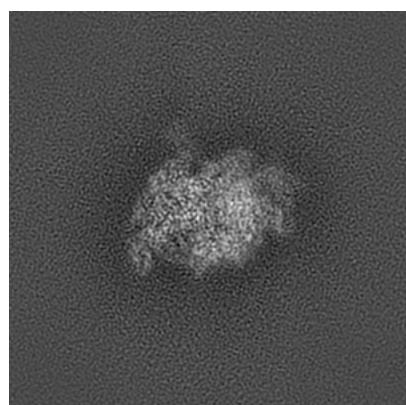
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21851. These allow visual inspection of the internal detail of the map and identification of artifacts.

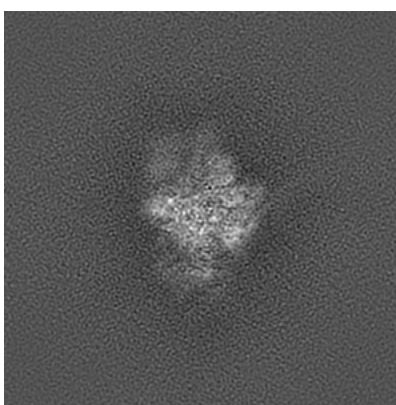
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

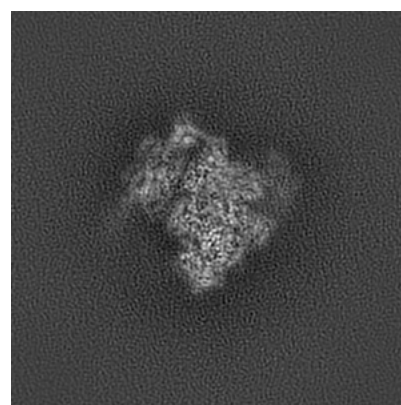
6.1.1 Primary map



X



Y

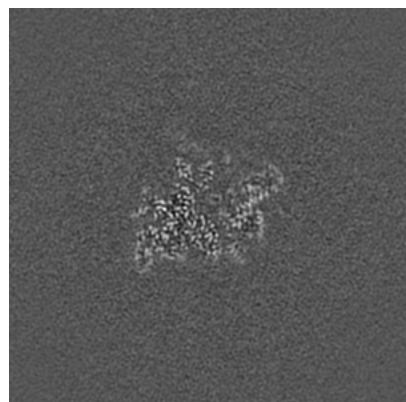


Z

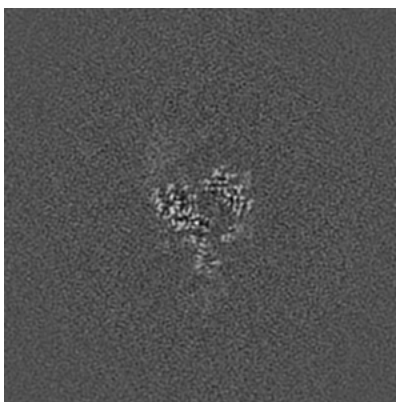
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

