



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:01 PM UTC

PDB ID : 9L0Y / pdb_00009l0y
EMDB ID : EMD-62728
Title : Cryo-EM structure of E.coli transcription initiation complex with Escherichia phage Mu middle transcription activator Mor
Authors : Lin, W.; Feng, Y.; Shi, J.
Deposited on : 2024-12-13
Resolution : 3.78 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:

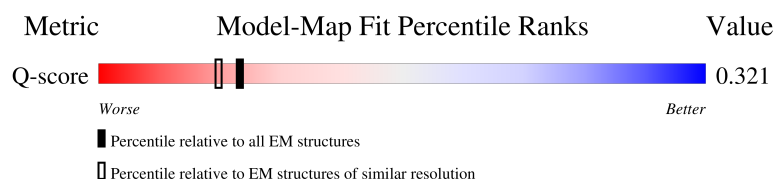
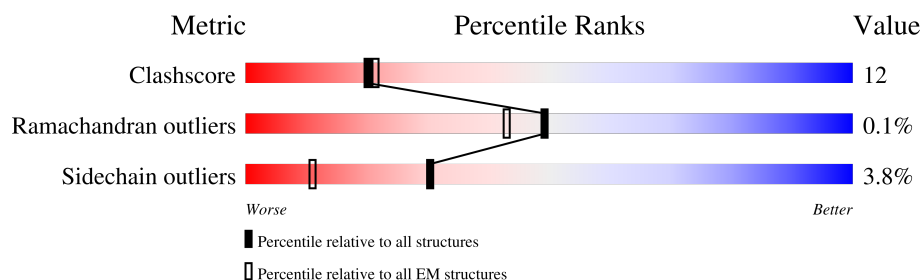
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

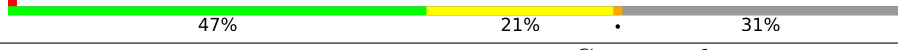
The reported resolution of this entry is 3.78 Å.

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



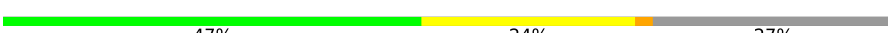
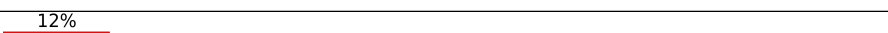
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10074 (3.28 - 4.27)

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	1	76	
2	2	76	
3	A	329	
3	B	329	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	P	329	
4	C	1342	
5	D	1407	
6	E	91	
7	F	613	
8	G	129	
8	J	129	
8	M	129	
8	N	129	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 35859 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 (76-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	73	Total	C	N	O	P	0	0
			1496	715	266	442	73		

- Molecule 2 is a DNA chain called DNA (76-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	73	Total	C	N	O	P	0	0
			1510	718	287	432	73		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	230	Total	C	N	O	S	0	0
			1786	1112	317	351	6		
3	B	228	Total	C	N	O	S	0	0
			1767	1100	312	349	6		
3	P	71	Total	C	N	O	S	0	0
			554	350	96	106	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	1340	Total	C	N	O	S	0	0
			10560	6627	1840	2050	43		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	516	VAL	ASP	conflict	UNP P0A8V2

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	1334	Total	C	N	O	S	0	0
			10369	6514	1849	1956	50		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	79	Total	C	N	O	S	0	0
			627	382	118	126	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	496	Total	C	N	O	S	0	0
			3977	2484	707	764	22		

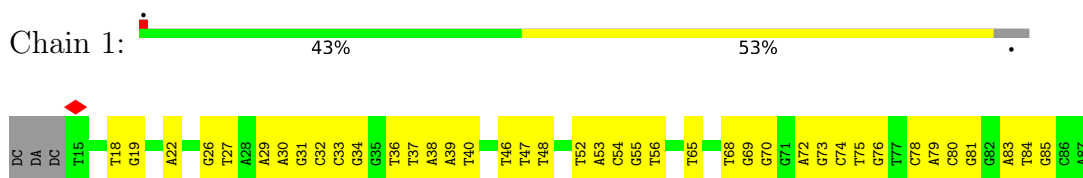
- Molecule 8 is a protein called Middle operon regulator.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	94	Total	C	N	O	S	0	0
			743	469	142	130	2		
8	J	109	Total	C	N	O	S	0	0
			855	536	160	157	2		
8	M	111	Total	C	N	O	S	0	0
			872	545	163	162	2		
8	N	94	Total	C	N	O	S	0	0
			743	469	142	130	2		

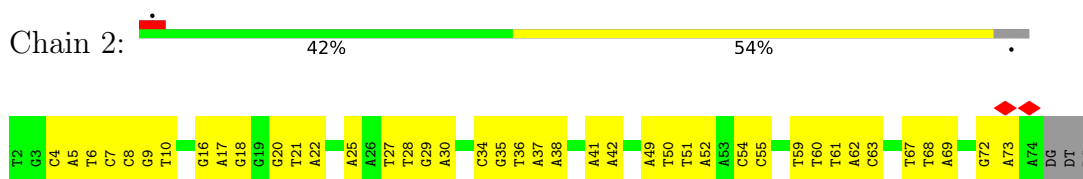
3 Residue-property plots

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.

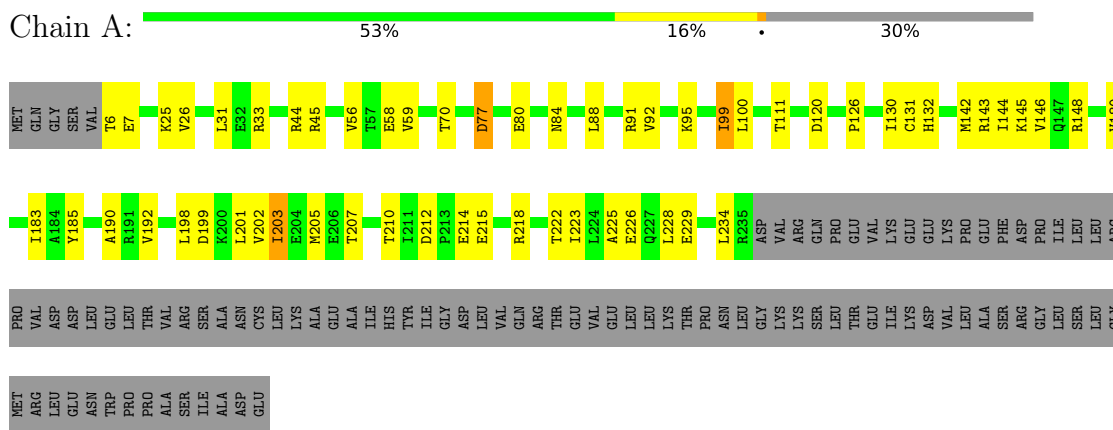
- Molecule 1: DNA (76-MER)



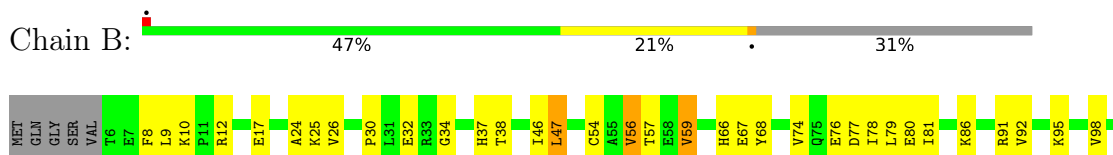
- Molecule 2: DNA (76-MER)

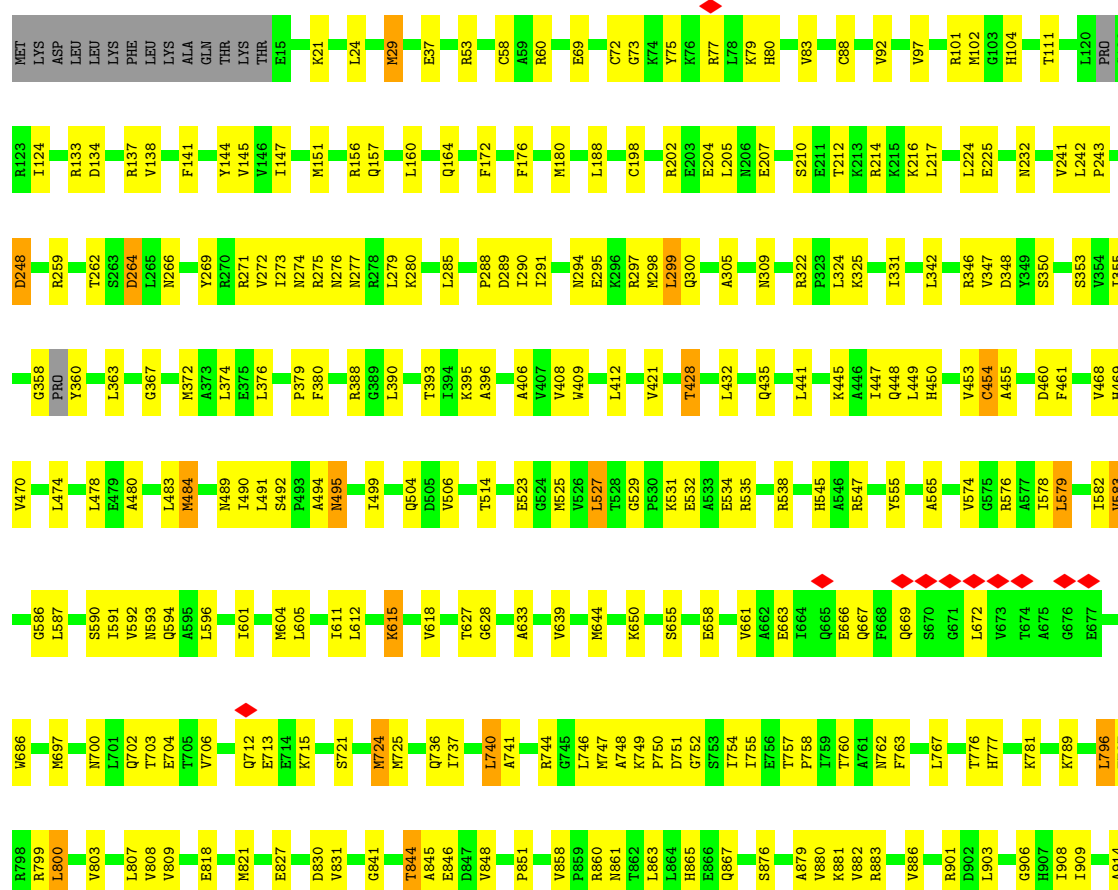


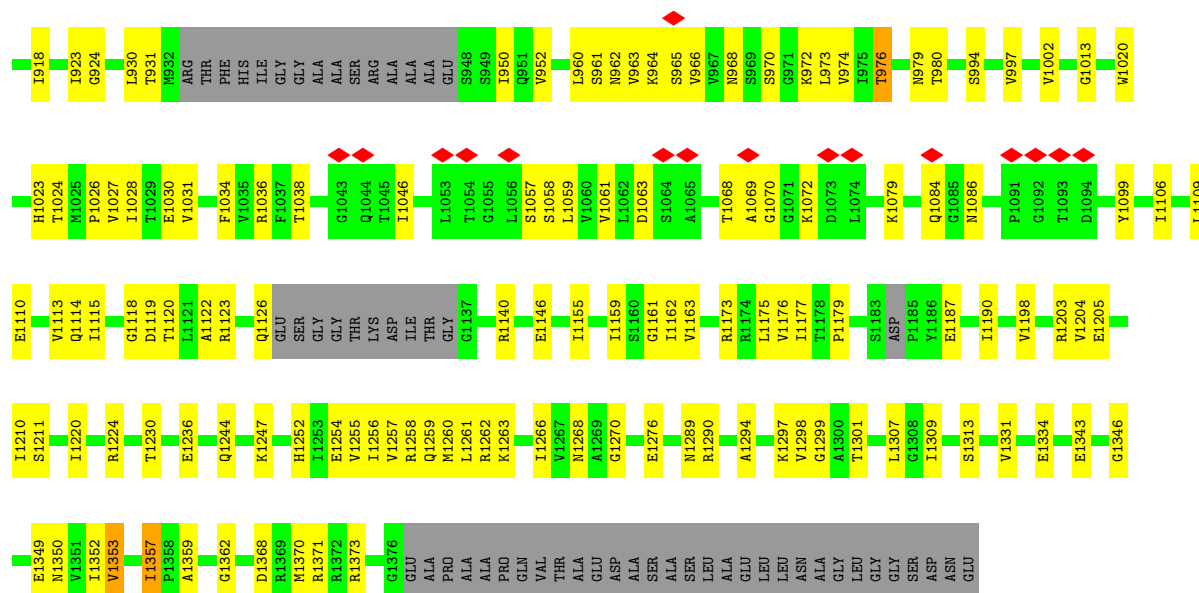
- Molecule 3: DNA-directed RNA polymerase subunit alpha



- Molecule 3: DNA-directed RNA polymerase subunit alpha



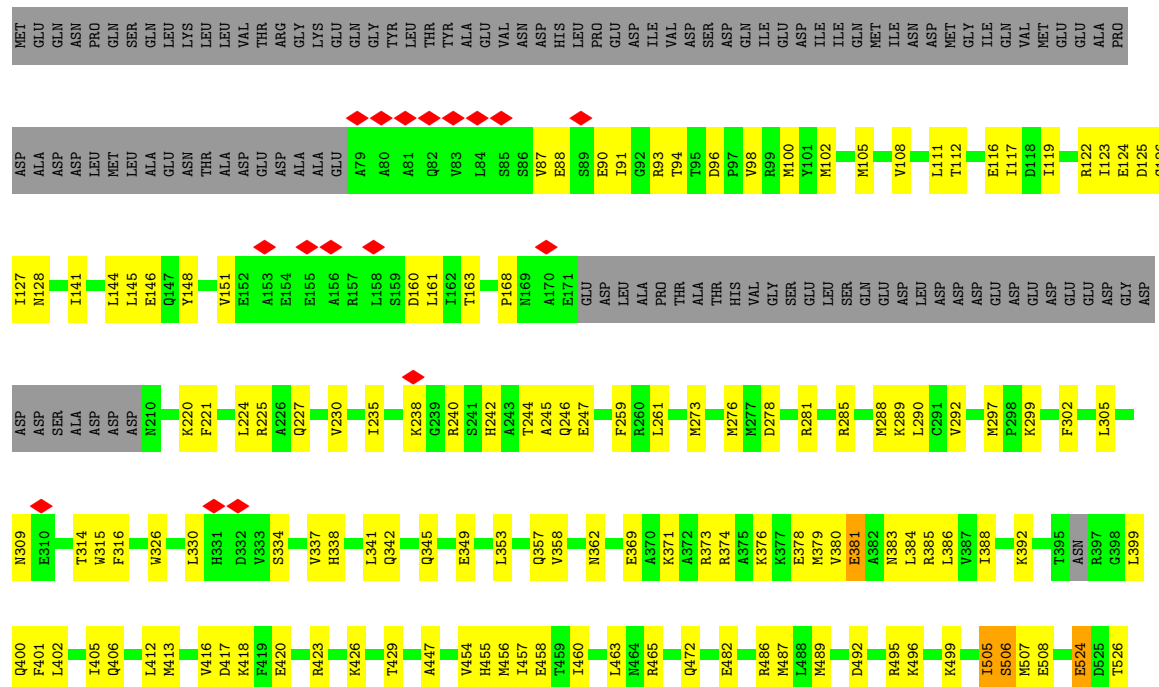


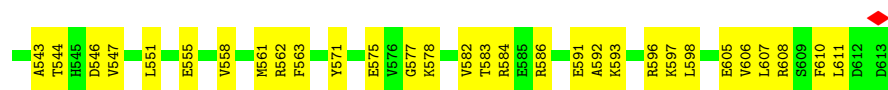


- Molecule 6: DNA-directed RNA polymerase subunit omega

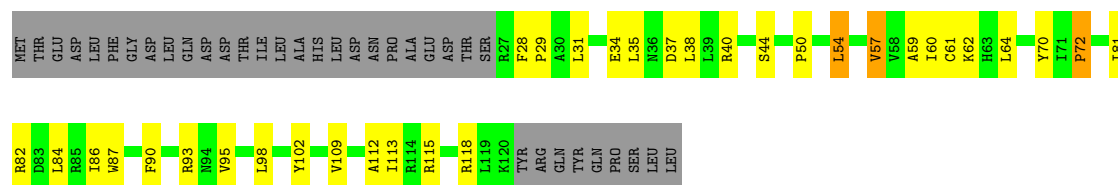


- Molecule 7: RNA polymerase sigma factor RpoD

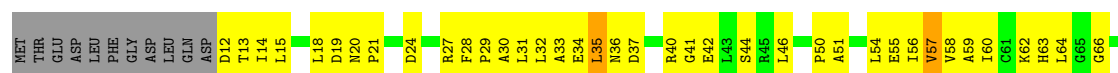




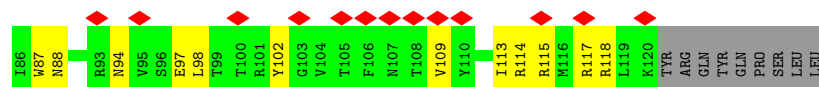
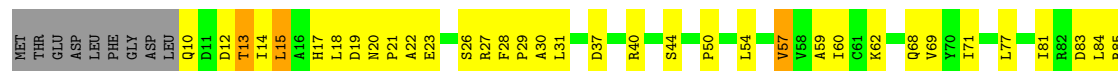
• Molecule 8: Middle operon regulator



