



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 10:05 AM UTC

PDB ID : 7MK9 / pdb_00007mk9
EMDB ID : EMD-23887
Title : Complex structure of trailing EC of EC+EC (trailing EC-focused)
Authors : Yang, C.; Murakami, K.
Deposited on : 2021-04-22
Resolution : 3.54 Å (reported)
Based on initial models : 3PO2, 5C4J

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:

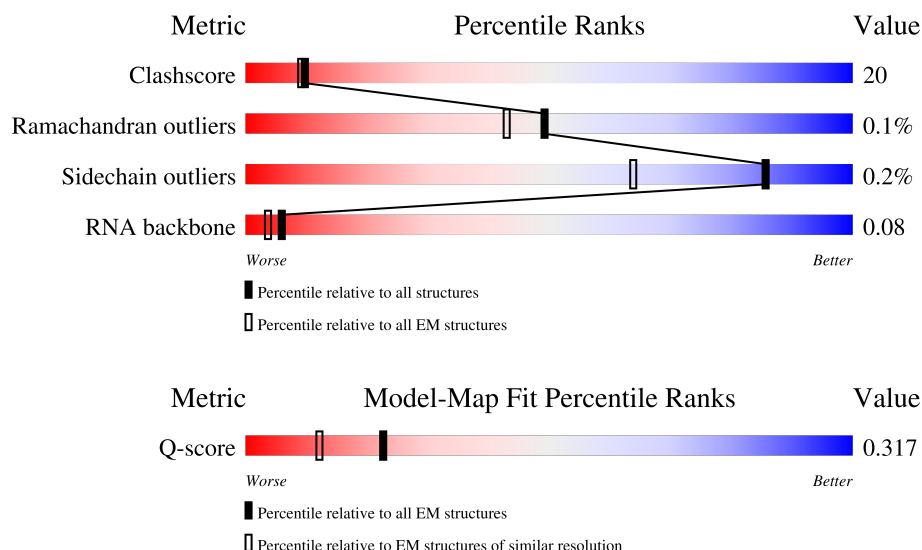
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.54 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12891 (3.04 - 4.04)

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	N	40	
2	O	40	
3	A	1733	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	B	1224	
5	C	318	
6	D	221	
7	E	215	
8	F	155	
9	G	171	
10	H	146	
11	I	122	
12	J	70	
13	K	120	
14	L	70	
15	R	15	
16	Q	735	
17	M	400	

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 36122 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 (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	40	Total	C	N	O	P	0	0
			822	393	162	227	40		

- Molecule 2 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	40	Total	C	N	O	P	0	0
			827	396	141	250	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1425	Total	C	N	O	S	0	0
			11167	7036	1948	2121	62		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	1166	Total	C	N	O	S	0	0
			9227	5823	1619	1729	56		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	265	Total	C	N	O	S	0	0
			2086	1312	347	414	13		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	168	Total	C	N	O	S	0	0
			1331	822	237	270	2		

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 8 is a protein called DNA-directed RNA polymerases I,II,and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	87	Total	C	N	O	S	0	0
			705	451	119	132	3		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	171	Total	C	N	O	S	0	0
			1335	858	221	248	8		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	135	Total	C	N	O	S	0	0
			1080	679	182	214	5		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	114	Total	C	N	O	S	0	0
			927	571	168	178	10		

- Molecule 12 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	66	Total	C	N	O	S	0	0
			540	345	94	95	6		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	115	Total	C	N	O	S	0	0
			924	593	157	172	2		

- Molecule 14 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 15 is a RNA chain called RNA (5'-R(P*UP*CP*GP*AP*GP*AP*GP*GP*AP*UP*CP*CP*CP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	15	Total	C	N	O	P	0	0
			312	141	56	100	15		

- Molecule 16 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	214	Total	C	N	O	S	0	0
			1619	1017	297	299	6		

- Molecule 17 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	135	Total	C	N	O	S	0	0
			1106	694	197	210	5		

- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

Continued on next page...

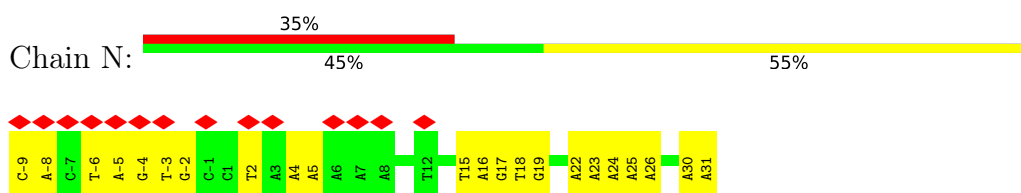
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
19	R	1	1	1	0

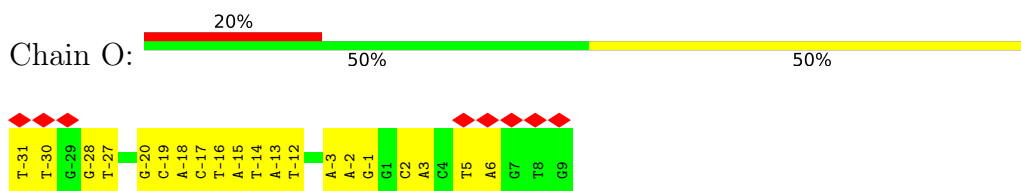
3 Residue-property plots [i](#)