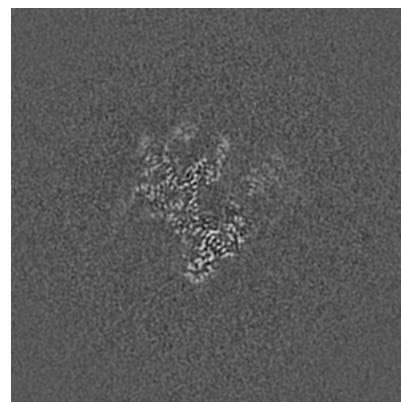
6.2.1 Primary map



X Index: 179



Y Index: 179

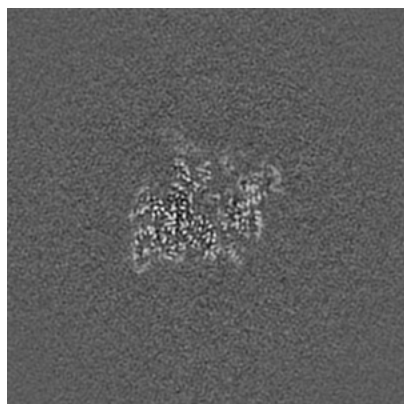


Z Index: 179

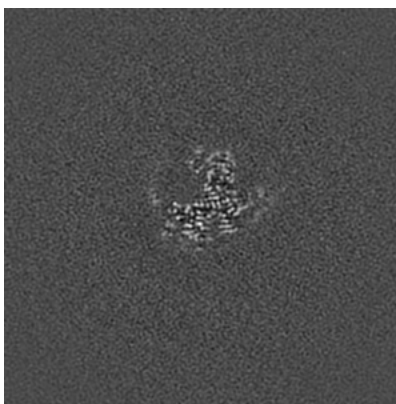
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