• Molecule 8: Middle operon regulator



• Molecule 8: Middle operon regulator



• Molecule 8: Middle operon regulator



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99820	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 ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.482	Depositor
Minimum map value	-0.191	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1	0.23	0/1676	0.46	0/2585
2	2	0.22	0/1698	0.42	0/2621
3	A	0.11	0/1808	0.28	0/2450
3	B	0.10	0/1789	0.28	0/2425
3	P	0.10	0/561	0.30	0/762
4	C	0.11	0/10728	0.29	0/14474
5	D	0.11	0/10521	0.31	1/14196 (0.0%)
6	E	0.11	0/629	0.33	0/847
7	F	0.11	0/4028	0.31	0/5421
8	G	0.11	0/755	0.33	0/1019
8	J	0.17	0/869	0.44	0/1177
8	M	0.13	0/886	0.40	0/1200
8	N	0.13	0/755	0.35	0/1019
All	All	0.13	0/36703	0.33	1/50196 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	124	ILE	N-CA-C	-6.94	107.11	113.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1496	0	827	47	0
2	2	1510	0	822	30	0
3	A	1786	0	1813	36	0
3	B	1767	0	1789	49	0
3	P	554	0	573	21	0
4	C	10560	0	10573	226	0
5	D	10369	0	10590	251	0
6	E	627	0	634	24	0
7	F	3977	0	4008	118	0
8	G	743	0	755	31	0
8	J	855	0	855	47	0
8	M	872	0	867	33	0
8	N	743	0	755	28	0
All	All	35859	0	34861	864	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 12.