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

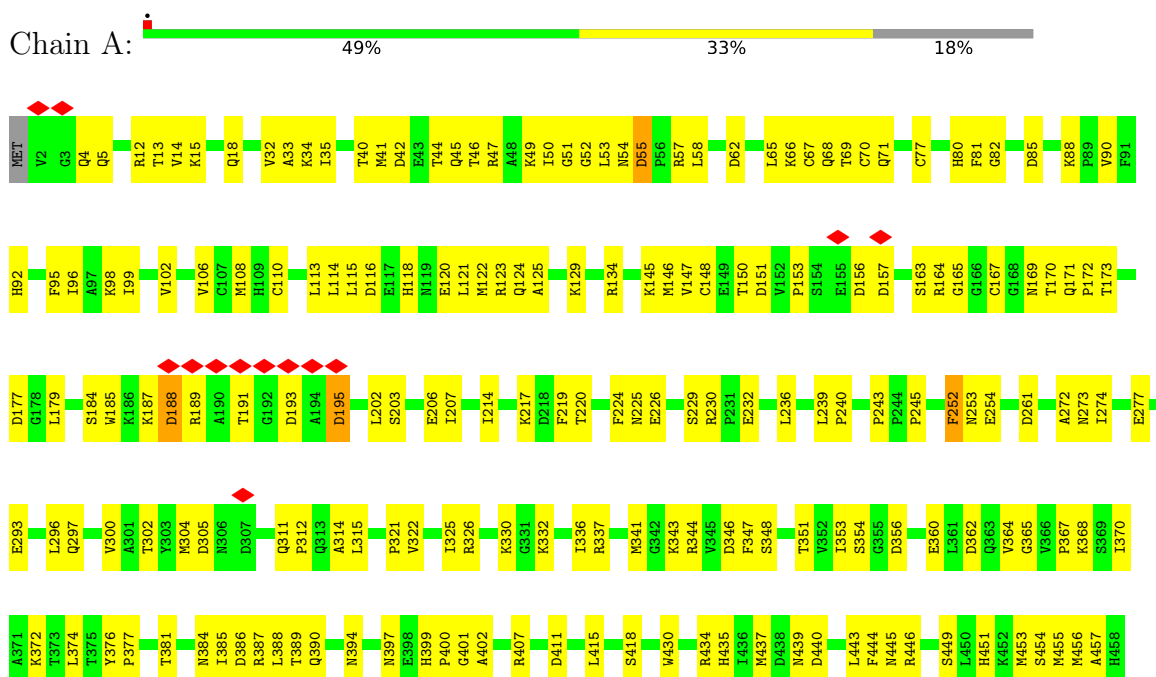
- Molecule 1: DNA (40-MER)



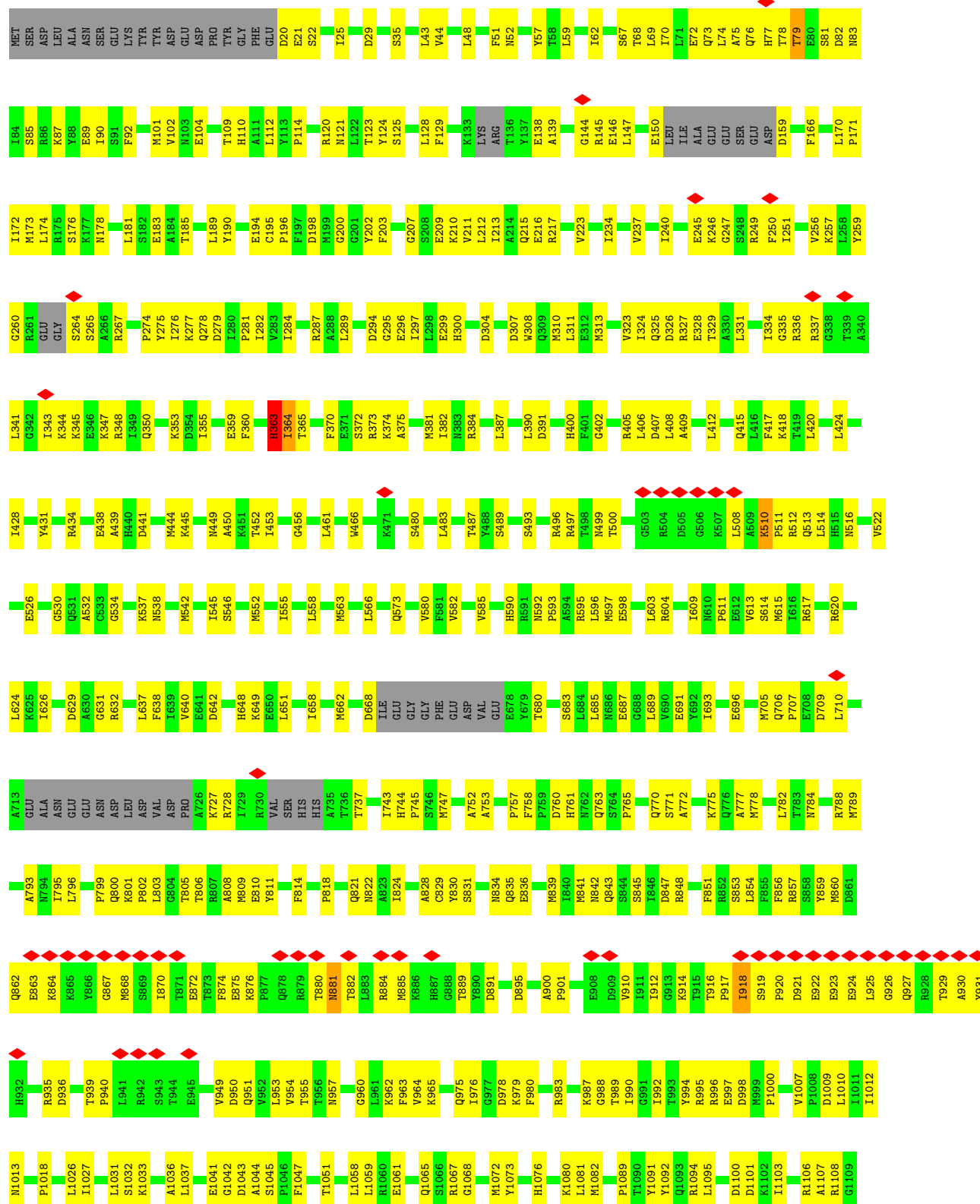
- Molecule 2: DNA (40-MER)