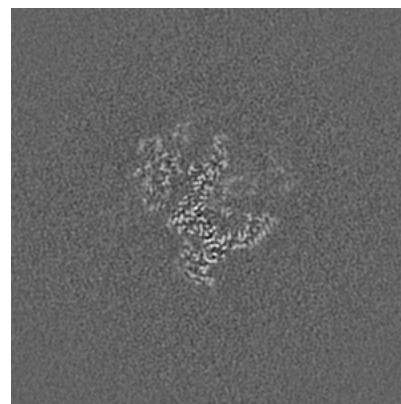
6.3.1 Primary map



X Index: 178



Y Index: 161



Z Index: 172

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

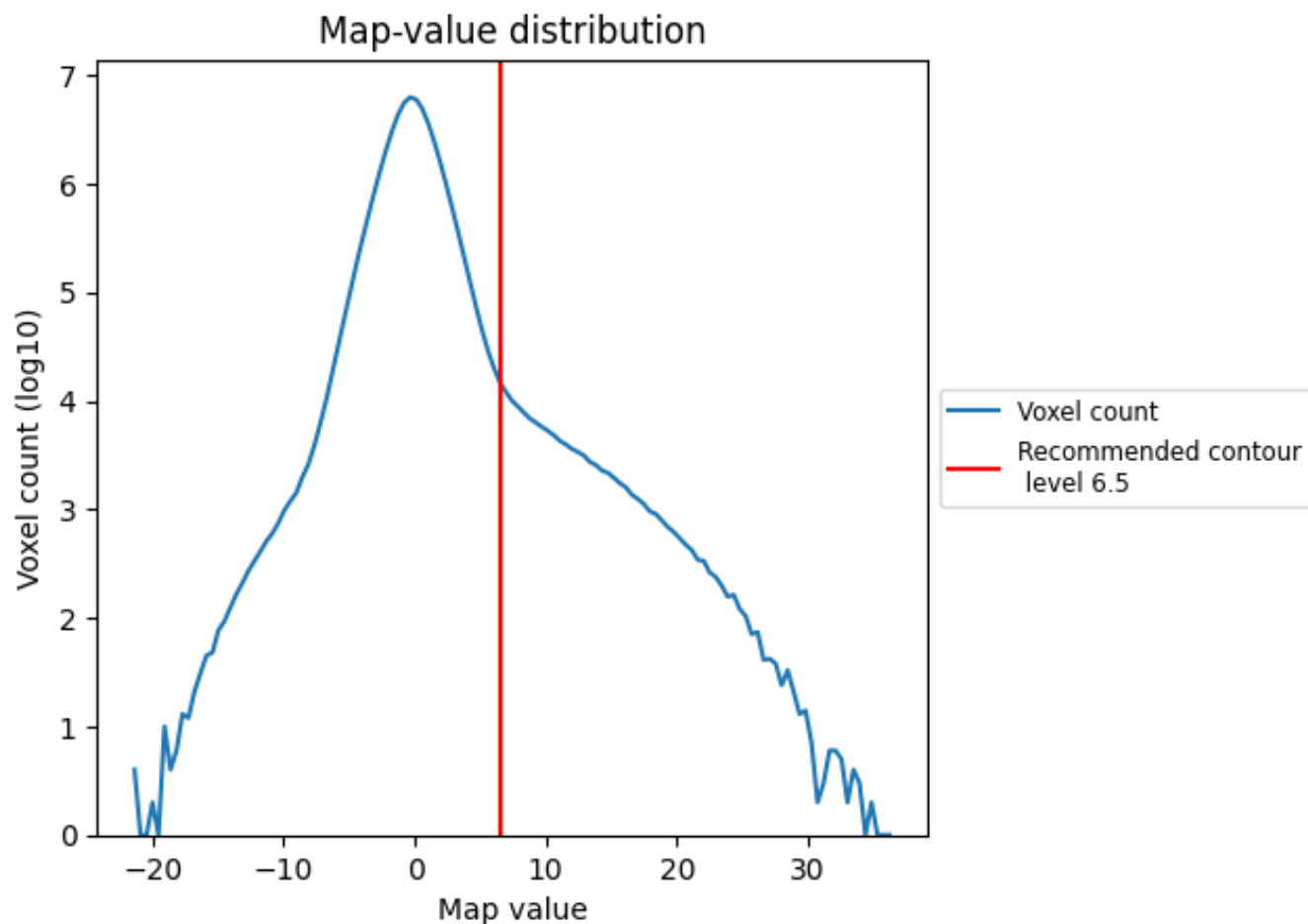