All (864) 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)
5:D:863:LEU:HD11	5:D:901:ARG:HB3	1.63	0.79
5:D:789:LYS:HD2	5:D:931:THR:HG23	1.63	0.78
7:F:482:GLU:HG2	7:F:486:ARG:HH22	1.50	0.77
7:F:592:ALA:HB1	7:F:596:ARG:HH21	1.51	0.76
3:A:91:ARG:HE	3:A:210:THR:HA	1.51	0.76
3:A:180:VAL:HA	3:A:207:THR:HG22	1.67	0.75
5:D:965:SER:HB3	5:D:973:LEU:HD11	1.69	0.75
4:C:560:PRO:HB2	5:D:776:THR:HG21	1.69	0.74
5:D:650:LYS:NZ	5:D:760:THR:O	2.20	0.74
7:F:145:LEU:HD11	7:F:224:LEU:HD13	1.70	0.74
4:C:812:PHE:O	5:D:504:GLN:NE2	2.21	0.74
7:F:381:GLU:HA	7:F:384:LEU:HD13	1.70	0.74
5:D:144:TYR:HB2	5:D:160:LEU:HB2	1.70	0.73
8:M:71:ILE:HG22	8:N:32:LEU:HD21	1.69	0.73
6:E:2:ALA:N	6:E:5:THR:O	2.23	0.72
5:D:706:VAL:HG12	5:D:715:LYS:HG2	1.71	0.71
7:F:399:LEU:HB2	7:F:447:ALA:HB2	1.71	0.71
2:2:27:DT:H2'	2:2:28:DT:C6	2.25	0.71
8:N:74:GLY:O	8:N:78:ASP:N	2.20	0.71
5:D:974:VAL:HG12	5:D:1002:VAL:HA	1.72	0.71
5:D:746:LEU:HG	5:D:758:PRO:HB3	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1137:GLU:HB3	4:C:1140:LYS:HB2	1.71	0.70
5:D:737:ILE:HA	5:D:740:LEU:HB2	1.73	0.70
4:C:975:ILE:HG22	4:C:994:ARG:HH21	1.55	0.70
6:E:3:ARG:HD3	6:E:4:VAL:HG13	1.75	0.69
1:1:36:DT:O4	8:N:107:ASN:ND2	2.25	0.69
3:A:77:ASP:OD1	3:A:77:ASP:N	2.23	0.69
1:1:47:DT:H2'	1:1:48:DT:H71	1.73	0.69
1:1:78:DC:H2''	1:1:79:DA:C8	2.28	0.69
8:J:15:LEU:HA	8:J:18:LEU:HB2	1.75	0.68
4:C:444:ASP:O	4:C:450:ASN:ND2	2.26	0.68
2:2:4:DC:H2'	2:2:5:DA:C8	2.27	0.68
4:C:1314:GLN:HE21	4:C:1315:MET:H	1.42	0.68
4:C:59:ILE:HD12	4:C:475:VAL:HG11	1.76	0.67
7:F:383:ASN:HB2	7:F:412:LEU:HD11	1.75	0.67
3:A:92:VAL:O	3:A:148:ARG:NH2	2.25	0.67
3:B:180:VAL:HA	3:B:207:THR:HG22	1.77	0.67
3:B:86:LYS:HZ1	3:B:176:CYS:HB2	1.59	0.66
4:C:368:ARG:NH2	7:F:90:GLU:O	2.29	0.66
4:C:490:GLN:HG2	7:F:472:GLN:HG3	1.77	0.66
4:C:1107:MET:HE1	5:D:736:GLN:HB3	1.78	0.66
7:F:388:ILE:HG22	7:F:405:ILE:HD12	1.78	0.66
4:C:243:PRO:O	4:C:247:ARG:NH2	2.29	0.65
4:C:1243:MET:HE3	5:D:445:LYS:HG3	1.77	0.65
1:1:47:DT:H2'	1:1:48:DT:C6	2.31	0.65
4:C:68:LEU:HD11	4:C:475:VAL:HG21	1.76	0.65
5:D:961:SER:O	5:D:980:THR:HA	1.97	0.65
4:C:1244:HIS:HD2	4:C:1268:GLN:HE22	1.44	0.65
5:D:803:VAL:HG11	5:D:1309:ILE:HG13	1.77	0.65
4:C:750:ILE:HD11	4:C:966:ILE:HG21	1.78	0.65
7:F:608:ARG:HA	7:F:611:LEU:HD23	1.79	0.64
3:A:58:GLU:HB2	3:A:145:LYS:HB2	1.77	0.64
8:N:115:ARG:HA	8:N:118:ARG:HD2	1.78	0.64
1:1:33:DC:H2''	1:1:34:DG:N7	2.12	0.64
8:G:44:SER:HB3	8:G:50:PRO:HG3	1.79	0.64
2:2:28:DT:H2'	2:2:29:DG:C8	2.32	0.64
5:D:1368:ASP:OD1	5:D:1371:ARG:NH2	2.31	0.63
3:P:273:GLU:HG2	3:P:284:ARG:HH12	1.63	0.63
5:D:242:LEU:HD12	5:D:243:PRO:HD2	1.81	0.63
5:D:72:CYS:SG	5:D:73:GLY:N	2.71	0.63
5:D:273:ILE:O	5:D:277:ASN:ND2	2.32	0.63
4:C:1066:MET:HE1	4:C:1234:LYS:HD2	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:363:LEU:HD13	5:D:618:VAL:HG23	1.80	0.62
8:G:93:ARG:NH2	3:P:268:ASN:O	2.32	0.62
4:C:342:ASP:OD1	4:C:439:LYS:NZ	2.33	0.62
8:J:84:LEU:HA	8:J:87:TRP:CE2	2.34	0.62
3:A:80:GLU:O	3:A:84:ASN:ND2	2.31	0.62
3:B:95:LYS:HE2	3:B:98:VAL:HG22	1.80	0.62
5:D:590:SER:O	5:D:594:GLN:NE2	2.33	0.62
8:J:115:ARG:HA	8:J:118:ARG:HD3	1.82	0.62
8:M:69:VAL:HG12	8:N:31:LEU:HD13	1.81	0.62
3:B:167:PRO:HD2	3:B:170:ARG:HE	1.65	0.62
5:D:160:LEU:HB3	5:D:164:GLN:HE22	1.64	0.62
5:D:960:LEU:HD13	5:D:963:VAL:HG21	1.82	0.62
7:F:122:ARG:HB3	7:F:371:LYS:HZ2	1.64	0.62
4:C:825:GLU:HG3	4:C:827:ARG:HG2	1.82	0.61
8:N:89:ASP:O	8:N:94:ASN:ND2	2.34	0.61
4:C:1032:LYS:HA	4:C:1035:LYS:HE3	1.82	0.61
7:F:124:GLU:O	7:F:128:ASN:ND2	2.33	0.61
3:A:70:THR:HG21	4:C:755:LYS:HE3	1.83	0.60
4:C:89:GLY:HA2	4:C:140:GLY:HA3	1.83	0.60
7:F:420:GLU:HB2	7:F:423:ARG:HG2	1.82	0.60
4:C:788:SER:O	4:C:788:SER:OG	2.17	0.60
4:C:820:GLU:OE1	4:C:824:GLN:NE2	2.34	0.60
5:D:264:ASP:OD1	5:D:264:ASP:N	2.22	0.60
7:F:168:PRO:HG3	7:F:220:LYS:HE3	1.83	0.60
4:C:1288:GLN:O	4:C:1292:THR:HB	2.01	0.60
5:D:586:GLY:HA3	5:D:612:LEU:HD11	1.82	0.60
4:C:204:LEU:HB3	4:C:208:ILE:HD12	1.83	0.60
5:D:741:ALA:O	5:D:762:ASN:ND2	2.34	0.60
2:2:27:DT:OP2	7:F:465:ARG:NH2	2.27	0.60
8:M:81:ILE:HD12	8:N:54:LEU:HB2	1.83	0.60
8:N:91:ASN:OD1	8:N:94:ASN:ND2	2.34	0.60
4:C:888:THR:HG23	4:C:914:LYS:HB3	1.82	0.60
7:F:119:ILE:HG12	7:F:122:ARG:HH21	1.65	0.60
8:J:29:PRO:HA	8:J:32:LEU:HG	1.84	0.60
4:C:192:ASP:HB3	4:C:346:TYR:HD1	1.67	0.60
5:D:523:GLU:OE2	5:D:547:ARG:NH1	2.33	0.60
5:D:1068:THR:HG22	5:D:1070:GLY:H	1.67	0.60
4:C:118:LYS:NZ	4:C:485:ASP:O	2.35	0.59
4:C:1142:ARG:NH1	4:C:1161:LEU:O	2.35	0.59
4:C:483:ASP:HB3	4:C:487:LEU:HB2	1.83	0.59
3:P:285:THR:HG22	3:P:315:GLY:HA2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1244:HIS:NE2	4:C:1266:GLY:O	2.34	0.59
5:D:799:ARG:NH1	5:D:1146:GLU:OE2	2.35	0.59
8:N:86:ILE:HG23	8:N:98:LEU:HD13	1.84	0.59
4:C:201:ARG:HB3	4:C:369:MET:HE2	1.84	0.59
5:D:1161:GLY:HA3	5:D:1179:PRO:HA	1.84	0.59
4:C:472:GLU:HA	4:C:475:VAL:HG12	1.84	0.59
5:D:1058:SER:OG	5:D:1059:LEU:N	2.35	0.59
5:D:1204:VAL:HG11	5:D:1210:ILE:HD11	1.85	0.59
8:J:29:PRO:O	8:J:33:ALA:N	2.34	0.59
5:D:276:ASN:OD1	5:D:280:LYS:NZ	2.35	0.59
7:F:221:PHE:HD1	7:F:224:LEU:HD12	1.68	0.59
8:J:31:LEU:O	8:J:34:GLU:HB3	2.03	0.59
4:C:813:GLU:HB2	5:D:461:PHE:HD2	1.68	0.58
3:A:56:VAL:HA	3:A:146:VAL:HG22	1.84	0.58
5:D:1028:ILE:HA	5:D:1120:THR:HA	1.85	0.58
8:J:59:ALA:HA	8:J:62:LYS:HG2	1.85	0.58
8:M:84:LEU:HA	8:M:87:TRP:CD1	2.39	0.58
3:A:234:LEU:HD11	3:B:12:ARG:HH22	1.67	0.58
5:D:212:THR:O	5:D:216:LYS:NZ	2.36	0.58
5:D:748:ALA:HA	5:D:754:ILE:HA	1.85	0.58
4:C:314:ASN:O	4:C:352:ARG:NH1	2.36	0.58
7:F:358:VAL:O	7:F:362:ASN:ND2	2.36	0.58
8:M:68:GLN:HA	8:N:70:TYR:HA	1.86	0.58
8:G:61:CYS:HA	8:J:71:ILE:HD11	1.85	0.58
3:A:192:VAL:HG21	3:A:198:LEU:HD12	1.84	0.58
3:P:283:GLN:O	3:P:317:ARG:NH2	2.30	0.58
4:C:120:GLN:NE2	4:C:488:MET:SD	2.76	0.57
4:C:533:LEU:HD21	4:C:571:LEU:HD13	1.85	0.57
5:D:966:VAL:HG13	5:D:974:VAL:HG23	1.84	0.57
6:E:59:ILE:HD12	6:E:64:LEU:HD11	1.85	0.57
4:C:302:ILE:HG22	4:C:309:LEU:HA	1.85	0.57
4:C:808:ASN:H	5:D:633:ALA:HB2	1.69	0.57
5:D:294:ASN:ND2	7:F:406:GLN:OE1	2.36	0.57
4:C:528:ARG:NH2	4:C:576:SER:O	2.37	0.57
8:J:32:LEU:O	8:J:35:LEU:HB2	2.04	0.57
8:J:82:ARG:HA	8:J:85:ARG:HD3	1.84	0.57
8:N:90:PHE:HB2	8:N:98:LEU:HD11	1.85	0.57
5:D:1350:ASN:HA	5:D:1353:VAL:HG12	1.86	0.57
4:C:149:LEU:N	4:C:531:SER:O	2.36	0.57
5:D:1026:PRO:HB2	5:D:1028:ILE:HG23	1.86	0.57
8:G:81:ILE:HD12	8:G:84:LEU:HD23	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:38:DA:H3'	7:F:586:ARG:HD2	1.87	0.57
4:C:716:ALA:HB3	4:C:784:ALA:H	1.70	0.57
5:D:495:ASN:ND2	5:D:1247:LYS:O	2.38	0.57
7:F:235:ILE:HD13	7:F:245:ALA:HB1	1.86	0.57
5:D:964:LYS:HD2	5:D:976:THR:HB	1.85	0.57
5:D:1109:LEU:HD12	5:D:1113:VAL:HG23	1.87	0.57
4:C:816:ILE:HB	4:C:1076:ILE:HD13	1.87	0.57
4:C:705:GLU:HB2	4:C:794:LEU:H	1.70	0.56
5:D:644:MET:HE1	5:D:740:LEU:HB3	1.87	0.56
1:1:52:DT:H2''	1:1:53:DA:C8	2.40	0.56
4:C:169:LYS:NZ	4:C:192:ASP:OD1	2.37	0.56
4:C:1126:ASP:HA	4:C:1129:ASN:ND2	2.21	0.56
5:D:1254:GLU:O	5:D:1258:ARG:N	2.34	0.56
7:F:125:ASP:HA	7:F:128:ASN:HD21	1.69	0.56
7:F:487:MET:HB3	7:F:489:MET:HG2	1.87	0.56
8:J:12:ASP:O	8:J:14:ILE:N	2.38	0.56
8:M:10:GLN:NE2	8:M:12:ASP:OD2	2.39	0.56
3:A:26:VAL:HB	3:A:203:ILE:HG23	1.86	0.56
4:C:660:VAL:HG13	4:C:661:VAL:HG13	1.86	0.56
3:B:57:THR:OG1	3:B:147:GLN:NE2	2.39	0.56
4:C:1122:LYS:HG2	4:C:1229:TYR:CZ	2.40	0.56
7:F:299:LYS:HA	7:F:302:PHE:HB3	1.88	0.56
5:D:432:LEU:HD12	5:D:435:GLN:HE22	1.71	0.56
5:D:579:LEU:HD13	5:D:582:ILE:HD12	1.86	0.56
6:E:42:GLU:OE2	6:E:52:ARG:NH2	2.39	0.56
1:1:39:DA:H2'	1:1:40:DT:H71	1.88	0.56
5:D:803:VAL:HG12	5:D:1313:SER:HB3	1.87	0.56
7:F:94:THR:HG22	7:F:96:ASP:H	1.71	0.56
8:J:36:ASN:HB3	8:J:57:VAL:HG11	1.88	0.56
5:D:529:GLY:N	5:D:532:GLU:OE2	2.39	0.56
1:1:31:DG:N2	2:2:59:DT:O2	2.39	0.56
4:C:348:SER:O	4:C:352:ARG:HG2	2.06	0.56
4:C:14:ASP:H	4:C:1157:GLN:HE22	1.54	0.55
5:D:406:ALA:HA	5:D:409:TRP:HD1	1.71	0.55
8:J:12:ASP:HB2	8:J:15:LEU:HD23	1.88	0.55
8:J:89:ASP:O	8:J:94:ASN:ND2	2.36	0.55
3:P:260:LEU:HD23	3:P:262:LEU:HD13	1.88	0.55
5:D:702:GLN:HG3	5:D:703:THR:HG23	1.87	0.55
7:F:240:ARG:HE	7:F:357:GLN:HE22	1.55	0.55
4:C:1314:GLN:HB2	6:E:28:ARG:HH22	1.71	0.55
5:D:274:ASN:HA	5:D:277:ASN:HD21	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:886:VAL:HA	5:D:1258:ARG:HD3	1.89	0.55
7:F:148:TYR:HA	7:F:151:VAL:HG22	1.89	0.55
8:G:31:LEU:HD13	8:J:69:VAL:HG12	1.88	0.55
3:P:285:THR:OG1	3:P:288:GLU:OE1	2.22	0.55
4:C:469:VAL:O	4:C:472:GLU:HG3	2.07	0.55
4:C:759:SER:OG	4:C:760:ASN:N	2.40	0.55
4:C:897:PRO:HA	4:C:900:LYS:HE3	1.88	0.55
3:B:56:VAL:HB	3:B:146:VAL:HG22	1.88	0.55
4:C:994:ARG:O	4:C:994:ARG:NH1	2.35	0.55
4:C:1280:ALA:HB1	5:D:918:ILE:HG22	1.88	0.55
5:D:744:ARG:HH22	5:D:767:LEU:HD21	1.72	0.55
4:C:794:LEU:HD21	4:C:796:LEU:HG	1.88	0.55
4:C:994:ARG:NH1	4:C:997:TRP:HB2	2.22	0.55
5:D:275:ARG:HG3	5:D:299:LEU:HD23	1.89	0.55
5:D:198:CYS:SG	5:D:202:ARG:NH2	2.80	0.54
7:F:119:ILE:HG21	7:F:379:MET:HB2	1.88	0.54
8:J:21:PRO:HA	8:J:24:ASP:HB2	1.89	0.54
4:C:135:THR:HG22	4:C:527:LYS:HZ3	1.72	0.54
4:C:1211:ARG:NH1	4:C:1213:TYR:OH	2.37	0.54
5:D:151:MET:HE1	5:D:176:PHE:HB3	1.89	0.54
8:J:40:ARG:HB2	8:J:50:PRO:HB3	1.88	0.54
4:C:590:PRO:HG2	4:C:655:VAL:HG21	1.88	0.54
5:D:156:ARG:HG2	5:D:157:GLN:HG3	1.88	0.54
6:E:30:MET:HE1	6:E:46:THR:HB	1.89	0.54
8:G:59:ALA:HA	8:G:62:LYS:HG2	1.89	0.54
1:1:76:DG:H5"	4:C:200:ARG:HH22	1.72	0.54
4:C:14:ASP:OD2	4:C:1156:ARG:NH2	2.40	0.54
4:C:318:SER:OG	4:C:320:ASP:OD1	2.23	0.54
4:C:842:ASP:HA	4:C:847:PRO:HA	1.90	0.54
5:D:1266:ILE:HD11	5:D:1276:GLU:HG2	1.88	0.54
4:C:134:GLY:O	4:C:527:LYS:NZ	2.40	0.54
4:C:236:LYS:HD2	4:C:286:GLU:HG3	1.89	0.54
7:F:358:VAL:HG22	7:F:362:ASN:HD21	1.73	0.54
4:C:1070:HIS:NE2	4:C:1114:GLU:OE1	2.39	0.54
5:D:288:PRO:HG2	7:F:380:VAL:HG21	1.89	0.54
5:D:1030:GLU:OE1	5:D:1099:TYR:OH	2.22	0.54
1:1:22:DA:H61	2:2:67:DT:H3	1.54	0.54
1:1:46:DT:H2"	1:1:47:DT:C6	2.43	0.54
4:C:867:GLU:HG2	4:C:943:LYS:HE2	1.89	0.54
4:C:978:VAL:HG21	4:C:1014:LEU:HD21	1.90	0.54
5:D:60:ARG:NH2	5:D:88:CYS:O	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1370:MET:HA	5:D:1373:ARG:HG2	1.89	0.54
4:C:41:GLN:NE2	4:C:73:TYR:O	2.40	0.54
5:D:355:ILE:HD11	5:D:449:LEU:HB2	1.90	0.54
5:D:1255:VAL:O	5:D:1258:ARG:HB3	2.08	0.54
7:F:144:LEU:HD13	7:F:261:LEU:HD21	1.90	0.54
5:D:846:GLU:HA	5:D:860:ARG:HG2	1.90	0.54
5:D:830:ASP:OD1	5:D:831:VAL:N	2.41	0.53
2:2:35:DG:H2'	2:2:36:DT:C6	2.43	0.53
3:A:45:ARG:NE	3:B:38:THR:OG1	2.29	0.53
4:C:14:ASP:OD1	4:C:15:PHE:N	2.42	0.53
5:D:495:ASN:OD1	5:D:495:ASN:N	2.41	0.53
5:D:1023:HIS:ND1	5:D:1126:GLN:O	2.41	0.53
4:C:387:ASN:HB3	4:C:394:ARG:HE	1.72	0.53
4:C:1125:GLY:HA3	4:C:1179:GLY:HA2	1.89	0.53
7:F:98:VAL:HG22	7:F:402:LEU:HD13	1.90	0.53
8:G:87:TRP:HE3	8:G:112:ALA:HB1	1.72	0.53
8:J:12:ASP:OD1	8:J:12:ASP:N	2.42	0.53
5:D:53:ARG:NH2	5:D:58:CYS:SG	2.81	0.53
5:D:865:HIS:CE1	5:D:867:GLN:HB2	2.43	0.53
8:M:98:LEU:HD22	8:M:102:TYR:HE2	1.74	0.53
3:B:77:ASP:OD1	3:B:78:ILE:N	2.34	0.53
4:C:483:ASP:OD1	4:C:486:THR:N	2.37	0.53
4:C:18:ARG:NH2	4:C:620:ASN:OD1	2.42	0.53
8:M:118:ARG:HH22	8:N:29:PRO:HB2	1.73	0.53
7:F:495:ARG:O	7:F:499:LYS:HG2	2.09	0.53
5:D:264:ASP:OD2	5:D:325:LYS:N	2.37	0.53
8:M:83:ASP:OD2	8:M:115:ARG:NH1	2.37	0.53
8:M:109:VAL:O	8:M:113:ILE:HG12	2.09	0.53
4:C:1184:THR:HG23	4:C:1189:GLY:HA2	1.91	0.53
5:D:747:MET:SD	5:D:747:MET:N	2.82	0.53
8:M:84:LEU:O	8:M:88:ASN:ND2	2.40	0.53
3:P:250:ASP:HB3	3:P:253:LEU:HD23	1.90	0.53
5:D:342:LEU:HD12	5:D:1352:ILE:HG23	1.90	0.52
4:C:490:GLN:NE2	7:F:472:GLN:O	2.42	0.52
8:J:42:GLU:O	8:J:46:LEU:N	2.37	0.52
8:J:83:ASP:OD2	8:J:115:ARG:NH1	2.41	0.52
4:C:1308:ILE:HD12	5:D:380:PHE:HE1	1.75	0.52
5:D:205:LEU:O	5:D:214:ARG:NH1	2.41	0.52
5:D:367:GLY:HA3	5:D:448:GLN:HB2	1.90	0.52
5:D:1256:ILE:O	5:D:1260:MET:N	2.41	0.52
8:M:15:LEU:HA	8:M:18:LEU:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:611:GLU:OE2	4:C:637:ARG:NH1	2.29	0.52
8:M:57:VAL:HA	8:M:60:ILE:HG12	1.90	0.52
2:2:54:DC:H2'	2:2:55:DC:C4	2.44	0.52
2:2:68:DT:H2''	2:2:69:DA:O5'	2.09	0.52
7:F:125:ASP:OD1	7:F:126:GLY:N	2.42	0.52
4:C:529:ARG:HD2	4:C:572:ILE:HG23	1.92	0.52
5:D:1203:ARG:NH1	5:D:1205:GLU:OE2	2.38	0.52
4:C:509:SER:OG	4:C:510:GLN:N	2.43	0.52
5:D:803:VAL:O	5:D:1259:GLN:HG2	2.10	0.52
8:G:72:PRO:HA	8:J:66:GLY:H	1.75	0.52
4:C:1313:HIS:CE1	6:E:31:GLN:HE22	2.28	0.52
3:B:158:ARG:HB3	3:B:172:LEU:HD21	1.92	0.51
4:C:263:VAL:HG11	4:C:269:ILE:HG13	1.92	0.51
7:F:221:PHE:O	7:F:225:ARG:HG2	2.09	0.51
8:J:40:ARG:HH12	8:J:51:ALA:HA	1.76	0.51
4:C:673:HIS:ND1	5:D:763:PHE:O	2.41	0.51
4:C:1020:GLU:HA	4:C:1023:HIS:CE1	2.45	0.51
4:C:1271:GLY:N	4:C:1274:GLU:OE2	2.43	0.51
3:A:84:ASN:HB3	3:A:130:ILE:HD12	1.92	0.51
7:F:227:GLN:HA	7:F:230:VAL:HG22	1.92	0.51
3:B:153:VAL:O	3:B:158:ARG:NH2	2.43	0.51
4:C:1026:GLU:O	4:C:1030:GLU:HG2	2.11	0.51
7:F:369:GLU:O	7:F:373:ARG:HG2	2.10	0.51
4:C:446:ASP:OD1	4:C:446:ASP:N	2.42	0.51
1:1:68:DT:C2	7:F:386:LEU:HG	2.45	0.51