- Molecule 3: DNA-directed RNA polymerase subunit

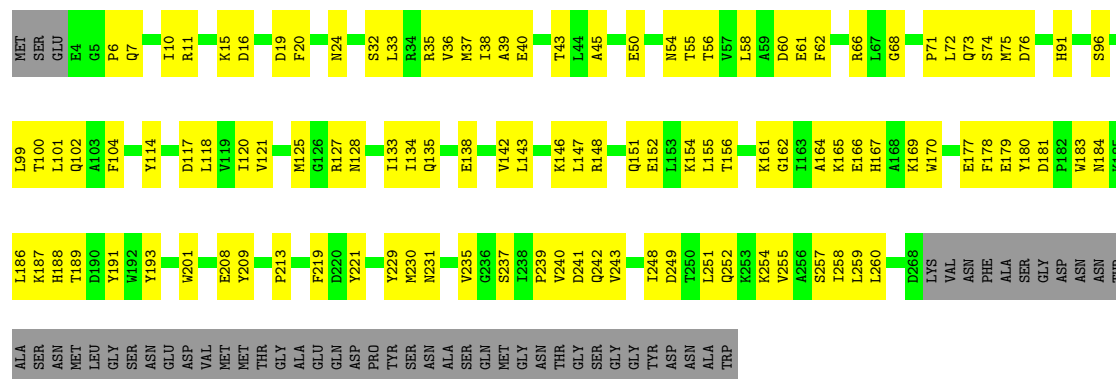


- Molecule 4: DNA-directed RNA polymerase subunit beta

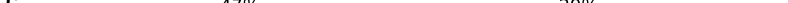


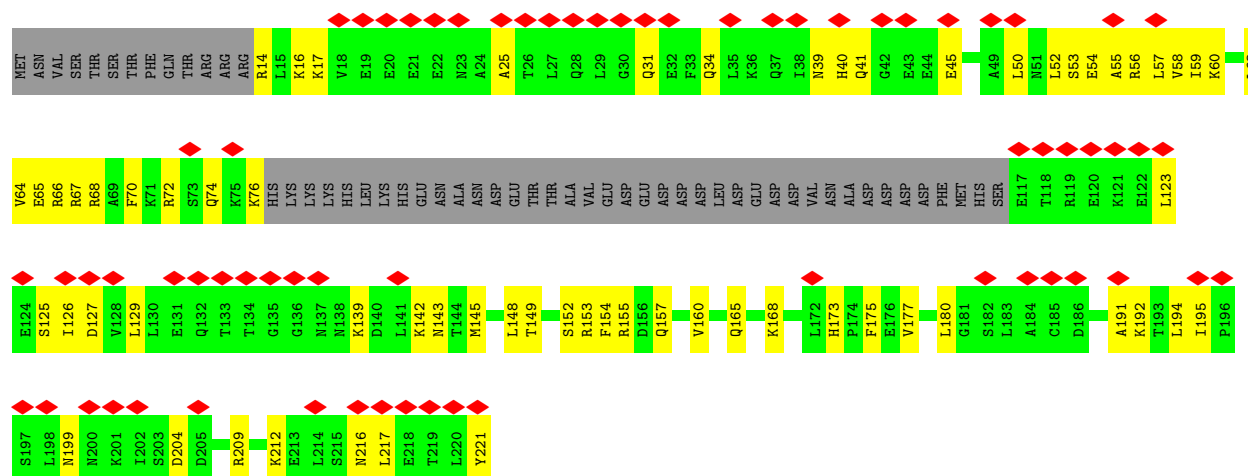
- Molecule 5: DNA-directed RNA polymerase II subunit RPB3

Chain C: 48% 35% 17%

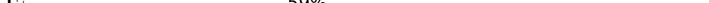


- Molecule 6: DNA-directed RNA polymerase II subunit RPB4

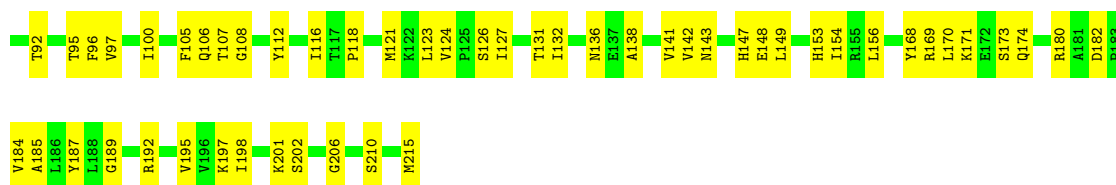
Chain D: 



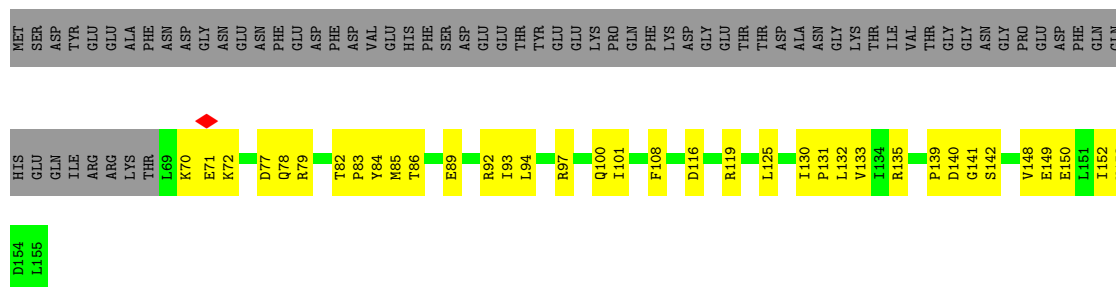
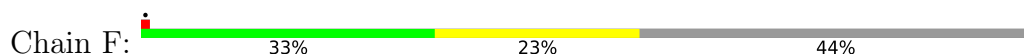
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:  59% 40%