6.5 Mask visualisation

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

7 Map analysis [i](#)

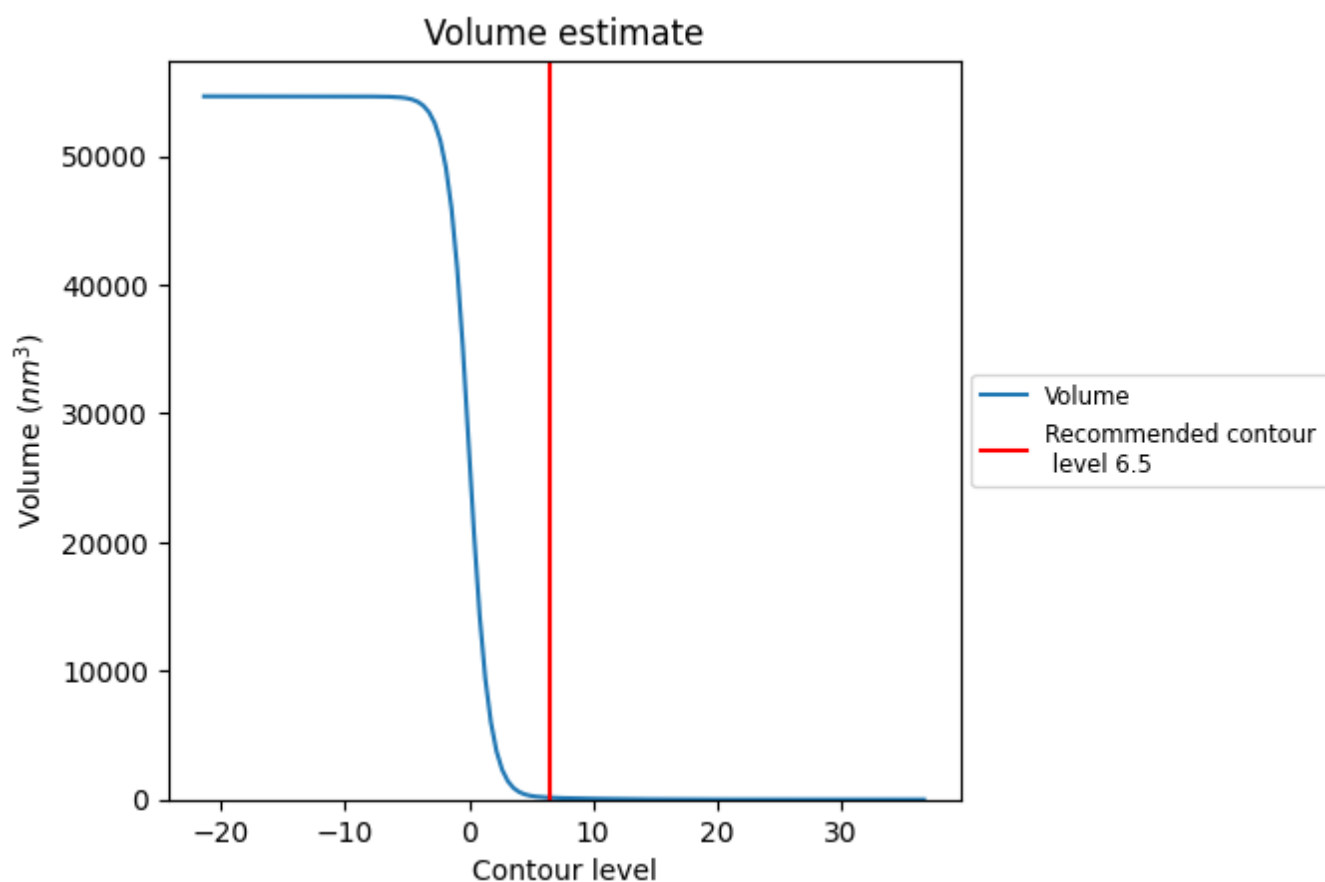
This section contains the results of statistical analysis of the map.