5:D:514:THR:HG21	5:D:596:LEU:HD12	1.92	0.51
6:E:10:VAL:O	6:E:14:GLY:N	2.37	0.51
7:F:238:LYS:HB3	7:F:242:HIS:CG	2.45	0.51
2:2:21:DT:H1'	2:2:22:DA:H5'	1.92	0.50
4:C:102:LEU:HB2	4:C:118:LYS:HB2	1.93	0.50
4:C:820:GLU:HA	4:C:1079:ILE:HD11	1.92	0.50
4:C:1313:HIS:HE1	6:E:31:GLN:HE22	1.57	0.50
5:D:844:THR:HA	5:D:882:VAL:HA	1.92	0.50
8:N:97:GLU:O	8:N:101:ARG:N	2.44	0.50
1:1:84:DT:H2''	1:1:85:DG:C8	2.46	0.50
4:C:14:ASP:HA	4:C:1183:ALA:HB3	1.92	0.50
4:C:1066:MET:HB3	4:C:1232:MET:HE3	1.93	0.50
5:D:248:ASP:OD1	5:D:248:ASP:N	2.40	0.50
5:D:721:SER:HA	5:D:724:MET:HE2	1.92	0.50
8:J:30:ALA:O	8:J:33:ALA:HB3	2.12	0.50
3:B:67:GLU:HB2	3:B:79:LEU:HD21	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:806:PRO:HD3	4:C:1100:PRO:HG3	1.93	0.50
4:C:972:PHE:HB3	4:C:976:ARG:HE	1.75	0.50
5:D:393:THR:HG21	5:D:395:LYS:HZ3	1.76	0.50
7:F:122:ARG:HA	7:F:125:ASP:OD2	2.11	0.50
7:F:316:PHE:CE1	7:F:341:LEU:HD11	2.46	0.50
8:G:115:ARG:HA	8:G:118:ARG:HD2	1.93	0.50
5:D:611:ILE:HG22	5:D:612:LEU:HD12	1.92	0.50
6:E:71:GLU:O	6:E:74:GLU:HG3	2.12	0.50
2:2:16:DG:H2''	2:2:17:DA:C8	2.46	0.50
4:C:483:ASP:OD1	4:C:485:ASP:N	2.42	0.50
4:C:525:THR:HG21	4:C:687:ARG:HD2	1.94	0.50
5:D:279:LEU:HD12	5:D:295:GLU:HG3	1.94	0.50
1:1:69:DG:H5'	1:1:69:DG:H8	1.76	0.50
3:B:215:GLU:OE2	3:B:219:ARG:NH2	2.44	0.50
5:D:751:ASP:OD1	5:D:752:GLY:N	2.45	0.50
8:N:87:TRP:HA	8:N:90:PHE:HB3	1.94	0.50
1:1:74:DC:H3'	1:1:75:DT:H2'	1.93	0.50
2:2:25:DA:H3'	7:F:465:ARG:HD3	1.92	0.50
8:J:32:LEU:HA	8:J:35:LEU:HD23	1.93	0.50
5:D:827:GLU:HA	5:D:994:SER:HB3	1.93	0.50
5:D:1230:THR:HG22	5:D:1257:VAL:HG11	1.94	0.50
5:D:1268:ASN:HB2	5:D:1301:THR:HG22	1.93	0.50
3:A:131:CYS:SG	3:A:132:HIS:N	2.85	0.50
5:D:358:GLY:O	5:D:360:TYR:N	2.44	0.50
7:F:278:ASP:HA	7:F:281:ARG:HG2	1.92	0.50
7:F:305:LEU:HB3	7:F:315:TRP:HB2	1.94	0.50
8:G:60:ILE:O	8:G:64:LEU:HB2	2.11	0.50
8:M:81:ILE:HD13	8:M:84:LEU:HD21	1.93	0.50
4:C:759:SER:HB2	4:C:765:ILE:HD11	1.94	0.49
5:D:1155:ILE:H	5:D:1211:SER:HB3	1.76	0.49
5:D:374:LEU:HB3	5:D:412:LEU:HD11	1.94	0.49
5:D:531:LYS:O	5:D:534:GLU:HG3	2.11	0.49
7:F:240:ARG:O	7:F:246:GLN:NE2	2.38	0.49
4:C:292:ILE:HG22	4:C:317:LEU:HD11	1.94	0.49
7:F:455:HIS:O	7:F:458:GLU:HG3	2.12	0.49
8:J:54:LEU:O	8:J:57:VAL:HG22	2.12	0.49
4:C:248:GLY:O	4:C:268:ARG:NH1	2.43	0.49
4:C:700:VAL:HA	4:C:1182:ILE:HG22	1.93	0.49
4:C:805:MET:HE1	4:C:807:TRP:HE3	1.76	0.49
4:C:1244:HIS:CD2	4:C:1268:GLN:HE22	2.29	0.49
5:D:224:LEU:HD12	5:D:225:GLU:HG3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:492:SER:HB2	5:D:499:ILE:HD11	1.94	0.49
5:D:818:GLU:HA	5:D:845:ALA:HB1	1.93	0.49
5:D:1173:ARG:HB3	5:D:1190:ILE:HG13	1.94	0.49
4:C:120:GLN:HE22	4:C:490:GLN:HB2	1.77	0.49
5:D:490:ILE:HG13	5:D:491:LEU:HG	1.94	0.49
7:F:383:ASN:HB3	7:F:386:LEU:HD12	1.95	0.49
1:1:55:DG:H2'	1:1:56:DT:H71	1.94	0.49
3:B:109:PRO:HA	3:B:132:HIS:HA	1.94	0.49
8:G:28:PHE:CG	8:G:29:PRO:HD3	2.48	0.49
1:1:47:DT:H2''	1:1:48:DT:O5'	2.12	0.49
3:B:153:VAL:HG13	3:B:158:ARG:HH21	1.78	0.49
4:C:985:GLU:HB3	4:C:988:LYS:HG3	1.95	0.49
4:C:263:VAL:HG21	4:C:269:ILE:HG13	1.95	0.49
5:D:271:ARG:O	5:D:275:ARG:HG2	2.13	0.49
7:F:288:MET:HA	7:F:292:VAL:HB	1.95	0.49
1:1:26:DG:H2'	1:1:27:DT:H72	1.94	0.49
5:D:755:ILE:HG22	5:D:757:THR:H	1.78	0.49
6:E:38:LEU:HD22	6:E:58:LEU:HD21	1.95	0.49
7:F:141:ILE:HD12	7:F:141:ILE:H	1.78	0.49
1:1:37:DT:H2''	1:1:38:DA:C8	2.48	0.49
4:C:74:ARG:NH1	4:C:121:GLU:OE2	2.44	0.49
4:C:657:THR:OG1	4:C:1187:PHE:HB2	2.13	0.49
4:C:801:ARG:HB3	4:C:1094:VAL:HG23	1.94	0.49
4:C:1041:ASP:N	4:C:1041:ASP:OD1	2.45	0.49
4:C:1194:GLU:OE1	4:C:1194:GLU:N	2.43	0.49
3:A:226:GLU:HG3	3:B:10:LYS:NZ	2.28	0.48
5:D:583:VAL:HG23	5:D:587:LEU:HD23	1.95	0.48
8:J:34:GLU:O	8:J:37:ASP:HB2	2.13	0.48
8:M:13:THR:OG1	8:M:14:ILE:N	2.44	0.48
4:C:976:ARG:HB3	4:C:997:TRP:HZ3	1.76	0.48
1:1:29:DA:H2''	1:1:30:DA:C8	2.48	0.48
1:1:54:DC:H2''	1:1:55:DG:C8	2.48	0.48
4:C:840:SER:HB2	4:C:850:ILE:HD11	1.94	0.48
8:N:95:VAL:O	8:N:98:LEU:HB2	2.13	0.48
7:F:555:GLU:N	7:F:555:GLU:OE1	2.46	0.48
8:J:36:ASN:O	8:J:40:ARG:N	2.28	0.48
8:M:84:LEU:HA	8:M:87:TRP:NE1	2.28	0.48
1:1:70:DG:H5''	7:F:392:LYS:HD3	1.95	0.48
5:D:388:ARG:HG3	5:D:390:LEU:HD23	1.96	0.48
8:G:84:LEU:HA	8:G:87:TRP:CE2	2.49	0.48
1:1:37:DT:H2''	1:1:38:DA:H8	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:745:GLU:OE1	4:C:745:GLU:N	2.46	0.48
4:C:797:GLY:N	4:C:1231:TYR:OH	2.45	0.48
5:D:901:ARG:HA	5:D:908:ILE:HA	1.95	0.48
3:B:102:LEU:HB2	3:B:115:ILE:HG13	1.95	0.48
4:C:84:GLU:HA	4:C:87:ILE:HB	1.94	0.48
5:D:1175:LEU:HB2	5:D:1190:ILE:HD13	1.94	0.48
7:F:606:VAL:HG13	7:F:607:LEU:HD22	1.94	0.48
1:1:38:DA:H2'	1:1:39:DA:C8	2.49	0.48
5:D:1254:GLU:OE1	5:D:1254:GLU:N	2.46	0.48
1:1:36:DT:H3'	8:J:27:ARG:HD2	1.95	0.48
3:B:9:LEU:HD13	3:B:30:PRO:HG2	1.95	0.48
3:B:91:ARG:HH21	3:B:210:THR:HA	1.78	0.48
4:C:93:SER:HA	4:C:128:PRO:HA	1.95	0.48
4:C:1305:TYR:HE1	5:D:379:PRO:HG3	1.78	0.48
6:E:75:GLN:O	6:E:79:GLU:HG2	2.14	0.48
7:F:102:MET:HA	7:F:105:MET:HG3	1.94	0.48
3:A:31:LEU:O	3:A:33:ARG:NH2	2.47	0.48
4:C:803:ALA:HB2	4:C:1227:VAL:HG22	1.96	0.48
5:D:395:LYS:HE3	7:F:610:PHE:HA	1.95	0.48
7:F:151:VAL:HG11	7:F:161:LEU:HD11	1.96	0.48
8:M:12:ASP:HB2	8:M:15:LEU:HB3	1.96	0.48
1:1:34:DG:OP2	8:N:82:ARG:NH1	2.47	0.47
1:1:80:DC:H2'	1:1:81:DG:C8	2.49	0.47
7:F:505:ILE:HG13	7:F:506:SER:H	1.79	0.47
7:F:582:VAL:O	7:F:584:ARG:NE	2.41	0.47
8:M:94:ASN:HB2	8:M:97:GLU:HB3	1.96	0.47
3:B:158:ARG:NH1	3:B:173:VAL:O	2.47	0.47
4:C:580:GLN:HG2	4:C:581:THR:H	1.79	0.47
5:D:506:VAL:HG13	5:D:628:GLY:HA3	1.96	0.47
5:D:1038:THR:OG1	5:D:1079:LYS:HG2	2.15	0.47
7:F:334:SER:HA	7:F:337:VAL:HG12	1.96	0.47
7:F:380:VAL:HG12	7:F:416:VAL:HG21	1.96	0.47
8:M:19:ASP:O	8:M:23:GLU:N	2.41	0.47
5:D:151:MET:HE2	5:D:172:PHE:CG	2.49	0.47
1:1:18:DT:H2'	1:1:19:DG:C8	2.48	0.47
4:C:86:GLN:HA	4:C:140:GLY:HA2	1.96	0.47
5:D:1069:ALA:HA	5:D:1072:LYS:HE2	1.96	0.47
5:D:1159:ILE:HG13	5:D:1177:ILE:HG21	1.96	0.47
8:M:85:ARG:HG2	8:M:102:TYR:HE1	1.79	0.47
4:C:971:LEU:O	4:C:975:ILE:HG12	2.14	0.47
8:N:84:LEU:HA	8:N:87:TRP:CE2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:38:DA:H3'	7:F:586:ARG:HH11	1.79	0.47
4:C:726:TYR:HB3	4:C:733:VAL:HB	1.96	0.47
4:C:1281:TYR:OH	5:D:489:ASN:ND2	2.48	0.47
5:D:1109:LEU:HD13	5:D:1115:ILE:HG23	1.96	0.47
8:J:55:GLU:O	8:J:58:VAL:HG12	2.14	0.47
3:P:280:ASP:OD1	3:P:321:TRP:NE1	2.45	0.47
3:P:303:ILE:HG13	3:P:304:LYS:HD3	1.97	0.47
3:B:78:ILE:HA	3:B:81:ILE:HG12	1.96	0.47
3:B:104:LYS:HD3	3:B:105:SER:N	2.30	0.47
4:C:101:ARG:HG2	4:C:119:GLU:HB2	1.96	0.47
4:C:1287:LEU:O	4:C:1291:LEU:HG	2.14	0.47
5:D:450:HIS:O	5:D:453:VAL:HG22	2.15	0.47
5:D:796:LEU:HD22	5:D:799:ARG:HH21	1.79	0.47
7:F:309:ASN:ND2	7:F:314:THR:OG1	2.48	0.47
7:F:412:LEU:O	7:F:416:VAL:HG23	2.14	0.47
7:F:482:GLU:HG2	7:F:486:ARG:NH2	2.24	0.47
7:F:492:ASP:O	7:F:496:LYS:HG2	2.14	0.47
8:M:54:LEU:O	8:M:57:VAL:HG12	2.14	0.47
5:D:69:GLU:HG2	5:D:77:ARG:HH22	1.80	0.47
5:D:97:VAL:HG22	5:D:101:ARG:HG3	1.96	0.47
5:D:527:LEU:HD12	5:D:527:LEU:HA	1.77	0.47
5:D:545:HIS:O	5:D:545:HIS:ND1	2.47	0.47
4:C:146:VAL:HG13	4:C:511:LEU:HD12	1.97	0.47
5:D:75:TYR:HD1	5:D:80:HIS:CE1	2.33	0.47
5:D:803:VAL:HG21	5:D:1309:ILE:HD11	1.97	0.47
2:2:36:DT:H2''	2:2:37:DA:C8	2.49	0.47
4:C:870:ILE:HG13	4:C:884:VAL:HG12	1.97	0.47
3:P:268:ASN:HA	3:P:271:LYS:HE2	1.97	0.47
2:2:17:DA:H2''	2:2:18:DG:C5	2.50	0.46
3:B:17:GLU:HB2	3:B:25:LYS:HE3	1.97	0.46
3:B:81:ILE:HD12	3:B:131:CYS:HB3	1.97	0.46
4:C:320:ASP:OD1	4:C:320:ASP:N	2.44	0.46
4:C:636:CYS:HB2	4:C:645:PHE:CD2	2.50	0.46
4:C:1212:LEU:HD23	4:C:1225:VAL:HB	1.97	0.46
5:D:494:ALA:HA	5:D:1252:HIS:CD2	2.50	0.46
5:D:1255:VAL:HG13	5:D:1256:ILE:HD12	1.96	0.46
3:B:229:GLU:HA	3:B:232:VAL:HG13	1.97	0.46
5:D:264:ASP:HB3	5:D:324:LEU:HD22	1.97	0.46
5:D:666:GLU:O	5:D:669:GLN:HG2	2.15	0.46
8:G:72:PRO:O	8:J:66:GLY:N	2.48	0.46
4:C:339:ASN:HB3	4:C:343:HIS:H	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:550:VAL:O	5:D:777:HIS:NE2	2.47	0.46
4:C:738:GLU:HA	4:C:741:MET:HG2	1.96	0.46
4:C:1230:MET:HE3	4:C:1230:MET:HB3	1.73	0.46
5:D:1115:ILE:HB	5:D:1119:ASP:HB3	1.97	0.46
7:F:108:VAL:HG11	7:F:381:GLU:HG3	1.97	0.46
1:1:46:DT:H2''	1:1:47:DT:H6	1.80	0.46
3:A:80:GLU:OE1	3:A:84:ASN:ND2	2.48	0.46
3:B:194:GLN:HG2	3:B:195:ARG:HG2	1.97	0.46
4:C:980:VAL:HG13	4:C:984:VAL:HG12	1.97	0.46
5:D:749:LYS:HG3	5:D:751:ASP:OD1	2.16	0.46
3:B:178:SER:HB2	5:D:535:ARG:HH22	1.80	0.46
4:C:358:ASP:N	4:C:358:ASP:OD1	2.49	0.46
4:C:562:GLU:OE2	4:C:574:SER:N	2.48	0.46
5:D:1140:ARG:NH2	5:D:1236:GLU:OE2	2.49	0.46
7:F:285:ARG:O	7:F:289:LYS:HG2	2.14	0.46
8:M:37:ASP:O	8:M:40:ARG:HG2	2.16	0.46
1:1:68:DT:H1'	7:F:385:ARG:HB3	1.97	0.46
3:A:95:LYS:NZ	3:A:120:ASP:OD2	2.47	0.46
4:C:65:ASN:HA	4:C:105:TYR:HB2	1.98	0.46
4:C:104:ILE:HD12	4:C:116:ASP:HB3	1.98	0.46
4:C:238:GLN:OE1	4:C:285:ILE:N	2.48	0.46
4:C:302:ILE:HG22	4:C:309:LEU:HD23	1.98	0.46
4:C:994:ARG:HH12	4:C:998:LEU:HD12	1.79	0.46
6:E:26:ARG:HD3	6:E:59:ILE:HD13	1.98	0.46
2:2:29:DG:H2'	2:2:30:DA:C8	2.50	0.46
4:C:721:GLY:H	4:C:779:ARG:HG2	1.79	0.46
5:D:262:THR:OG1	5:D:266:ASN:ND2	2.48	0.46
5:D:574:VAL:O	5:D:578:ILE:HG12	2.16	0.46
3:B:24:ALA:HB3	3:B:205:MET:SD	2.56	0.46
4:C:491:ASP:OD1	7:F:472:GLN:NE2	2.39	0.46
4:C:755:LYS:HA	4:C:755:LYS:HD3	1.59	0.46
4:C:1172:LEU:O	4:C:1176:LEU:HG	2.16	0.46
4:C:1278:LEU:HD23	4:C:1287:LEU:HB3	1.97	0.46
6:E:24:ALA:O	6:E:28:ARG:HG2	2.16	0.46
7:F:338:HIS:O	7:F:342:GLN:HG2	2.15	0.46
7:F:506:SER:OG	7:F:508:GLU:N	2.42	0.46
8:J:41:GLY:O	8:J:44:SER:OG	2.24	0.46
1:1:72:DA:OP1	1:1:73:DG:N2	2.48	0.46
4:C:375:PRO:HG3	7:F:87:VAL:HG21	1.98	0.46
8:G:90:PHE:HB2	8:G:98:LEU:HD11	1.98	0.46
8:J:116:MET:HA	8:J:116:MET:HE2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:460:ASP:OD1	5:D:460:ASP:N	2.49	0.46
5:D:532:GLU:O	5:D:535:ARG:HG2	2.16	0.46
4:C:142:GLU:OE1	4:C:517:GLN:NE2	2.49	0.45
4:C:477:GLU:OE1	4:C:477:GLU:N	2.49	0.45
7:F:88:GLU:HA	7:F:91:ILE:HG23	1.99	0.45
7:F:242:HIS:HB3	7:F:245:ALA:HB3	1.98	0.45
7:F:326:TRP:CD1	7:F:326:TRP:H	2.33	0.45
3:A:6:THR:OG1	3:A:7:GLU:N	2.49	0.45
3:B:54:CYS:SG	3:B:148:ARG:NH1	2.89	0.45
4:C:629:PHE:HE2	4:C:650:VAL:HG11	1.81	0.45
4:C:1024:GLU:OE1	4:C:1028:LYS:NZ	2.49	0.45
5:D:591:ILE:HG23	5:D:592:VAL:HG13	1.98	0.45
5:D:655:SER:HA	5:D:658:GLU:HG3	1.99	0.45
5:D:1357:ILE:O	5:D:1362:GLY:HA3	2.16	0.45
7:F:401:PHE:O	7:F:405:ILE:HG12	2.16	0.45
8:N:40:ARG:HB2	8:N:50:PRO:HB3	1.98	0.45
4:C:270:THR:OG1	4:C:273:HIS:ND1	2.40	0.45
5:D:204:GLU:O	5:D:207:GLU:HG2	2.16	0.45
5:D:1297:LYS:NZ	5:D:1299:GLY:O	2.36	0.45
8:G:70:TYR:HD2	8:G:72:PRO:HD3	1.81	0.45
3:P:275:ILE:HG21	3:P:281:LEU:HB3	1.98	0.45
3:P:300:LEU:HG	3:P:301:THR:HG23	1.98	0.45
4:C:811:ASN:HA	4:C:815:SER:HB3	1.97	0.45
6:E:7:GLN:O	6:E:10:VAL:HG22	2.16	0.45
7:F:605:GLU:OE1	7:F:605:GLU:N	2.46	0.45
3:P:284:ARG:HE	3:P:288:GLU:HG2	1.80	0.45
3:P:300:LEU:O	3:P:304:LYS:NZ	2.35	0.45
3:B:109:PRO:HB3	3:B:132:HIS:CD2	2.51	0.45
4:C:13:LYS:HB3	4:C:1182:ILE:HD12	1.98	0.45
4:C:192:ASP:HB3	4:C:346:TYR:CD1	2.51	0.45
5:D:1198:VAL:HG21	5:D:1204:VAL:HG21	1.98	0.45
3:P:254:LEU:H	3:P:254:LEU:HD23	1.82	0.45
2:2:49:DA:H2'	2:2:50:DT:H71	1.97	0.45
4:C:1160:ASP:OD2	4:C:1162:SER:OG	2.34	0.45
5:D:29:MET:HB3	5:D:29:MET:HE3	1.79	0.45
5:D:37:GLU:HB3	5:D:104:HIS:CE1	2.52	0.45
5:D:1034:PHE:HD1	5:D:1036:ARG:HH22	1.63	0.45
7:F:353:LEU:HD23	7:F:358:VAL:HB	1.98	0.45
8:N:109:VAL:O	8:N:113:ILE:HG12	2.17	0.45
1:1:36:DT:OP2	8:G:72:PRO:HG2	2.17	0.45
2:2:41:DA:H2''	2:2:42:DA:C8	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:104:LYS:HD2	3:B:110:VAL:HG12	1.99	0.45
4:C:741:MET:HE1	4:C:747:GLY:O	2.16	0.45
5:D:372:MET:SD	5:D:372:MET:N	2.90	0.45
1:1:65:DT:H6	1:1:65:DT:H5'	1.81	0.45
1:1:72:DA:H2''	1:1:73:DG:H5''	1.98	0.45
3:A:190:ALA:H	3:A:199:ASP:HA	1.82	0.45
3:B:118:ASP:OD1	3:B:118:ASP:N	2.48	0.45
3:B:179:PRO:HG3	3:B:211:ILE:HD12	1.98	0.45
5:D:350:SER:OG	5:D:469:HIS:ND1	2.44	0.45
5:D:601:ILE:O	5:D:604:MET:HG3	2.17	0.45
5:D:901:ARG:NE	5:D:906:GLY:O	2.35	0.45
7:F:374:ARG:HH12	7:F:378:GLU:HG3	1.81	0.45
7:F:524:GLU:HG3	7:F:526:THR:HG23	1.99	0.45
4:C:901:LEU:HD12	7:F:563:PHE:HD2	1.82	0.45
7:F:273:MET:O	7:F:276:MET:HG3	2.17	0.45
8:J:19:ASP:OD1	8:J:20:ASN:N	2.45	0.45
3:A:111:THR:OG1	3:A:126:PRO:O	2.30	0.44
5:D:1259:GLN:O	5:D:1262:ARG:NH1	2.50	0.44
6:E:30:MET:HE3	6:E:30:MET:HB3	1.83	0.44
7:F:457:ILE:HA	7:F:460:ILE:HG22	1.98	0.44
8:M:27:ARG:HB3	8:M:28:PHE:H	1.50	0.44
3:B:147:GLN:OE1	3:B:147:GLN:N	2.50	0.44
5:D:950:ILE:HG12	5:D:1020:TRP:HZ3	1.82	0.44
7:F:551:LEU:HD11	7:F:598:LEU:HD21	1.99	0.44
8:M:20:ASN:HB2	8:M:21:PRO:HD3	1.99	0.44
2:2:51:DT:H2''	2:2:52:DA:C8	2.51	0.44
4:C:563:THR:OG1	4:C:569:ILE:O	2.22	0.44
5:D:818:GLU:HB3	5:D:881:LYS:HE2	1.99	0.44
5:D:1290:ARG:HD2	5:D:1298:VAL:HB	1.99	0.44
6:E:36:ASP:N	6:E:36:ASP:OD1	2.48	0.44
7:F:577:GLY:HA3	7:F:584:ARG:HH22	1.82	0.44
3:P:260:LEU:O	3:P:310:ARG:NH2	2.50	0.44
3:B:67:GLU:HA	3:B:78:ILE:HD11	1.99	0.44
4:C:942:ASP:OD1	4:C:943:LYS:N	2.45	0.44