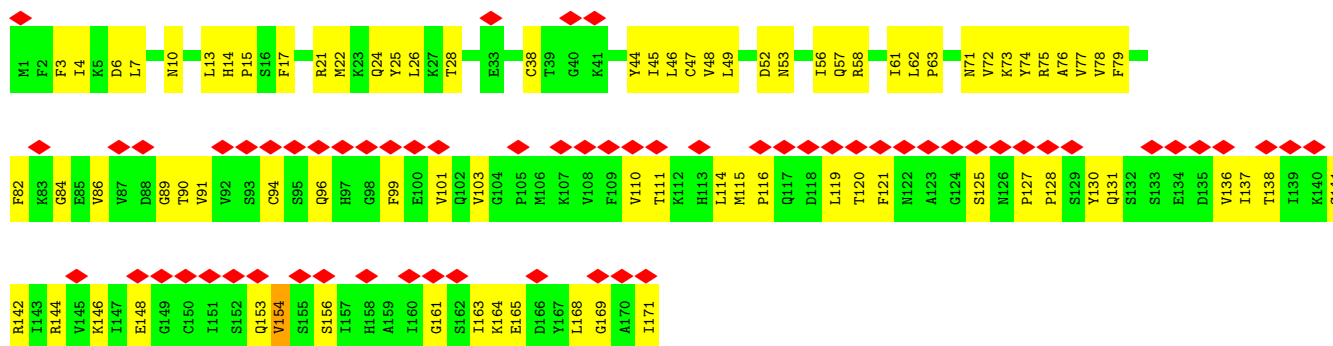




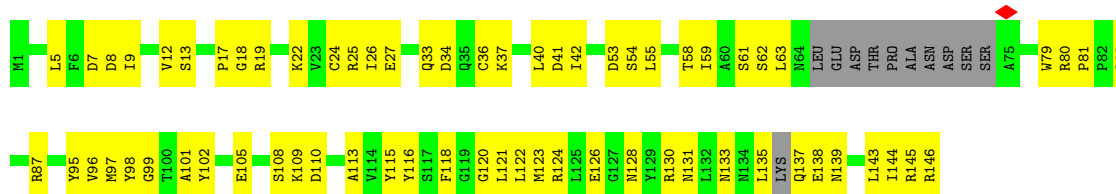
- Molecule 8: DNA-directed RNA polymerases I,II,and III subunit RPABC2



- Molecule 9: DNA-directed RNA polymerase II subunit RPB7

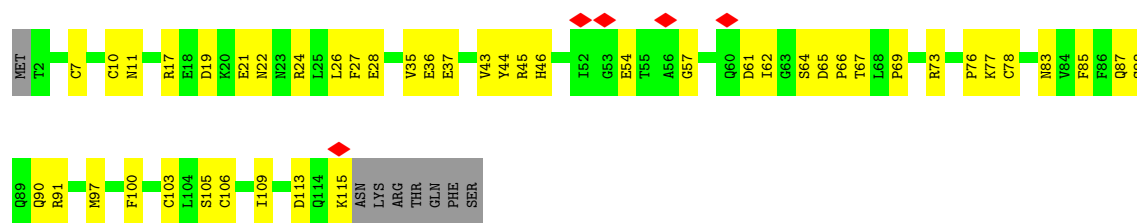


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 11: DNA-directed RNA polymerase II subunit RPB9





LEU VAL LYS GLY PRO TYR ALA PHE LYS TYR THR LEU ARG PRO GLU TYR LYS LYS LEU LYS LYS GLU GLU GLU ARG LYS LYS ALA THR LEU GLY GLU LEU ALA ASP GLU GLN THR GLY SER ALA GLY ASP ASN ALA GLN GLY ASP ALA GLU ALA ASP LEU GLU ASP GLU TLE GLU MET GLU ASP

VAL VAL

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66261	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.056	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0084	Depositor
Map size ($\text{\AA}$)	237.6, 237.6, 237.6	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	N	0.19	0/926	0.34	0/1425
2	O	0.28	0/925	0.53	0/1429
3	A	0.27	0/11368	0.49	2/15383 (0.0%)
4	B	0.28	0/9402	0.54	4/12680 (0.0%)
5	C	0.25	0/2124	0.44	0/2879
6	D	0.14	0/1339	0.39	0/1793
7	E	0.23	0/1788	0.42	0/2406
8	F	0.29	0/717	0.54	0/967
9	G	0.19	0/1363	0.48	0/1840
10	H	0.24	0/1097	0.47	0/1484
11	I	0.19	0/945	0.40	0/1273
12	J	0.36	0/549	0.59	0/738
13	K	0.25	0/942	0.44	0/1272
14	L	0.21	0/354	0.71	0/468
15	R	0.49	0/347	0.74	0/536
16	Q	0.17	0/1648	0.41	1/2226 (0.0%)
17	M	0.16	0/1124	0.43	0/1517
All	All	0.26	0/36958	0.49	7/50316 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	3
4	B	0	3
9	G	0	1
All	All	0	7

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	421	PRO	N-CA-CB	7.66	110.16	103.27
4	B	79	THR	CA-C-N	6.46	133.32	121.70
4	B	79	THR	C-N-CA	6.46	133.32	121.70
4	B	918	ILE	CA-C-N	5.26	131.16	121.70
4	B	918	ILE	C-N-CA	5.26	131.16	121.70
3	A	1107	VAL	CA-C-N	5.08	130.85	121.70
3	A	1107	VAL	C-N-CA	5.08	130.85	121.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	252	PHE	Peptide
3	A	55	ASP	Peptide
3	A	750	GLY	Peptide
4	B	363	HIS	Peptide
4	B	510	LYS	Peptide
4	B	881	ASN	Peptide
9	G	154	VAL	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	N	822	0	449	19	0
2	O	827	0	458	19	0
3	A	11167	0	11188	485	0
4	B	9227	0	9200	418	0
5	C	2086	0	2045	98	0
6	D	1331	0	1344	57	0
7	E	1752	0	1776	70	0
8	F	705	0	731	33	0
9	G	1335	0	1346	58	0
10	H	1080	0	1049	61	0
11	I	927	0	881	37	0
12	J	540	0	553	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	K	924	0	934	42	0
14	L	352	0	375	20	0
15	R	312	0	165	12	0
16	Q	1619	0	1452	44	0
17	M	1106	0	1099	48	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	C	1	0	0	0	0
18	I	2	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
19	A	1	0	0	0	0
19	R	1	0	0	0	0
All	All	36122	0	35045	1403	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 20.