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.

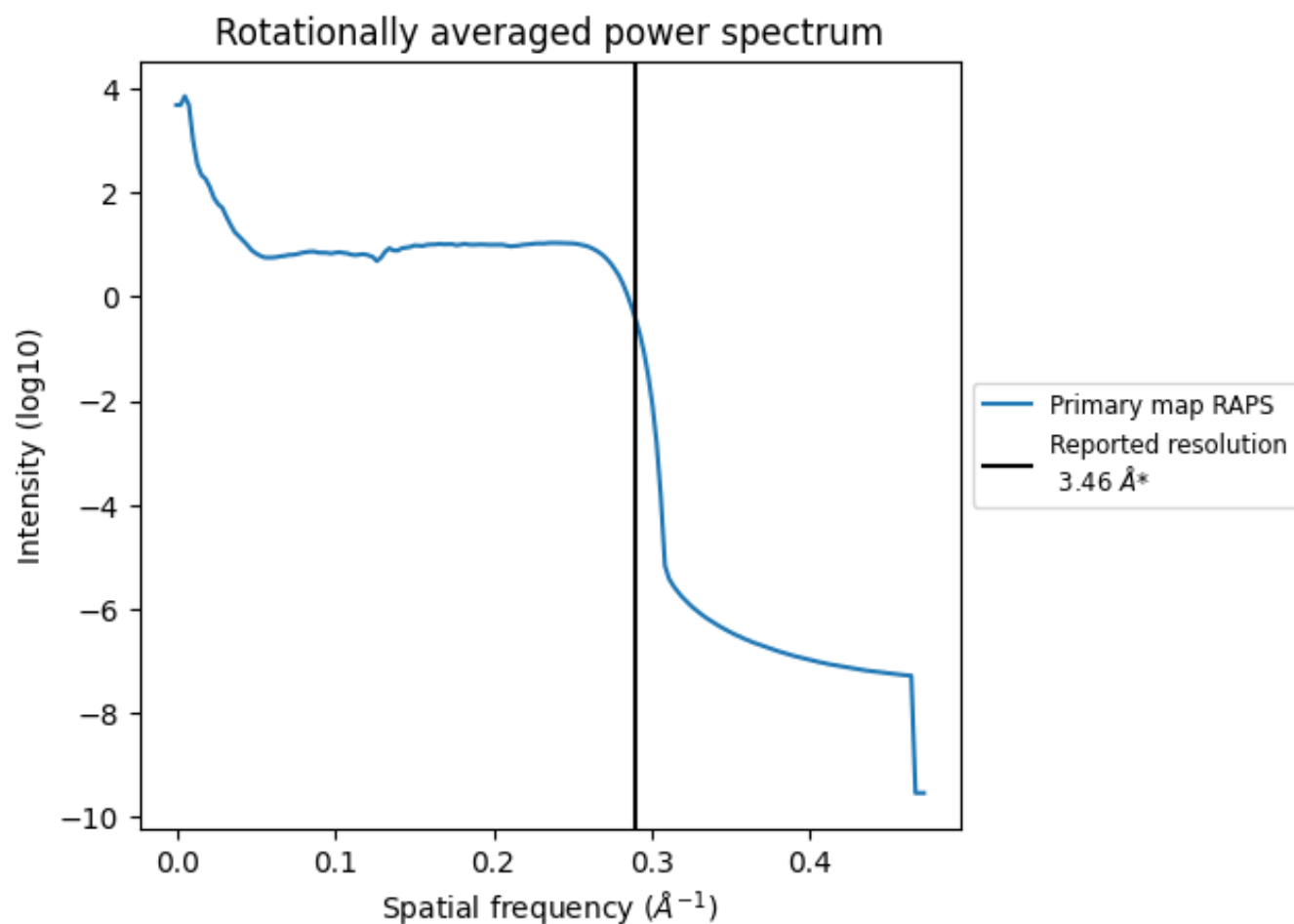
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 153 nm³; this corresponds to an approximate mass of 138 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 ⓘ