4:C:1192:GLU:O	4:C:1196:LYS:HG2	2.17	0.44
5:D:1084:GLN:HE21	5:D:1086:ASN:HD21	1.65	0.44
5:D:1220:ILE:HD12	5:D:1224:ARG:HH21	1.82	0.44
8:M:26:SER:O	8:M:29:PRO:HD2	2.18	0.44
2:2:72:DG:H2''	2:2:73:DA:C8	2.53	0.44
5:D:582:ILE:HD11	5:D:627:THR:HG21	2.00	0.44
5:D:841:GLY:HA2	5:D:901:ARG:HD3	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:575:GLU:HA	7:F:578:LYS:HE3	2.00	0.44
8:G:86:ILE:HG12	8:G:102:TYR:CD2	2.52	0.44
3:B:158:ARG:HD2	3:B:172:LEU:HD11	1.99	0.44
4:C:35:PHE:CG	4:C:130:MET:HG3	2.52	0.44
4:C:962:GLU:O	4:C:965:GLN:HG3	2.17	0.44
5:D:480:ALA:HA	5:D:484:MET:HB2	2.00	0.44
5:D:797:THR:HG22	5:D:924:GLY:HA3	1.99	0.44
5:D:848:VAL:HG11	5:D:880:VAL:HG12	2.00	0.44
5:D:970:SER:OG	5:D:972:LYS:NZ	2.46	0.44
5:D:1263:LYS:HG3	5:D:1307:LEU:HD11	1.99	0.44
7:F:125:ASP:HA	7:F:128:ASN:ND2	2.31	0.44
1:1:72:DA:H1'	1:1:73:DG:C8	2.52	0.44
3:A:33:ARG:NH2	3:A:198:LEU:HA	2.33	0.44
5:D:821:MET:SD	5:D:879:ALA:HB1	2.58	0.44
8:J:20:ASN:HB3	8:J:21:PRO:HD3	2.00	0.44
8:M:44:SER:HB3	8:M:50:PRO:HG3	2.00	0.44
2:2:34:DC:H1'	2:2:35:DG:C8	2.52	0.44
3:A:214:GLU:OE2	3:A:218:ARG:NH2	2.51	0.44
4:C:231:GLU:HA	4:C:331:LYS:O	2.17	0.44
4:C:800:MET:SD	4:C:800:MET:N	2.90	0.44
7:F:400:GLN:HG3	7:F:401:PHE:H	1.83	0.44
7:F:543:ALA:HA	7:F:546:ASP:OD2	2.17	0.44
8:G:57:VAL:O	8:G:60:ILE:HB	2.18	0.44
8:N:105:THR:HG23	8:N:108:THR:H	1.83	0.44
3:B:192:VAL:HG21	3:B:198:LEU:HD12	1.99	0.44
7:F:105:MET:HE1	7:F:385:ARG:HG3	2.00	0.44
7:F:224:LEU:HD11	7:F:259:PHE:CZ	2.53	0.44
4:C:817:LEU:HB3	4:C:1097:VAL:HB	1.99	0.43
4:C:1255:THR:O	4:C:1257:GLN:NE2	2.50	0.43
5:D:555:TYR:CE2	5:D:565:ALA:HB2	2.52	0.43
5:D:663:GLU:O	5:D:667:GLN:HG2	2.18	0.43
5:D:1024:THR:HG23	5:D:1123:ARG:HB3	1.99	0.43
7:F:292:VAL:HG22	7:F:297:MET:HB2	1.98	0.43
7:F:562:ARG:NH1	7:F:571:TYR:O	2.51	0.43
8:G:109:VAL:O	8:G:113:ILE:HG12	2.18	0.43
2:2:62:DA:H2''	2:2:63:DC:H5''	2.00	0.43
4:C:548:ARG:HA	4:C:570:GLY:HA3	2.00	0.43
4:C:702:THR:HG23	4:C:704:MET:H	1.83	0.43
8:M:71:ILE:HD12	8:N:61:CYS:HA	1.99	0.43
3:A:212:ASP:HB3	3:A:215:GLU:HG2	2.00	0.43
4:C:149:LEU:HD21	4:C:451:ARG:HD3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:230:PHE:HB2	4:C:333:ILE:HB	2.00	0.43
4:C:297:VAL:HA	4:C:335:THR:HG22	2.01	0.43
4:C:838:CYS:O	4:C:1049:ILE:HD12	2.18	0.43
4:C:1270:PHE:HB2	5:D:347:VAL:HB	1.99	0.43
5:D:579:LEU:HD22	5:D:579:LEU:HA	1.83	0.43
7:F:583:THR:OG1	7:F:586:ARG:HB3	2.18	0.43
8:M:19:ASP:HA	8:M:22:ALA:HB3	2.00	0.43
8:M:85:ARG:HG2	8:M:102:TYR:CE1	2.53	0.43
2:2:37:DA:H2''	2:2:38:DA:C8	2.54	0.43
4:C:1026:GLU:N	4:C:1026:GLU:OE1	2.51	0.43
4:C:1151:LEU:HA	4:C:1151:LEU:HD12	1.85	0.43
5:D:79:LYS:HG3	5:D:80:HIS:CE1	2.54	0.43
8:G:37:ASP:OD1	8:G:38:LEU:N	2.51	0.43
1:1:53:DA:C8	1:1:53:DA:H5'	2.52	0.43
3:B:92:VAL:O	3:B:148:ARG:NH1	2.51	0.43
4:C:10:ARG:NH1	4:C:697:LYS:HD3	2.34	0.43
4:C:636:CYS:HB2	4:C:645:PHE:HD2	1.83	0.43
4:C:1264:GLN:HE22	4:C:1266:GLY:HA3	1.84	0.43
7:F:244:THR:O	7:F:247:GLU:HG3	2.18	0.43
1:1:32:DC:H2''	1:1:33:DC:C6	2.54	0.43
5:D:305:ALA:HA	5:D:309:ASN:HA	2.01	0.43
5:D:700:ASN:O	5:D:704:GLU:HB3	2.19	0.43
7:F:456:MET:HE2	7:F:456:MET:H	1.84	0.43
3:A:185:TYR:HB2	3:A:201:LEU:HD11	2.00	0.43
3:B:220:ALA:HA	3:B:223:ILE:HG22	2.01	0.43
4:C:459:MET:O	4:C:463:GLN:HG2	2.19	0.43
4:C:543:ALA:HB3	4:C:548:ARG:HH21	1.84	0.43
4:C:1337:ILE:HD12	5:D:21:LYS:O	2.19	0.43
5:D:851:PRO:HG3	5:D:876:SER:H	1.84	0.43
6:E:2:ALA:N	6:E:55:GLU:OE2	2.52	0.43
7:F:426:LYS:O	7:F:429:THR:OG1	2.36	0.43
4:C:1287:LEU:HD21	5:D:1357:ILE:HG21	2.00	0.43
5:D:24:LEU:HG	5:D:232:ASN:HD21	1.84	0.43
5:D:962:ASN:HB3	5:D:979:ASN:O	2.18	0.43
8:J:56:ILE:O	8:J:60:ILE:HG12	2.18	0.43
1:1:47:DT:H2'	1:1:48:DT:C7	2.46	0.43
5:D:1057:SER:O	5:D:1110:GLU:HG2	2.18	0.43
6:E:8:ASP:HB2	6:E:55:GLU:OE1	2.18	0.43
7:F:506:SER:HG	7:F:508:GLU:H	1.62	0.43
8:N:84:LEU:HD23	8:N:87:TRP:HE1	1.84	0.43
4:C:99:LYS:HA	4:C:121:GLU:HA	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:347:ILE:HD11	4:C:433:ILE:HD11	2.01	0.43
4:C:1160:ASP:CG	4:C:1162:SER:HG	2.27	0.43
4:C:1330:ILE:HG23	4:C:1337:ILE:HG21	2.01	0.43
5:D:1063:ASP:OD1	5:D:1063:ASP:N	2.52	0.43
6:E:30:MET:SD	6:E:49:ILE:HD11	2.59	0.43
8:J:33:ALA:HA	8:J:36:ASN:ND2	2.33	0.43
3:B:205:MET:HE2	3:B:205:MET:HB2	1.80	0.42
4:C:1289:GLU:O	4:C:1294:LYS:HG2	2.18	0.42
7:F:593:LYS:O	7:F:596:ARG:HG2	2.19	0.42
8:J:84:LEU:HA	8:J:87:TRP:CD2	2.53	0.42
8:M:14:ILE:O	8:M:17:HIS:N	2.52	0.42
3:P:279:GLY:HA2	3:P:282:VAL:HG12	2.00	0.42
5:D:807:LEU:HD13	5:D:807:LEU:HA	1.90	0.42
5:D:1177:ILE:HG22	5:D:1179:PRO:HD3	1.99	0.42
5:D:1261:LEU:HD13	5:D:1261:LEU:HA	1.91	0.42
7:F:116:GLU:OE2	7:F:117:ILE:HG12	2.19	0.42
7:F:376:LYS:O	7:F:380:VAL:HG13	2.19	0.42
7:F:558:VAL:HA	7:F:561:MET:HG2	2.01	0.42
8:G:90:PHE:HZ	3:P:271:LYS:HD2	1.84	0.42
3:P:262:LEU:HD23	3:P:262:LEU:H	1.84	0.42
1:1:74:DC:H2'	1:1:75:DT:C2	2.54	0.42
2:2:9:DG:H2'	2:2:10:DT:H71	2.02	0.42
2:2:20:DG:OP2	5:D:259:ARG:NH2	2.51	0.42
4:C:202:ARG:HG2	4:C:369:MET:SD	2.60	0.42
4:C:991:LYS:HE3	4:C:991:LYS:HB3	1.92	0.42
5:D:495:ASN:HA	5:D:903:LEU:HD13	2.01	0.42
5:D:604:MET:HE2	5:D:604:MET:HB2	1.93	0.42
5:D:952:VAL:HG13	5:D:1013:GLY:HA2	2.01	0.42
5:D:1289:ASN:HB2	5:D:1294:ALA:HB3	2.01	0.42
7:F:100:MET:HB2	7:F:100:MET:HE2	1.79	0.42
3:A:100:LEU:HB2	3:A:144:ILE:HB	2.01	0.42
3:B:59:VAL:HG13	3:B:171:LEU:HB2	2.00	0.42
4:C:214:ASN:OD1	4:C:359:ARG:HD2	2.19	0.42
5:D:353:SER:HB2	5:D:447:ILE:HG12	2.00	0.42
5:D:672:LEU:HD23	5:D:672:LEU:H	1.85	0.42
5:D:968:ASN:HA	5:D:1118:GLY:HA3	2.00	0.42
7:F:123:ILE:O	7:F:127:ILE:HG12	2.19	0.42
8:G:82:ARG:O	8:G:86:ILE:HG13	2.19	0.42
3:P:282:VAL:HA	3:P:314:LEU:HD23	2.00	0.42
1:1:26:DG:H2'	1:1:27:DT:C7	2.49	0.42
4:C:1269:ARG:HA	5:D:346:ARG:HD3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:454:CYS:SG	5:D:455:ALA:N	2.92	0.42
3:B:57:THR:HA	3:B:173:VAL:HB	2.02	0.42
4:C:257:ALA:N	4:C:260:LYS:O	2.53	0.42
4:C:550:VAL:HB	5:D:777:HIS:HD2	1.85	0.42
4:C:1023:HIS:O	4:C:1027:LYS:HD3	2.20	0.42
4:C:1138:VAL:HG22	4:C:1170:MET:HE3	2.01	0.42
5:D:291:ILE:HD12	5:D:291:ILE:HA	1.92	0.42
5:D:1034:PHE:HA	5:D:1114:GLN:HB3	2.01	0.42
6:E:71:GLU:O	6:E:75:GLN:HG2	2.20	0.42
7:F:551:LEU:HD22	7:F:597:LYS:HE3	2.00	0.42
8:G:38:LEU:HD11	8:J:63:HIS:HB3	2.00	0.42
8:J:35:LEU:HD13	8:J:35:LEU:HA	1.84	0.42
8:N:44:SER:HB3	8:N:50:PRO:HG3	2.02	0.42
1:1:38:DA:H2''	1:1:39:DA:H8	1.85	0.42
1:1:80:DC:H2''	1:1:81:DG:O4'	2.20	0.42
4:C:262:TYR:OH	4:C:280:ASP:OD2	2.28	0.42
5:D:525:MET:SD	5:D:527:LEU:HD13	2.59	0.42
5:D:697:MET:HE2	5:D:697:MET:HB2	1.90	0.42
5:D:1257:VAL:HA	5:D:1260:MET:HB3	2.01	0.42
8:G:86:ILE:HG12	8:G:102:TYR:CG	2.55	0.42
8:M:59:ALA:O	8:M:62:LYS:HG3	2.19	0.42
2:2:60:DT:H6	2:2:60:DT:H2'	1.68	0.42
4:C:1314:GLN:HE21	4:C:1315:MET:N	2.14	0.42
5:D:322:ARG:HH22	7:F:508:GLU:HG2	1.84	0.42
5:D:428:THR:O	5:D:428:THR:OG1	2.30	0.42
5:D:682:VAL:HA	5:D:685:ILE:HG12	2.01	0.42
6:E:2:ALA:HA	6:E:55:GLU:HG3	2.02	0.42
7:F:345:GLN:O	7:F:349:GLU:HG2	2.20	0.42
4:C:590:PRO:HB2	4:C:655:VAL:HG11	2.02	0.42
4:C:632:ASP:N	4:C:632:ASP:OD1	2.53	0.42
4:C:1128:ILE:HD13	4:C:1176:LEU:HD13	2.01	0.42
4:C:1154:ASP:OD1	4:C:1154:ASP:N	2.52	0.42
5:D:441:LEU:HD23	5:D:441:LEU:HA	1.89	0.42
5:D:576:ARG:HD3	5:D:593:ASN:HA	2.02	0.42
7:F:454:VAL:HA	7:F:457:ILE:HG12	2.01	0.42
8:N:57:VAL:HA	8:N:60:ILE:HG12	2.01	0.42
8:N:57:VAL:O	8:N:60:ILE:HG12	2.19	0.42
8:N:84:LEU:HD23	8:N:87:TRP:NE1	2.35	0.42
1:1:83:DA:H2'	1:1:84:DT:H71	2.01	0.42
2:2:8:DC:H2''	2:2:9:DG:C8	2.55	0.42
3:A:142:MET:HE3	3:A:142:MET:HB3	1.95	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:218:ARG:O	3:A:222:THR:HG23	2.20	0.42
3:B:47:LEU:HD13	3:B:47:LEU:HA	1.90	0.42
4:C:1326:LEU:HG	5:D:331:ILE:HD11	2.02	0.42
5:D:224:LEU:HD12	5:D:225:GLU:N	2.35	0.42
5:D:865:HIS:HE1	5:D:867:GLN:HB2	1.83	0.42
8:J:109:VAL:O	8:J:113:ILE:HG12	2.20	0.42
5:D:217:LEU:HD13	5:D:217:LEU:HA	1.92	0.41
5:D:289:ASP:OD1	5:D:289:ASP:N	2.51	0.41
5:D:950:ILE:HG12	5:D:1020:TRP:CZ3	2.55	0.41
5:D:1046:ILE:HG22	5:D:1061:VAL:HG22	2.01	0.41
5:D:1346:GLY:N	5:D:1349:GLU:OE1	2.51	0.41
4:C:524:ILE:HD11	4:C:712:SER:HA	2.02	0.41
4:C:1286:THR:O	4:C:1290:MET:HG2	2.19	0.41
5:D:269:TYR:HA	5:D:272:VAL:HG22	2.00	0.41
8:G:35:LEU:HD23	8:J:64:LEU:HD22	2.01	0.41
8:G:54:LEU:O	8:G:57:VAL:HG22	2.20	0.41
8:J:56:ILE:H	8:J:56:ILE:HD12	1.85	0.41
3:A:99:ILE:HD11	3:A:143:ARG:HD3	2.03	0.41
4:C:1199:LEU:HD11	4:C:1206:THR:HA	2.02	0.41
5:D:111:THR:OG1	5:D:300:GLN:OE1	2.28	0.41
5:D:861:ASN:HB3	5:D:883:ARG:NH2	2.35	0.41
7:F:309:ASN:OD1	7:F:309:ASN:N	2.52	0.41
7:F:330:LEU:O	7:F:334:SER:N	2.53	0.41
8:G:64:LEU:HD11	8:J:35:LEU:HD21	2.02	0.41
3:B:178:SER:HB2	5:D:535:ARG:NH2	2.35	0.41
4:C:623:LEU:HD21	4:C:626:GLU:HA	2.02	0.41
4:C:1128:ILE:O	4:C:1131:MET:HG3	2.20	0.41
5:D:141:PHE:HD1	5:D:297:ARG:HG3	1.85	0.41
6:E:28:ARG:O	6:E:32:VAL:HG22	2.20	0.41
4:C:71:VAL:HG21	4:C:101:ARG:HG3	2.02	0.41
5:D:134:ASP:O	5:D:138:VAL:HG23	2.20	0.41
8:N:95:VAL:HA	8:N:98:LEU:HD12	2.01	0.41
2:2:4:DC:H2''	2:2:5:DA:O4'	2.20	0.41
3:B:8:PHE:HD2	3:B:32:GLU:HG3	1.85	0.41
5:D:133:ARG:HB2	7:F:93:ARG:CZ	2.50	0.41
5:D:682:VAL:HG22	5:D:686:TRP:CD1	2.56	0.41
5:D:712:GLN:HG2	5:D:713:GLU:H	1.84	0.41
5:D:750:PRO:HA	5:D:781:LYS:HE2	2.03	0.41
7:F:544:THR:HA	7:F:547:VAL:HG12	2.02	0.41
8:G:35:LEU:HD22	8:J:64:LEU:HD13	2.02	0.41
3:P:290:LEU:HD11	3:P:300:LEU:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:69:DG:H5'	1:1:69:DG:C8	2.53	0.41
4:C:81:ASP:N	4:C:84:GLU:OE2	2.43	0.41
4:C:1009:ASN:O	4:C:1012:GLU:HG3	2.20	0.41
5:D:202:ARG:NH2	5:D:225:GLU:OE2	2.53	0.41
5:D:1331:VAL:HA	5:D:1334:GLU:HG2	2.03	0.41
2:2:6:DT:C2	2:2:7:DC:C5	3.09	0.41
3:A:33:ARG:HH22	3:A:198:LEU:HA	1.86	0.41
3:A:44:ARG:HG3	3:A:183:ILE:HG13	2.03	0.41
5:D:480:ALA:HA	5:D:484:MET:HE2	2.02	0.41
5:D:800:LEU:HG	5:D:923:ILE:HD11	2.02	0.41
5:D:808:VAL:HG12	5:D:914:ALA:HA	2.03	0.41
5:D:963:VAL:HA	5:D:980:THR:OG1	2.21	0.41
5:D:1030:GLU:HG2	5:D:1031:VAL:HG13	2.03	0.41
5:D:1357:ILE:O	5:D:1359:ALA:N	2.48	0.41
7:F:160:ASP:O	7:F:163:THR:OG1	2.35	0.41
2:2:35:DG:H2''	2:2:36:DT:O5'	2.20	0.41
2:2:61:DT:O4	2:2:62:DA:N6	2.54	0.41
3:A:45:ARG:HE	3:B:38:THR:HG1	1.58	0.41
4:C:373:GLY:HA2	7:F:91:ILE:HG22	2.02	0.41
4:C:447:HIS:CD2	4:C:553:THR:HG21	2.55	0.41
4:C:581:THR:HG22	4:C:582:ASN:O	2.21	0.41
4:C:672:GLU:OE1	4:C:672:GLU:N	2.49	0.41
5:D:137:ARG:HG3	7:F:93:ARG:HH12	1.85	0.41
5:D:725:MET:HE2	5:D:725:MET:HB2	1.96	0.41
7:F:417:ASP:OD1	7:F:418:LYS:N	2.54	0.41
3:A:205:MET:SD	3:A:207:THR:HG23	2.61	0.41
3:B:76:GLU:HB3	3:B:80:GLU:HG3	2.02	0.41
5:D:615:LYS:HG2	6:E:7:GLN:NE2	2.36	0.41
3:A:45:ARG:NH2	3:B:34:GLY:O	2.48	0.40
3:B:66:HIS:CD2	3:B:68:TYR:HB2	2.56	0.40
4:C:178:PRO:HA	4:C:397:LEU:HD23	2.03	0.40
4:C:478:ARG:HD2	4:C:478:ARG:HA	1.83	0.40
5:D:1176:VAL:HG13	5:D:1187:GLU:HG2	2.04	0.40
8:J:98:LEU:HD22	8:J:102:TYR:HE2	1.87	0.40
8:M:77:LEU:HD21	8:N:58:VAL:HG22	2.04	0.40
4:C:1243:MET:O	4:C:1262:LYS:NZ	2.42	0.40
5:D:658:GLU:HA	5:D:661:VAL:HB	2.02	0.40
5:D:1027:VAL:HG12	5:D:1122:ALA:H	1.85	0.40
5:D:1175:LEU:HD12	5:D:1190:ILE:HD13	2.02	0.40
5:D:1198:VAL:HG11	5:D:1204:VAL:HG22	2.03	0.40
7:F:413:MET:HE2	7:F:413:MET:HB2	1.81	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:84:LEU:HD12	8:G:87:TRP:NE1	2.35	0.40
8:M:114:ARG:HH21	8:M:117:ARG:HD2	1.86	0.40
1:1:47:DT:H2'	1:1:48:DT:C5	2.57	0.40
4:C:484:LEU:H	4:C:484:LEU:HD23	1.87	0.40
4:C:550:VAL:HB	5:D:777:HIS:CD2	2.57	0.40
4:C:1294:LYS:HB3	5:D:348:ASP:H	1.85	0.40
5:D:295:GLU:O	5:D:298:MET:HG2	2.21	0.40
7:F:555:GLU:HA	7:F:558:VAL:HG12	2.03	0.40
3:A:80:GLU:CD	3:A:84:ASN:HD21	2.29	0.40
5:D:147:ILE:O	5:D:156:ARG:NH1	2.55	0.40
5:D:393:THR:HG23	5:D:396:ALA:H	1.87	0.40
5:D:534:GLU:O	5:D:538:ARG:HG2	2.21	0.40
5:D:1270:GLY:C	5:D:1290:ARG:HH12	2.28	0.40
8:G:34:GLU:HA	8:G:37:ASP:OD2	2.21	0.40
8:G:37:ASP:O	8:G:40:ARG:HG2	2.22	0.40
3:A:225:ALA:O	3:A:229:GLU:HG3	2.22	0.40
4:C:214:ASN:HD21	4:C:359:ARG:NH1	2.20	0.40
4:C:1321:GLU:O	4:C:1325:VAL:HG13	2.22	0.40
5:D:210:SER:O	5:D:214:ARG:HG2	2.21	0.40
5:D:474:LEU:HD12	5:D:474:LEU:HA	1.87	0.40
5:D:1162:ILE:HD13	5:D:1203:ARG:HB2	2.04	0.40
8:J:27:ARG:HD3	8:J:28:PHE:CD1	2.56	0.40
8:J:75:GLN:H	8:J:75:GLN:CD	2.28	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	
3	A	228/329 (69%)	221 (97%)	7 (3%)	0	100	100
3	B	226/329 (69%)	224 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	67/329 (20%)	65 (97%)	2 (3%)	0	100	100
4	C	1338/1342 (100%)	1304 (98%)	34 (2%)	0	100	100
5	D	1322/1407 (94%)	1279 (97%)	43 (3%)	0	100	100
6	E	77/91 (85%)	72 (94%)	5 (6%)	0	100	100
7	F	490/613 (80%)	468 (96%)	22 (4%)	0	100	100
8	G	92/129 (71%)	86 (94%)	5 (5%)	1 (1%)	11	40
8	J	107/129 (83%)	97 (91%)	9 (8%)	1 (1%)	14	44
8	M	109/129 (84%)	101 (93%)	6 (6%)	2 (2%)	6	32
8	N	92/129 (71%)	86 (94%)	5 (5%)	1 (1%)	11	40
All	All	4148/4956 (84%)	4003 (96%)	140 (3%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	M	30	ALA
8	N	72	PRO
8	J	13	THR
8	M	13	THR
8	G	72	PRO