All (1403) 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)
4:B:510:LYS:HG3	4:B:511:PRO:HD3	1.45	0.98
12:J:8:PHE:H	12:J:49:MET:HE1	1.27	0.97
14:L:48:CYS:SG	14:L:51:CYS:HB2	2.09	0.93
3:A:110:CYS:HB3	3:A:167:CYS:SG	2.09	0.92
3:A:802:ASN:HD21	3:A:806:ARG:HB2	1.35	0.91
4:B:334:ILE:HA	4:B:347:LYS:HG3	1.52	0.90
4:B:763:GLN:HG2	4:B:765:PRO:HD2	1.53	0.89
3:A:148:CYS:HB2	3:A:171:GLN:HE22	1.41	0.86
14:L:28:LYS:HB2	14:L:39:SER:HA	1.57	0.86
3:A:1266:THR:O	3:A:1270:ASN:HB2	1.76	0.86
3:A:397:ASN:O	13:K:2:ASN:ND2	2.08	0.85
4:B:799:PRO:HB2	4:B:818:PRO:HG2	1.59	0.85
16:Q:105:ALA:HB1	17:M:87:LEU:HD12	1.59	0.84
10:H:55:LEU:HA	10:H:146:ARG:HH12	1.42	0.83
9:G:91:VAL:HG22	9:G:101:VAL:HG22	1.61	0.83
3:A:202:LEU:HB3	3:A:207:ILE:HD11	1.62	0.80
4:B:805:THR:OG1	4:B:809:MET:SD	2.39	0.80
4:B:880:THR:HA	4:B:931:TYR:H	1.47	0.79
8:F:125:LEU:HA	8:F:130:ILE:HD11	1.64	0.78
4:B:526:GLU:O	4:B:538:ASN:ND2	2.17	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:75:ALA:HB2	4:B:83:ASN:H	1.48	0.77
8:F:97:ARG:HD2	8:F:100:GLN:HE22	1.49	0.77
3:A:368:LYS:HD3	13:K:3:ALA:HA	1.66	0.77
4:B:1166:CYS:SG	6:D:16:LYS:NZ	2.57	0.77
4:B:246:LYS:HE2	4:B:249:ARG:HD2	1.67	0.76
4:B:829:CYS:HA	4:B:834:ASN:HD21	1.48	0.76
10:H:80:ARG:HD3	10:H:81:PRO:HD2	1.67	0.76
9:G:21:ARG:HH22	9:G:25:TYR:HB2	1.49	0.76
15:R:14:C:O2'	15:R:14:C:O2	2.02	0.76
6:D:153:ARG:HH22	6:D:160:VAL:HA	1.49	0.76
3:A:367:PRO:HB3	3:A:466:SER:HA	1.67	0.76
4:B:841:MET:HE1	4:B:980:PHE:HE2	1.51	0.76
4:B:85:SER:HB3	4:B:138:GLU:HB3	1.68	0.75
3:A:1430:LEU:HB3	3:A:1432:GLN:HE22	1.51	0.75
16:Q:106:ILE:HG22	17:M:87:LEU:HD11	1.69	0.74
3:A:1420:ASP:OD2	3:A:1422:ARG:NH1	2.21	0.74
12:J:10:CYS:SG	12:J:11:GLY:N	2.60	0.74
4:B:74:LEU:HA	4:B:85:SER:HA	1.69	0.73
14:L:61:THR:HG22	14:L:63:ARG:H	1.50	0.73
4:B:978:ASP:OD2	4:B:1094:ARG:NH2	2.21	0.73
3:A:368:LYS:HZ2	13:K:4:PRO:HD3	1.54	0.73
3:A:18:GLN:HB3	4:B:1215:ARG:HB2	1.70	0.72
3:A:1208:THR:OG1	3:A:1211:GLN:OE1	2.07	0.72
5:C:165:LYS:HE2	13:K:9:LEU:HD11	1.69	0.72
6:D:152:SER:HB2	6:D:155:ARG:HH21	1.54	0.72
12:J:1:MET:HA	12:J:57:ILE:HG23	1.69	0.72
3:A:15:LYS:HD3	4:B:1219:ASP:HA	1.72	0.72
3:A:252:PHE:O	3:A:254:GLU:N	2.21	0.72
4:B:842:ASN:ND2	4:B:845:SER:OG	2.21	0.72
3:A:855:THR:OG1	3:A:857:ARG:NH1	2.23	0.72
9:G:47:CYS:SG	9:G:48:VAL:N	2.62	0.72
3:A:40:THR:HG22	3:A:53:LEU:HB2	1.72	0.72
5:C:177:GLU:HB2	5:C:231:ASN:HB3	1.70	0.72
6:D:64:VAL:HG23	6:D:68:ARG:HH22	1.53	0.71
16:Q:375:LEU:HB2	16:Q:387:ILE:HB	1.72	0.71
4:B:384:ARG:HH21	4:B:387:LEU:HD11	1.55	0.71
4:B:806:THR:HG23	4:B:808:ALA:H	1.56	0.71
15:R:13:U:H5''	15:R:14:C:H5''	1.73	0.71
6:D:39:ASN:ND2	6:D:41:GLN:OE1	2.23	0.71
6:D:70:PHE:O	6:D:74:GLN:NE2	2.23	0.71
4:B:190:TYR:HE2	4:B:196:PRO:HD3	1.56	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:81:PRO:O	10:H:87:ARG:NH2	2.24	0.70
3:A:273:ASN:HA	3:A:296:LEU:HD21	1.73	0.70
4:B:287:ARG:NH1	4:B:324:ILE:O	2.23	0.70
4:B:1165:ILE:N	4:B:1190:ASP:OD1	2.17	0.70
4:B:313:MET:HE1	4:B:390:LEU:HD13	1.74	0.70
3:A:474:VAL:HA	3:A:521:MET:HE1	1.73	0.70
4:B:822:ASN:O	12:J:48:ARG:NH2	2.24	0.70
14:L:47:ARG:HH21	14:L:54:ARG:HE	1.40	0.70
4:B:234:ILE:HG21	4:B:257:LYS:HD2	1.73	0.69
4:B:365:THR:HG21	4:B:370:PHE:HB2	1.73	0.69
14:L:31:CYS:HA	14:L:56:LEU:HA	1.74	0.69
17:M:96:ARG:NH2	17:M:103:LYS:O	2.25	0.69
3:A:1397:LEU:HD23	3:A:1429:ILE:HD11	1.75	0.69