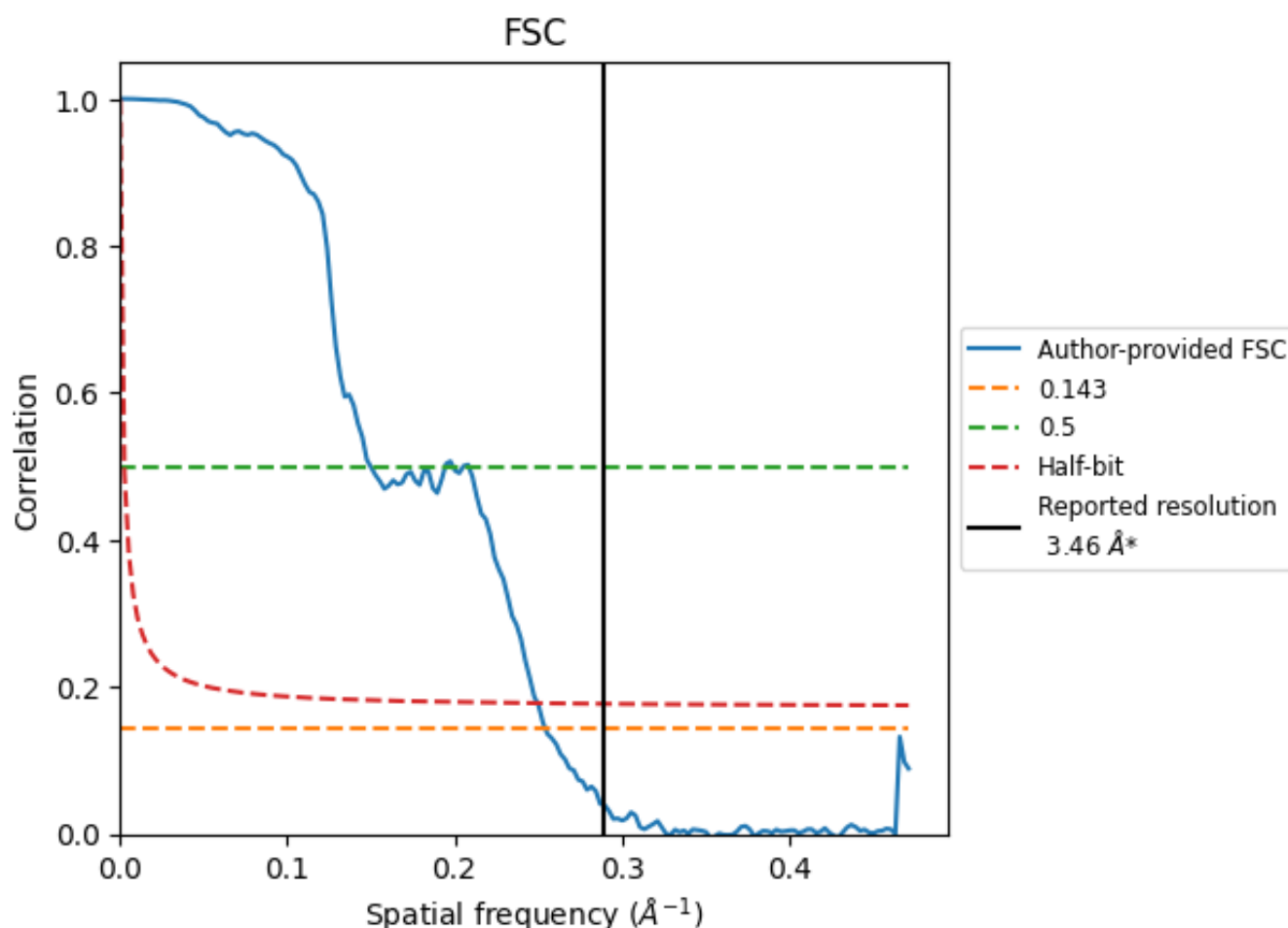


*Reported resolution corresponds to spatial frequency of 0.289 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.289 Å⁻¹

8.2 Resolution estimates [i](#)

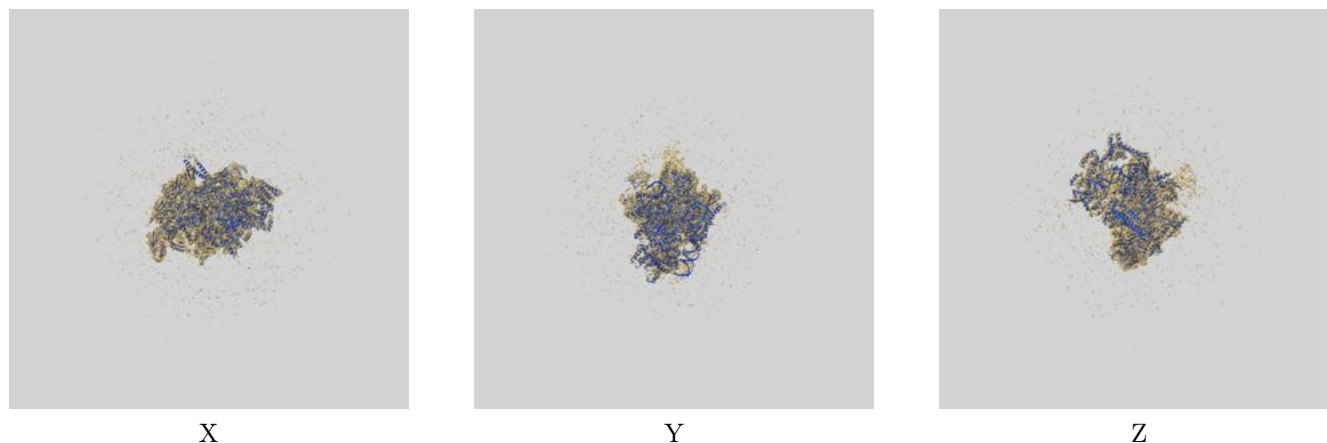
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.46	-	-
Author-provided FSC curve	3.93	6.67	4.00
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.93 differs from the reported value 3.46 by more than 10 %