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	
3	A	198/286 (69%)	189 (96%)	9 (4%)	24	48
3	B	196/286 (68%)	185 (94%)	11 (6%)	19	44
3	P	63/286 (22%)	61 (97%)	2 (3%)	34	55
4	C	1152/1157 (100%)	1111 (96%)	41 (4%)	31	53
5	D	1115/1168 (96%)	1068 (96%)	47 (4%)	26	50
6	E	67/75 (89%)	66 (98%)	1 (2%)	57	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	F	430/540 (80%)	419 (97%)	11 (3%)	40	60
8	G	77/112 (69%)	74 (96%)	3 (4%)	28	52
8	J	90/112 (80%)	87 (97%)	3 (3%)	33	55
8	M	92/112 (82%)	89 (97%)	3 (3%)	33	55
8	N	77/112 (69%)	72 (94%)	5 (6%)	15	41
All	All	3557/4246 (84%)	3421 (96%)	136 (4%)	30	52

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	25	LYS
3	A	59	VAL
3	A	77	ASP
3	A	88	LEU
3	A	99	ILE
3	A	202	VAL
3	A	203	ILE
3	A	223	ILE
3	A	228	LEU
3	B	26	VAL
3	B	37	HIS
3	B	46	ILE
3	B	47	LEU
3	B	56	VAL
3	B	59	VAL
3	B	74	VAL
3	B	153	VAL
3	B	202	VAL
3	B	203	ILE
3	B	224	LEU
4	C	59	ILE
4	C	98	VAL
4	C	102	LEU
4	C	114	VAL
4	C	135	THR
4	C	146	VAL
4	C	184	LEU
4	C	229	ILE
4	C	237	LEU
4	C	306	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	C	442	VAL
4	C	461	GLU
4	C	488	MET
4	C	498	ILE
4	C	504	GLU
4	C	509	SER
4	C	515	MET
4	C	569	ILE
4	C	589	THR
4	C	615	VAL
4	C	630	VAL
4	C	657	THR
4	C	662	SER
4	C	663	VAL
4	C	759	SER
4	C	788	SER
4	C	819	SER
4	C	878	THR
4	C	888	THR
4	C	933	VAL
4	C	953	LEU
4	C	959	ASP
4	C	1046	VAL
4	C	1051	LYS
4	C	1052	VAL
4	C	1117	LEU
4	C	1141	LEU
4	C	1159	VAL
4	C	1195	ILE
4	C	1253	LEU
4	C	1340	GLU
5	D	29	MET
5	D	83	VAL
5	D	92	VAL
5	D	102	MET
5	D	145	VAL
5	D	180	MET
5	D	188	LEU
5	D	241	VAL
5	D	248	ASP
5	D	264	ASP
5	D	285	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	D	290	ILE
5	D	299	LEU
5	D	376	LEU
5	D	408	VAL
5	D	421	VAL
5	D	428	THR
5	D	454	CYS
5	D	468	VAL
5	D	470	VAL
5	D	478	LEU
5	D	483	LEU
5	D	484	MET
5	D	495	ASN
5	D	527	LEU
5	D	579	LEU
5	D	583	VAL
5	D	605	LEU
5	D	615	LYS
5	D	639	VAL
5	D	724	MET
5	D	740	LEU
5	D	796	LEU
5	D	800	LEU
5	D	809	VAL
5	D	844	THR
5	D	858	VAL
5	D	909	ILE
5	D	930	LEU
5	D	976	THR
5	D	997	VAL
5	D	1106	ILE
5	D	1163	VAL
5	D	1244	GLN
5	D	1343	GLU
5	D	1353	VAL
5	D	1357	ILE
6	E	29	GLN
7	F	111	LEU
7	F	112	THR
7	F	146	GLU
7	F	290	LEU
7	F	381	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	F	463	LEU
7	F	505	ILE
7	F	506	SER
7	F	507	MET
7	F	524	GLU
7	F	591	GLU
8	G	54	LEU
8	G	57	VAL
8	G	95	VAL
8	J	35	LEU
8	J	57	VAL
8	J	118	ARG
8	M	15	LEU
8	M	31	LEU
8	M	57	VAL
8	N	54	LEU
8	N	61	CYS
8	N	70	TYR
8	N	71	ILE
8	N	107	ASN
3	P	270	LEU
3	P	282	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	128	HIS
3	B	41	ASN
3	B	66	HIS
3	B	84	ASN
3	B	117	HIS
3	B	128	HIS
3	B	137	ASN
4	C	36	GLN
4	C	120	GLN
4	C	387	ASN
4	C	582	ASN
4	C	686	GLN
4	C	760	ASN
4	C	808	ASN
4	C	856	ASN
4	C	952	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	C	1010	GLN
4	C	1061	GLN
4	C	1257	GLN
4	C	1268	GLN
4	C	1312	ASN
4	C	1314	GLN
5	D	232	ASN
5	D	266	ASN
5	D	277	ASN
5	D	341	ASN
5	D	435	GLN
5	D	450	HIS
5	D	489	ASN
5	D	921	GLN
5	D	1010	GLN
5	D	1238	GLN
5	D	1244	GLN
6	E	31	GLN
7	F	128	ASN
7	F	362	ASN
7	F	461	ASN
8	G	36	ASN
8	G	88	ASN
8	M	10	GLN
8	N	68	GLN
8	N	88	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no ligands in this entry.