3:A:69:THR:HA	3:A:71:GLN:HE22	1.57	0.69
3:A:1059:HIS:ND1	8:F:86:THR:OG1	2.23	0.69
3:A:871:ASP:OD2	3:A:1366:ARG:NH2	2.25	0.69
4:B:82:ASP:H	4:B:83:ASN:HA	1.57	0.69
4:B:582:VAL:O	4:B:585:VAL:HG12	1.92	0.69
3:A:747:VAL:HG12	3:A:753:GLY:HA3	1.73	0.69
9:G:4:ILE:HD12	9:G:49:LEU:HD11	1.75	0.69
3:A:1136:SER:HB2	3:A:1274:ARG:HH22	1.57	0.69
4:B:44:VAL:HG11	4:B:200:GLY:HA2	1.75	0.69
4:B:611:PRO:HG2	4:B:685:LEU:HD21	1.75	0.69
13:K:95:ILE:HD12	13:K:98:LEU:HD11	1.75	0.69
3:A:365:GLY:HA3	3:A:469:ARG:HB3	1.74	0.68
4:B:510:LYS:O	4:B:512:ARG:N	2.27	0.68
10:H:97:MET:HE1	10:H:118:PHE:CG	2.27	0.68
5:C:10:ILE:HD12	5:C:20:PHE:HB3	1.75	0.68
4:B:757:PRO:HD3	4:B:983:ARG:HE	1.59	0.68
3:A:346:ASP:H	4:B:1154:ALA:HB1	1.58	0.68
4:B:526:GLU:OE2	4:B:753:ALA:N	2.20	0.67
4:B:542:MET:HE1	4:B:747:MET:HB3	1.75	0.67
3:A:46:THR:O	3:A:47:ARG:NE	2.28	0.67
3:A:454:SER:O	3:A:455:MET:HE2	1.93	0.67
4:B:706:GLN:HB2	4:B:709:ASP:HB3	1.77	0.67
3:A:883:LEU:HD23	3:A:885:THR:H	1.58	0.67
4:B:930:ALA:HA	4:B:931:TYR:C	2.20	0.67
3:A:821:ARG:HD3	4:B:514:LEU:HB2	1.76	0.67
3:A:830:LYS:NZ	3:A:1079:MET:O	2.28	0.67
3:A:884:ASP:OD2	3:A:1025:ARG:NE	2.27	0.67
4:B:642:ASP:HA	4:B:649:LYS:HE3	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:124:LEU:HD23	17:M:222:CYS:HB3	1.76	0.67
3:A:311:GLN:HG2	3:A:312:PRO:HD3	1.77	0.67
3:A:788:SER:HB2	11:I:69:PRO:HG3	1.77	0.67
4:B:72:GLU:HA	4:B:87:LYS:HA	1.77	0.66
4:B:839:MET:HG3	4:B:1012:ILE:HG22	1.77	0.66
8:F:85:MET:HE3	8:F:153:VAL:HG12	1.77	0.66
9:G:148:GLU:H	9:G:161:GLY:HA2	1.60	0.66
3:A:1161:THR:HG22	3:A:1163:ILE:H	1.60	0.66
4:B:210:LYS:NZ	4:B:480:SER:O	2.29	0.66
4:B:365:THR:O	4:B:374:LYS:NZ	2.28	0.66
7:E:136:ASN:HD21	7:E:138:ALA:HB3	1.60	0.66
3:A:868:TYR:HD1	3:A:1058:VAL:HG21	1.60	0.66
3:A:1126:ALA:HA	3:A:1304:TRP:HD1	1.60	0.66
7:E:97:VAL:HA	7:E:100:ILE:HD12	1.77	0.66
9:G:153:GLN:HG3	9:G:154:VAL:H	1.60	0.66
3:A:569:LYS:NZ	5:C:221:TYR:O	2.29	0.66
3:A:1159:ARG:HH12	3:A:1186:ASP:HB2	1.60	0.66
4:B:363:HIS:O	4:B:365:THR:N	2.29	0.66
3:A:1107:VAL:HA	3:A:1108:ALA:HB3	1.78	0.65
4:B:864:LYS:H	4:B:872:GLU:HG3	1.60	0.65
5:C:10:ILE:HG21	13:K:112:GLN:HG3	1.79	0.65
3:A:1318:THR:HG22	7:E:141:VAL:HG11	1.78	0.65
4:B:771:SER:O	4:B:775:LYS:NZ	2.29	0.65
4:B:884:ARG:NH2	4:B:936:ASP:O	2.30	0.65
4:B:1161:HIS:HB3	4:B:1191:ILE:HD11	1.77	0.65
3:A:528:LEU:HD11	3:A:619:LYS:HB3	1.76	0.65
3:A:802:ASN:ND2	3:A:807:GLY:O	2.29	0.65
6:D:139:LYS:HA	6:D:142:LYS:HE3	1.78	0.65
6:D:165:GLN:HA	6:D:168:LYS:HE3	1.76	0.65
3:A:1444:MET:HB3	8:F:133:VAL:HG23	1.78	0.65
4:B:172:ILE:HD11	4:B:178:ASN:HB2	1.78	0.65
3:A:81:PHE:HE1	3:A:243:PRO:HD3	1.60	0.65
4:B:48:LEU:O	4:B:52:ASN:ND2	2.27	0.65
5:C:148:ARG:HH12	12:J:65:PRO:HD2	1.61	0.65
3:A:1128:GLN:OE1	3:A:1304:TRP:NE1	2.30	0.65
17:M:138:GLN:HG3	17:M:211:LYS:HB3	1.78	0.65
4:B:173:MET:HB3	4:B:176:SER:HB3	1.79	0.65
10:H:33:GLN:HG3	10:H:36:CYS:H	1.61	0.65
4:B:604:ARG:NH1	4:B:691:GLU:OE2	2.30	0.64
3:A:390:GLN:NE2	3:A:394:ASN:OD1	2.29	0.64
3:A:4:GLN:O	4:B:1159:ARG:NH2	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:334:ILE:HG13	4:B:335:GLY:H	1.60	0.64
4:B:796:LEU:HA	4:B:853:SER:HA	1.78	0.64
6:D:40:HIS:HB2	9:G:73:LYS:HZ2	1.62	0.64
7:E:124:VAL:HG13	7:E:132:ILE:HB	1.79	0.64
16:Q:376:LEU:HD12	17:M:71:VAL:HG21	1.78	0.64
4:B:822:ASN:OD1	12:J:48:ARG:NH2	2.31	0.64
3:A:226:GLU:HG2	3:A:230:ARG:HE	1.63	0.64