9 Map-model fit [i](#)

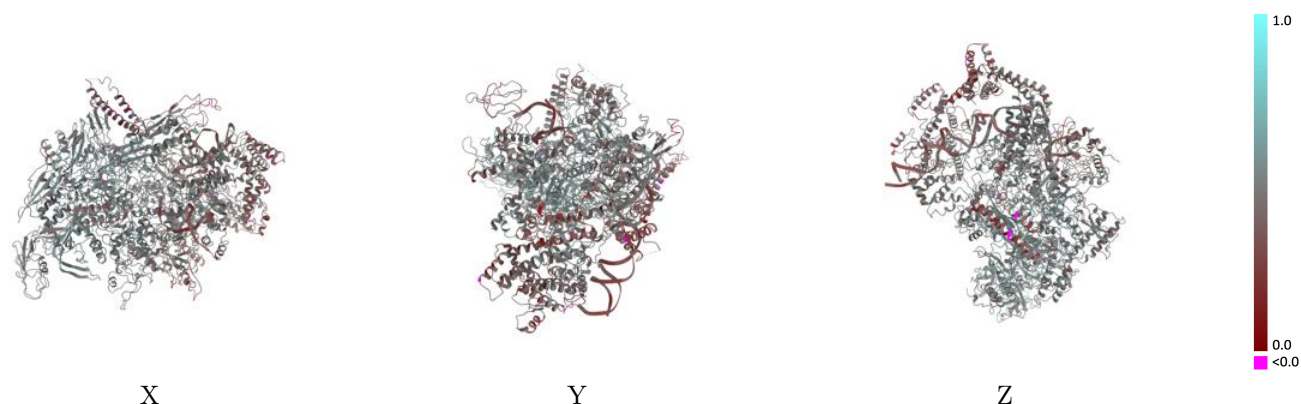
This section contains information regarding the fit between EMDB map EMD-21851 and PDB model 6WMR. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



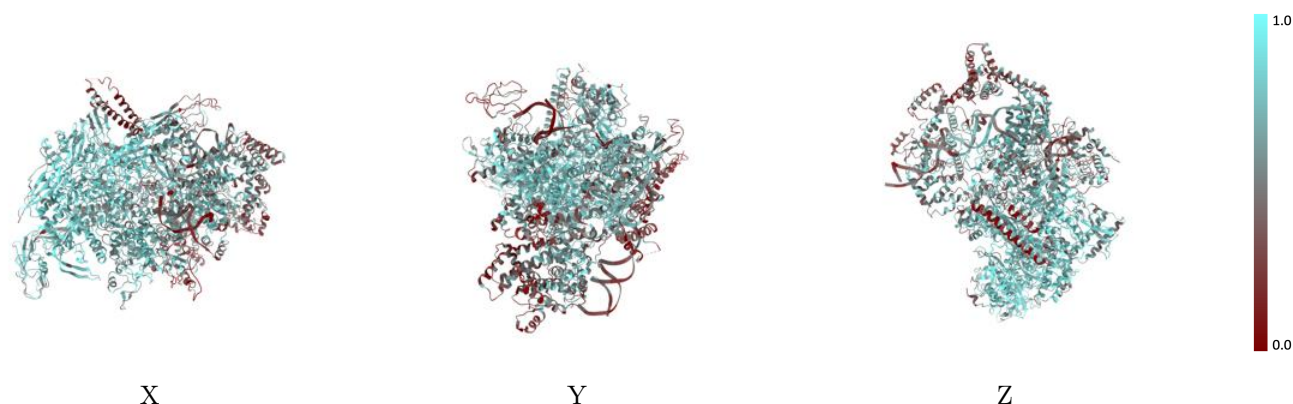
The images above show the 3D surface view of the map at the recommended contour level 6.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