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.

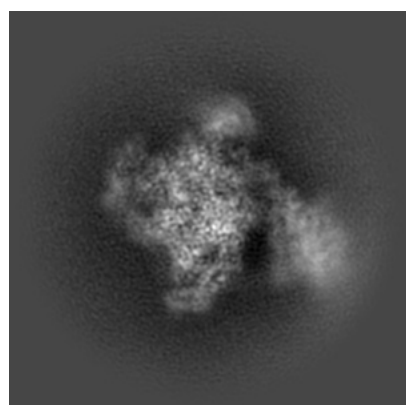
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62728. These allow visual inspection of the internal detail of the map and identification of artifacts.

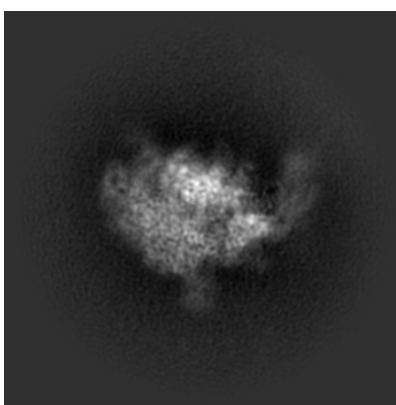
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

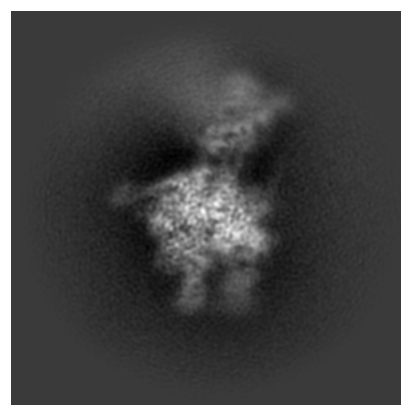
6.1.1 Primary map



X



Y

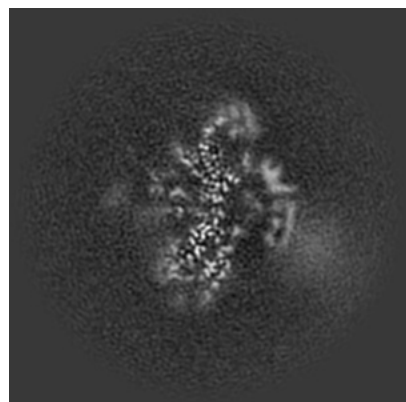


Z

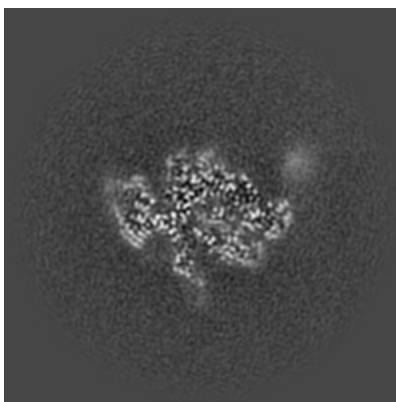
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

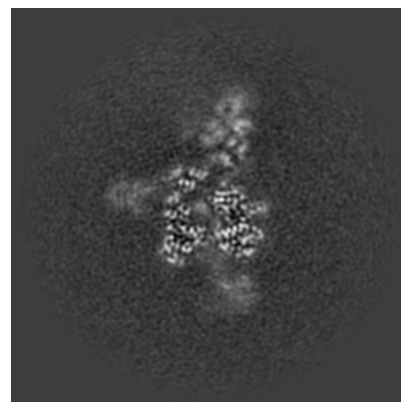
6.2.1 Primary map



X Index: 150



Y Index: 150

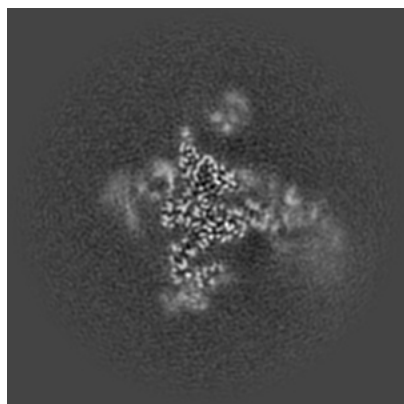


Z Index: 150

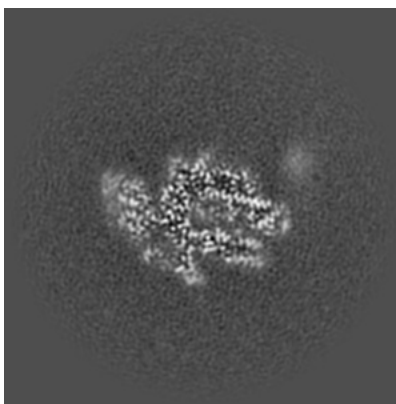
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

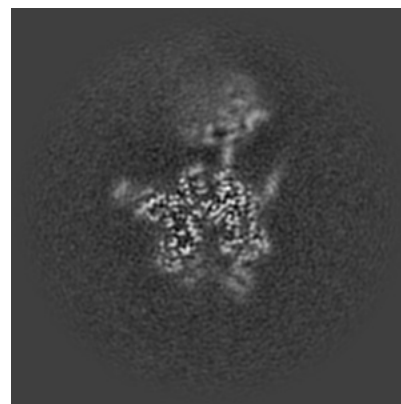
6.3.1 Primary map



X Index: 162



Y Index: 146

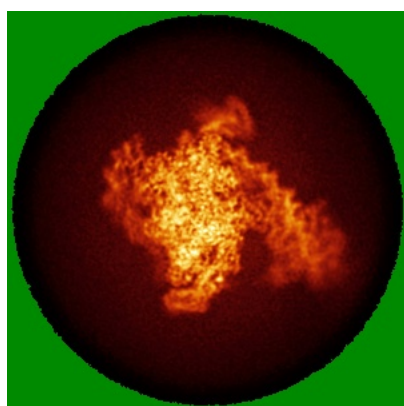


Z Index: 137

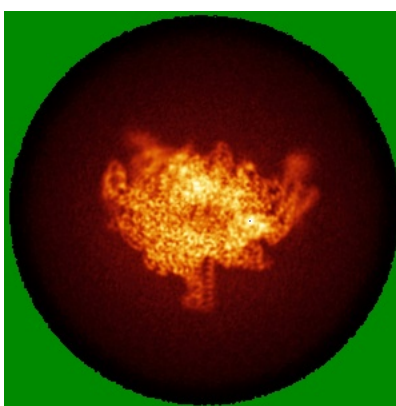
The images above show the largest variance slices of the map in three orthogonal directions.

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

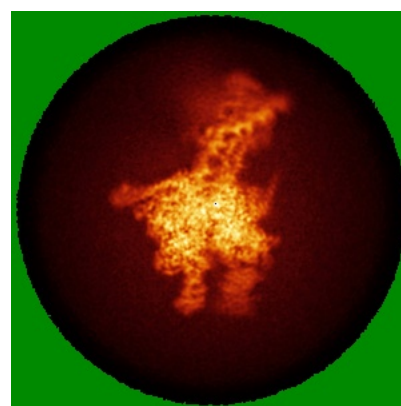
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

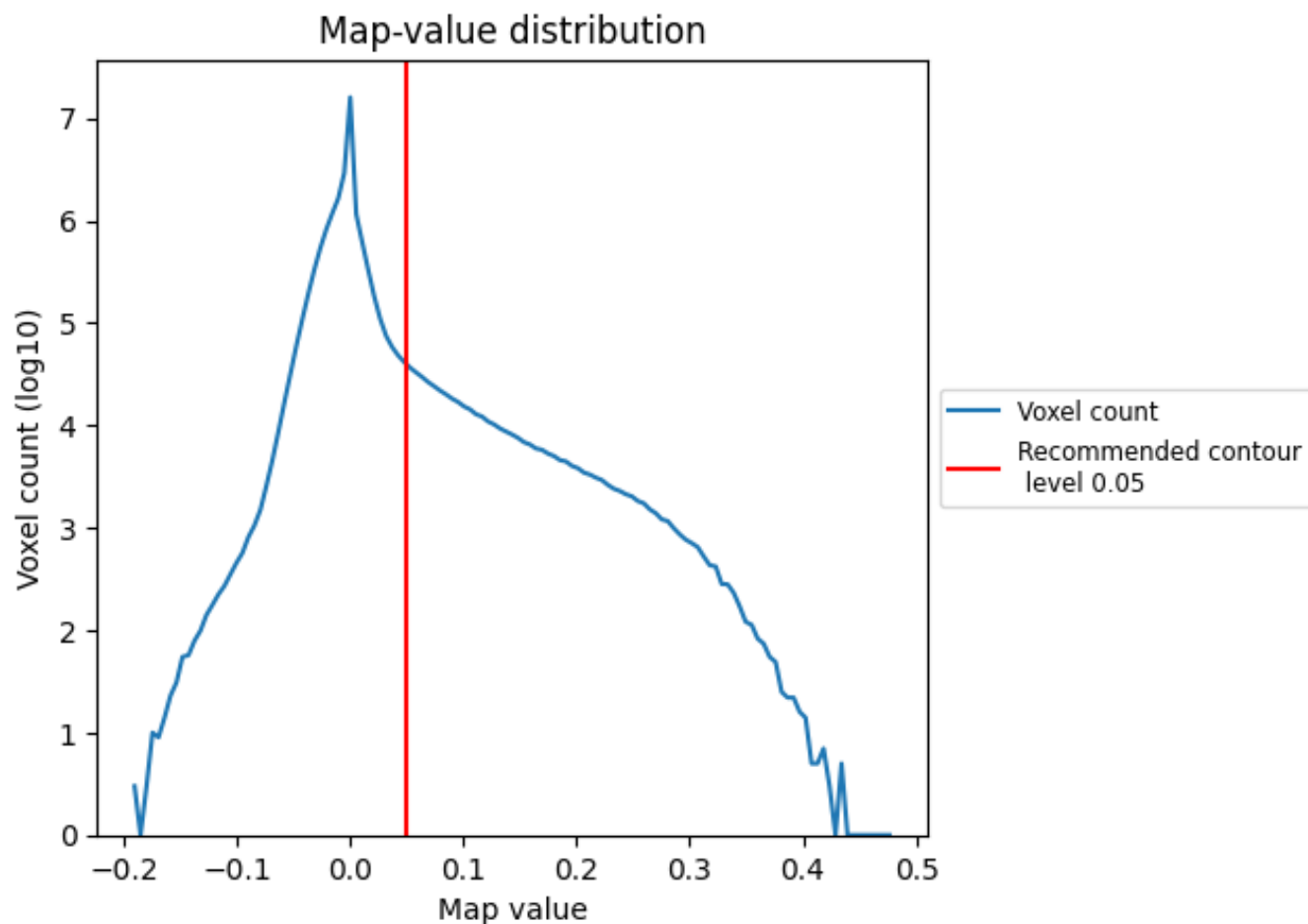
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