8:F:86:THR:N	8:F:89:GLU:OE2	2.29	0.64
3:A:356:ASP:HB2	3:A:469:ARG:HD2	1.79	0.64
4:B:493:SER:OG	4:B:497:ARG:NH2	2.31	0.64
4:B:1033:LYS:HD2	4:B:1059:LEU:HD11	1.80	0.64
6:D:139:LYS:NZ	6:D:143:ASN:OD1	2.21	0.64
4:B:79:THR:HB	4:B:81:SER:H	1.63	0.64
17:M:226:PRO:HG3	17:M:236:ILE:HD11	1.80	0.64
7:E:62:ALA:O	7:E:77:SER:OG	2.15	0.63
3:A:77:CYS:SG	3:A:80:HIS:CE1	2.79	0.63
3:A:567:LYS:HB3	3:A:568:PRO:HD3	1.81	0.63
7:E:169:ARG:NH2	8:F:142:SER:OG	2.31	0.63
9:G:52:ASP:OD1	9:G:53:ASN:N	2.32	0.63
7:E:88:VAL:HG21	7:E:116:ILE:HG12	1.80	0.63
1:N:17:DG:H2''	1:N:18:DT:H5'	1.78	0.63
3:A:826:ASP:OD2	3:A:827:THR:N	2.31	0.63
4:B:980:PHE:HE1	4:B:1094:ARG:HG3	1.64	0.63
4:B:1135:ARG:NH2	4:B:1136:ASP:OD1	2.31	0.63
3:A:1197:LEU:HB2	3:A:1236:LEU:HB3	1.81	0.63
4:B:327:ARG:HG2	16:Q:398:ARG:HH12	1.64	0.63
14:L:40:LEU:HD12	14:L:44:ASP:HB2	1.80	0.63
3:A:959:ASN:OD1	3:A:960:ILE:N	2.32	0.62
3:A:1433:MET:HE1	3:A:1439:GLY:HA2	1.81	0.62
4:B:344:LYS:HZ2	4:B:347:LYS:HA	1.64	0.62
4:B:563:MET:HE1	4:B:590:HIS:HB2	1.80	0.62
6:D:123:LEU:HG	6:D:145:MET:HE1	1.81	0.62
3:A:894:GLU:HB2	3:A:898:ARG:HB2	1.81	0.62
4:B:1072:MET:HB3	4:B:1081:LEU:HD12	1.81	0.62
3:A:367:PRO:HG2	3:A:370:ILE:HG12	1.81	0.62
4:B:194:GLU:HA	4:B:784:ASN:HD22	1.65	0.62
4:B:1163:CYS:O	4:B:1167:GLY:N	2.23	0.62
9:G:46:LEU:HB2	9:G:77:VAL:HG13	1.81	0.62
14:L:30:ILE:HB	14:L:57:LEU:HB2	1.82	0.62
4:B:1106:ARG:NH2	4:B:1110:PRO:O	2.32	0.62
10:H:8:ASP:OD1	10:H:9:ILE:N	2.31	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:55:ASP:HA	3:A:58:LEU:HD23	1.81	0.62
3:A:169:ASN:OD1	3:A:170:THR:N	2.31	0.62
4:B:104:GLU:OE2	4:B:110:HIS:HE1	1.82	0.62
9:G:21:ARG:O	9:G:22:MET:HE2	1.99	0.62
3:A:500:GLU:OE2	4:B:1146:PHE:N	2.31	0.62
16:Q:97:GLU:OE2	17:M:96:ARG:NH1	2.32	0.62
3:A:203:SER:O	3:A:206:GLU:HG2	2.00	0.62
4:B:841:MET:HE2	4:B:990:ILE:HG12	1.82	0.62
3:A:664:THR:OG1	3:A:668:ASP:OD2	2.16	0.62
3:A:512:VAL:HA	3:A:519:PRO:HA	1.80	0.62
3:A:827:THR:HA	3:A:830:LYS:HG2	1.80	0.62
3:A:1200:ALA:O	3:A:1204:ASP:HB2	2.00	0.62
16:Q:141:ARG:NH1	16:Q:345:GLU:O	2.33	0.62
3:A:526:ASP:OD1	3:A:527:THR:N	2.31	0.61
4:B:334:ILE:HG13	4:B:335:GLY:N	2.16	0.61
3:A:146:MET:O	3:A:171:GLN:N	2.32	0.61
3:A:885:THR:O	3:A:940:ARG:NH1	2.32	0.61
7:E:147:HIS:HE1	7:E:149:LEU:HD13	1.65	0.61
3:A:598:LEU:O	10:H:25:ARG:NH2	2.27	0.61
4:B:20:ASP:OD1	4:B:21:GLU:N	2.33	0.61
4:B:1134:GLU:OE1	4:B:1134:GLU:N	2.28	0.61
3:A:834:THR:OG1	3:A:1076:ALA:HB1	2.00	0.61
4:B:795:ILE:O	4:B:854:LEU:N	2.32	0.61
11:I:45:ARG:HE	11:I:46:HIS:H	1.46	0.61
13:K:8:GLU:HA	13:K:37:LYS:HZ2	1.66	0.61
3:A:134:ARG:NH2	3:A:220:THR:O	2.33	0.61
3:A:1044:TRP:O	3:A:1048:ASN:ND2	2.33	0.61
3:A:1385:THR:OG1	3:A:1388:GLY:N	2.31	0.61
4:B:1010:LEU:HD11	4:B:1092:TYR:HE2	1.65	0.61
8:F:116:ASP:OD2	8:F:119:ARG:N	2.30	0.61
12:J:44:TYR:HA	12:J:47:ARG:HB3	1.83	0.61
3:A:789:LYS:NZ	11:I:67:THR:OG1	2.32	0.61
4:B:875:GLU:OE2	4:B:881:ASN:ND2	2.34	0.61
7:E:55:ARG:HA	7:E:58:MET:HE3	1.81	0.61
3:A:384:ASN:HB2	3:A:388:LEU:HD13	1.82	0.61
4:B:867:GLY:HA3	4:B:868:MET:C	2.25	0.61
13:K:36:GLU:N	13:K:36:GLU:OE1	2.34	0.61
4:B:1160:VAL:HG11	4:B:1169:MET:HE3	1.83	0.60
17:M:223:GLN:NE2	17:M:224:VAL:O	2.33	0.60
3:A:81:PHE:CE1	3:A:243:PRO:HD3	2.35	0.60
4:B:341:LEU:HB3	4:B:344:LYS:HD2	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:126:LYS:HD3	17:M:130:GLU:HB2	1.84	0.60