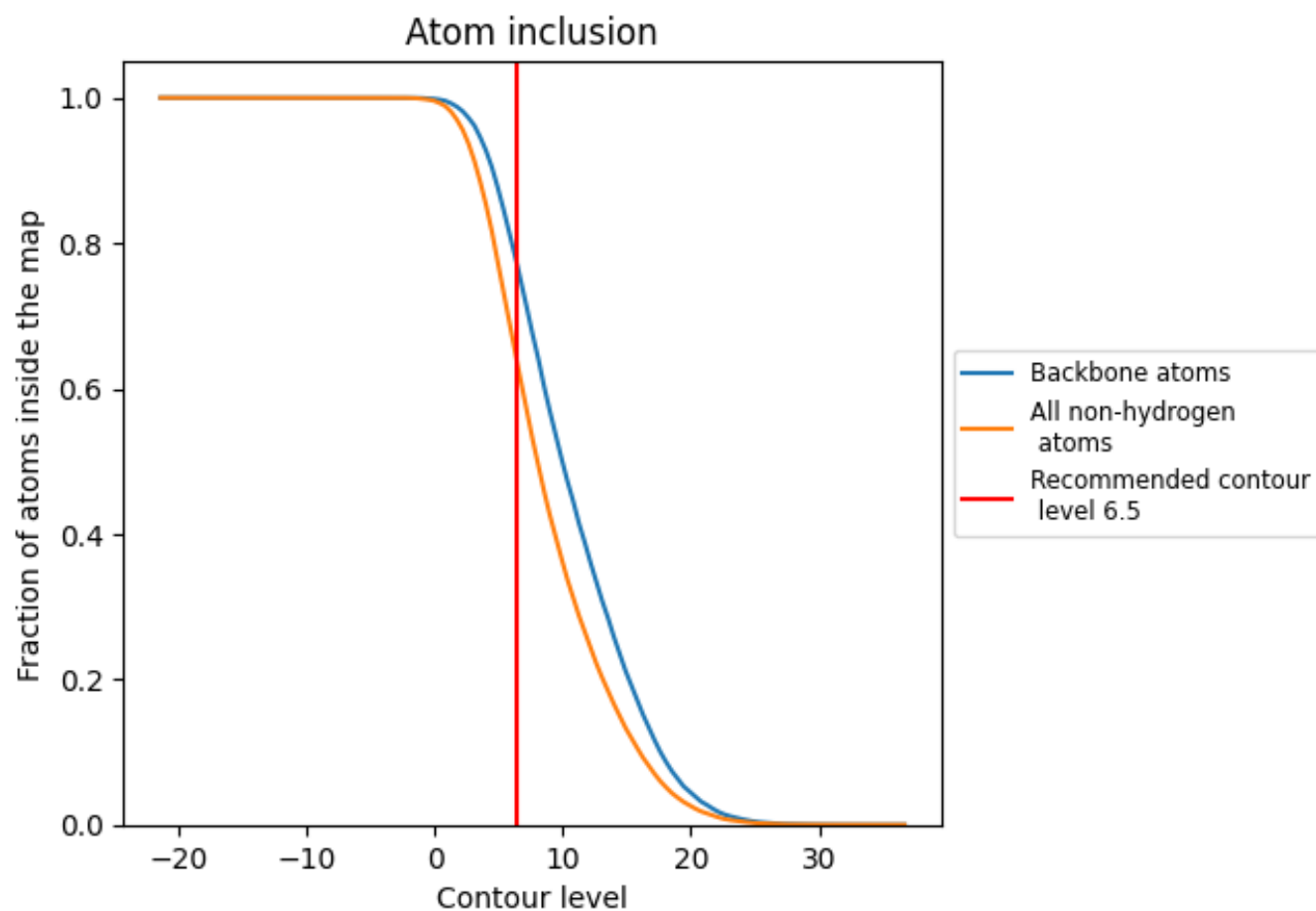
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 63% 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 (6.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6319	<div></div> 0.4660
A	<div></div> 0.7678	<div></div> 0.4990
B	<div></div> 0.7047	<div></div> 0.4850
C	<div></div> 0.6855	<div></div> 0.4920
D	<div></div> 0.7083	<div></div> 0.4960
E	<div></div> 0.5054	<div></div> 0.4550
G	<div></div> 0.4569	<div></div> 0.3820
H	<div></div> 0.4743	<div></div> 0.3540
J	<div></div> 0.3142	<div></div> 0.3640
M	<div></div> 0.4423	<div></div> 0.3980
S	<div></div> 0.4746	<div></div> 0.4170
X	<div></div> 0.1111	<div></div> 0.2730
Z	<div></div> 0.5008	<div></div> 0.4110