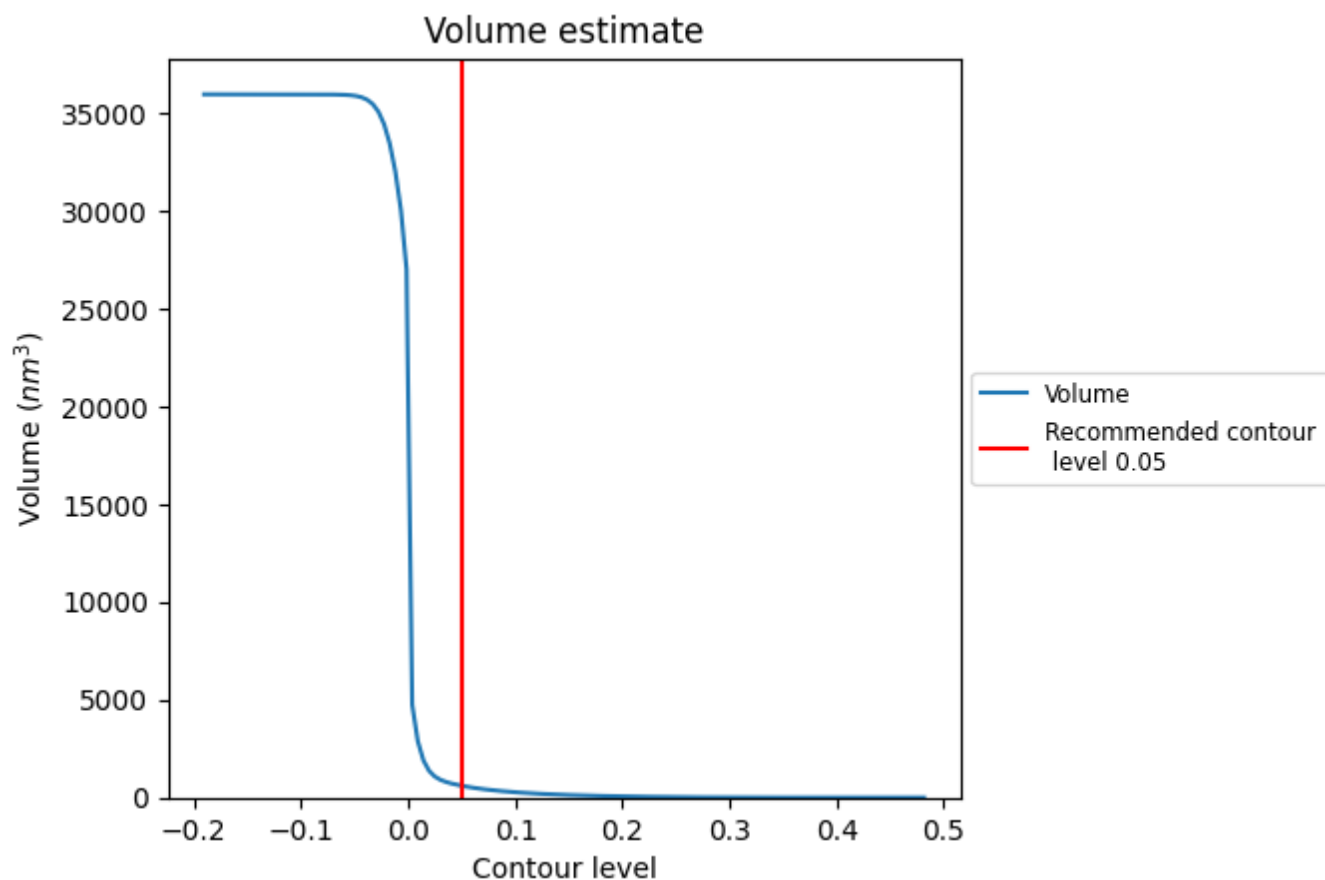
This section contains the results of statistical analysis of the map.

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.

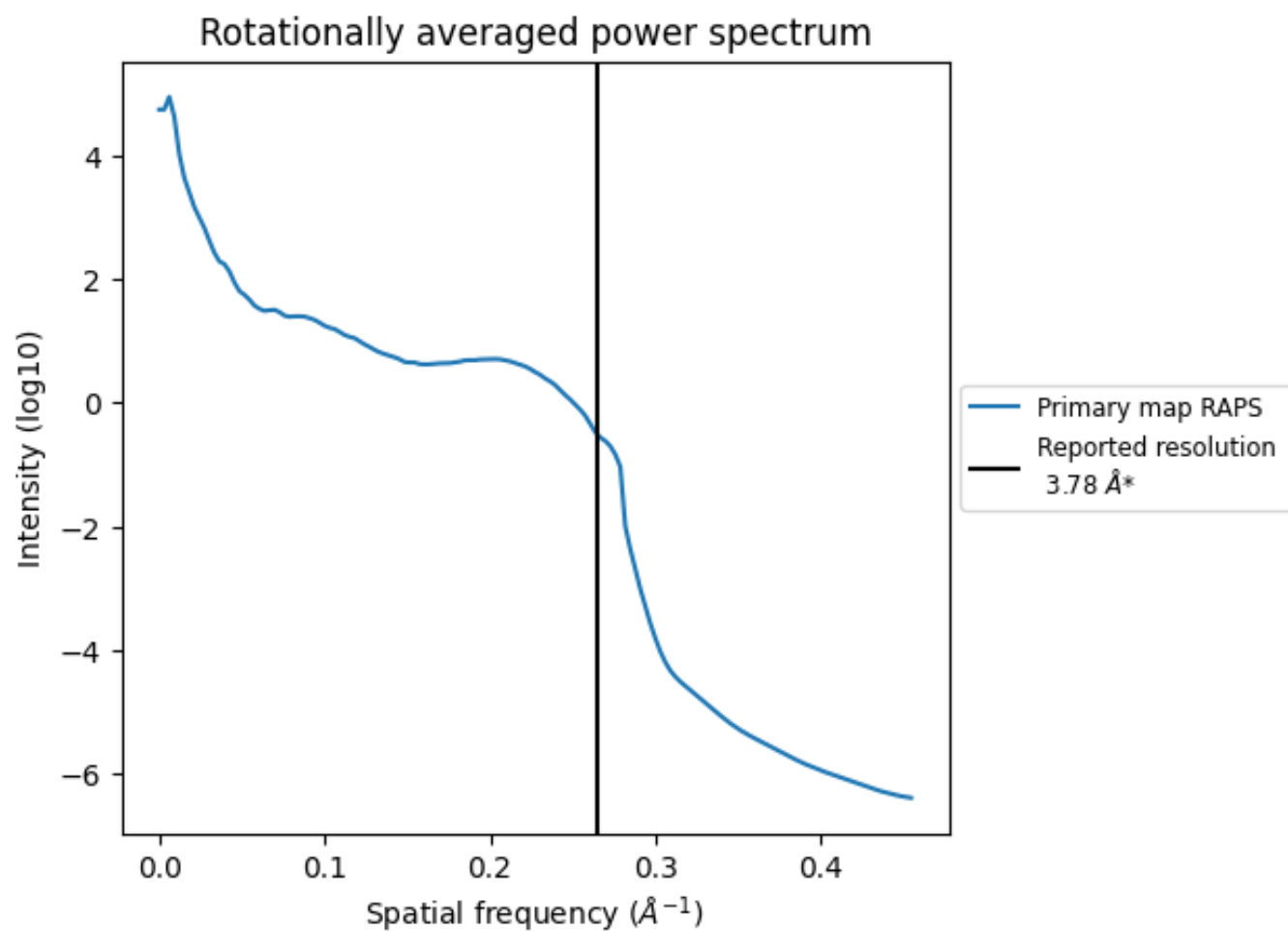
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 602 nm^3 ; this corresponds to an approximate mass of 544 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 0.265 Å⁻¹

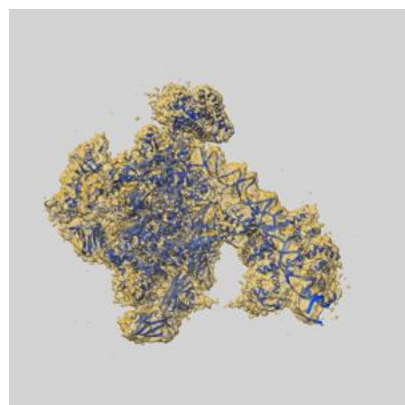
8 Fourier-Shell correlation ⓘ

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

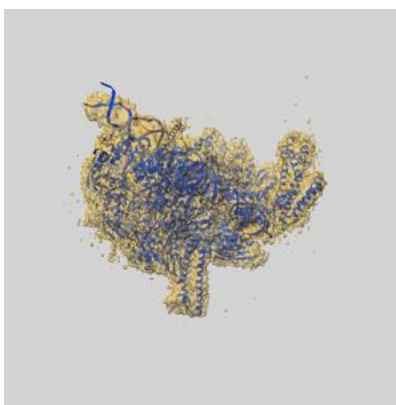
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62728 and PDB model 9L0Y. Per-residue inclusion information can be found in section [3](#) on page [6](#).

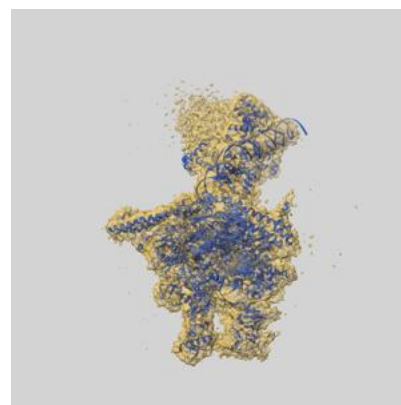
9.1 Map-model overlay [i](#)



X



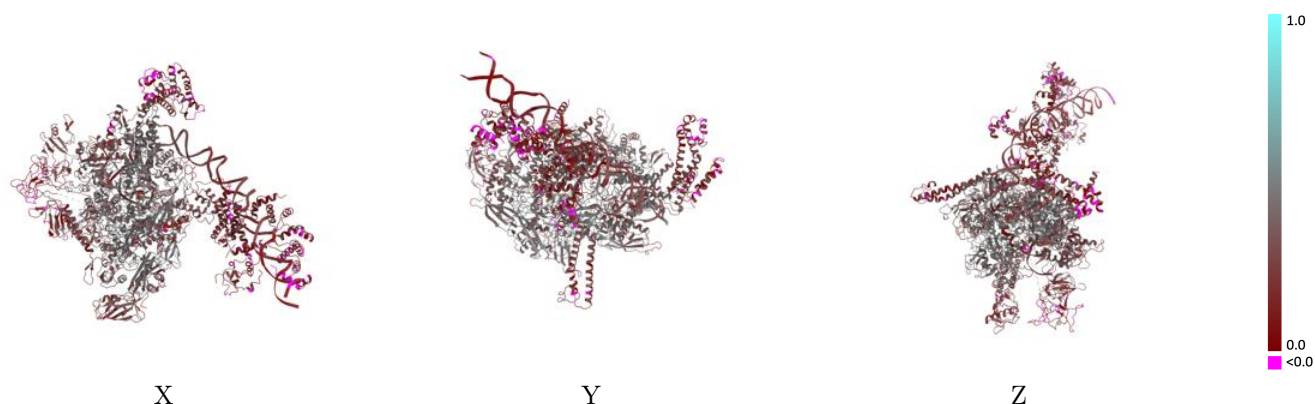
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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](#)

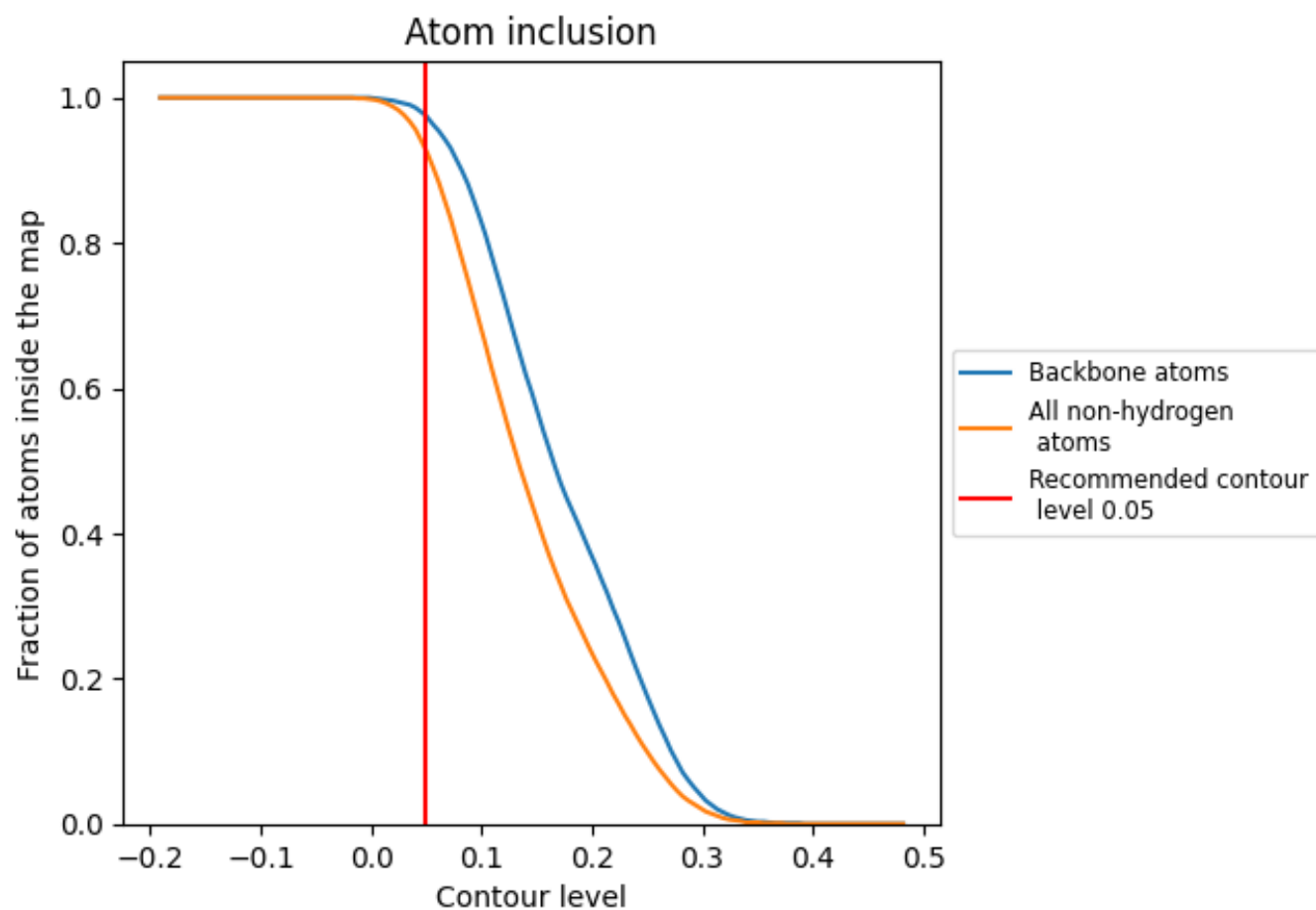


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 93% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9270	 0.3210
1	 0.9600	 0.2500
2	 0.9170	 0.2400
A	 0.9470	 0.4010
B	 0.9390	 0.3130
C	 0.9540	 0.3930
D	 0.9200	 0.3490
E	 0.9200	 0.2680
F	 0.9090	 0.2600
G	 0.9120	 0.1780
J	 0.7700	 0.1550
M	 0.8050	 0.0880
N	 0.9580	 0.1400
P	 0.9470	 0.1930