5:C:125:MET:SD	5:C:127:ARG:NE	2.73	0.60
9:G:89:GLY:HA3	9:G:103:VAL:HG22	1.83	0.60
3:A:453:MET:O	3:A:454:SER:OG	2.17	0.60
3:A:1063:MET:HE3	3:A:1436:ILE:HG23	1.83	0.60
5:C:162:GLY:HA3	5:C:170:TRP:CE2	2.37	0.60
5:C:240:VAL:O	5:C:243:VAL:HG22	2.01	0.60
3:A:886:ILE:HD11	3:A:943:LEU:HB3	1.84	0.60
4:B:114:PRO:HG3	4:B:181:LEU:HD11	1.84	0.60
4:B:296:GLU:O	4:B:300:HIS:ND1	2.28	0.60
3:A:147:VAL:HA	3:A:170:THR:HA	1.83	0.60
3:A:502:SER:OG	3:A:503:GLN:NE2	2.29	0.60
3:A:115:LEU:HD21	3:A:145:LYS:HD3	1.83	0.60
4:B:1037:LEU:O	12:J:47:ARG:NH1	2.35	0.60
5:C:167:HIS:CE1	5:C:169:LYS:HG3	2.37	0.60
10:H:12:VAL:HG12	10:H:53:ASP:H	1.65	0.60
3:A:148:CYS:HB2	3:A:171:GLN:NE2	2.15	0.60
3:A:840:ARG:NH1	3:A:1384:VAL:O	2.34	0.60
3:A:1142:THR:O	3:A:1145:SER:OG	2.18	0.60
5:C:143:LEU:HD21	5:C:146:LYS:HE3	1.84	0.60
3:A:1113:THR:O	3:A:1330:ASN:ND2	2.35	0.60
3:A:1168:GLU:O	3:A:1171:GLN:NE2	2.35	0.60
3:A:326:ARG:O	3:A:330:LYS:N	2.35	0.59
4:B:209:GLU:OE1	4:B:788:ARG:NH2	2.25	0.59
7:E:168:TYR:HB3	7:E:170:LEU:HD23	1.84	0.59
9:G:84:GLY:HA2	9:G:146:LYS:HD2	1.84	0.59
11:I:78:CYS:SG	11:I:105:SER:OG	2.60	0.59
3:A:905:ASP:OD1	3:A:906:HIS:N	2.35	0.59
4:B:801:LYS:O	12:J:52:THR:OG1	2.18	0.59
4:B:924:GLU:HG2	4:B:925:LEU:HD12	1.83	0.59
4:B:997:GLU:OE1	4:B:997:GLU:N	2.33	0.59
3:A:590:ARG:NH2	3:A:620:LYS:HB3	2.17	0.59
4:B:146:GLU:HG2	4:B:147:LEU:H	1.65	0.59
9:G:154:VAL:O	9:G:156:SER:N	2.34	0.59
5:C:178:PHE:CD1	5:C:230:MET:HE1	2.37	0.59
9:G:116:PRO:HD2	9:G:119:LEU:HD22	1.83	0.59
3:A:871:ASP:OD1	3:A:872:GLY:N	2.34	0.59
4:B:876:LYS:HB2	4:B:895:ASP:HA	1.83	0.59
10:H:5:LEU:HD11	10:H:61:SER:HB3	1.83	0.59
3:A:589:GLN:HB3	3:A:591:PHE:HE2	1.68	0.59
4:B:295:GLY:HA3	11:I:11:ASN:HB3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:99:GLY:HA3	10:H:118:PHE:CD1	2.38	0.59
10:H:135:LEU:HD13	10:H:137:GLN:HB3	1.85	0.59
4:B:510:LYS:HG3	4:B:511:PRO:CD	2.27	0.59
4:B:770:GLN:O	4:B:770:GLN:NE2	2.35	0.59
16:Q:379:GLU:N	16:Q:383:SER:O	2.25	0.59
3:A:33:ALA:H	3:A:82:GLY:HA2	1.67	0.59
3:A:618:GLU:HG3	3:A:620:LYS:H	1.65	0.59
10:H:128:ASN:OD1	10:H:131:ASN:ND2	2.34	0.59
4:B:372:SER:OG	4:B:373:ARG:NH1	2.34	0.59
3:A:32:VAL:O	3:A:57:ARG:NH1	2.35	0.59
4:B:1058:LEU:O	4:B:1061:GLU:HG3	2.02	0.59
5:C:66:ARG:NH2	12:J:3:VAL:O	2.35	0.59
10:H:62:SER:OG	10:H:63:LEU:N	2.36	0.59
10:H:130:ARG:H	10:H:130:ARG:HD3	1.68	0.59
11:I:45:ARG:HE	11:I:46:HIS:N	2.01	0.59
3:A:1054:LEU:HB3	8:F:84:TYR:HE1	1.68	0.58
4:B:79:THR:HG22	4:B:82:ASP:HA	1.85	0.58
6:D:56:ARG:NH2	6:D:154:PHE:O	2.31	0.58
9:G:144:ARG:HB2	9:G:169:GLY:H	1.67	0.58
3:A:1129:GLU:OE1	3:A:1129:GLU:N	2.33	0.58
4:B:687:GLU:OE1	4:B:687:GLU:N	2.26	0.58
3:A:1209:MET:HA	3:A:1212:VAL:HG22	1.85	0.58
4:B:70:ILE:HG22	4:B:89:GLU:HA	1.86	0.58
3:A:239:LEU:HD12	3:A:240:PRO:HD2	1.85	0.58
4:B:668:ASP:OD2	16:Q:28:ARG:NH2	2.36	0.58
5:C:239:PRO:HB2	5:C:242:GLN:HG2	1.85	0.58
9:G:56:ILE:HG13	9:G:57:GLN:H	1.68	0.58
10:H:99:GLY:HA3	10:H:118:PHE:HD1	1.68	0.58
2:O:-13:DA:H1'	3:A:835:GLY:HA3	1.86	0.58
4:B:75:ALA:O	4:B:76:GLN:HG2	2.03	0.58
4:B:275:TYR:HB3	4:B:337:ARG:HD2	1.86	0.58
4:B:307:ASP:OD1	4:B:308:TRP:N	2.37	0.58
6:D:40:HIS:HB2	9:G:73:LYS:NZ	2.19	0.58
4:B:412:LEU:HB3	4:B:466:TRP:CZ2	2.39	0.58
9:G:120:THR:OG1	9:G:131:GLN:O	2.22	0.58
3:A:1118:VAL:HB	3:A:1306:LEU:HB2	1.86	0.57
1:N:18:DT:H1'	1:N:19:DG:C8	2.39	0.57
3:A:1390:ASN:HD22	3:A:1402:PHE:HD2	1.52	0.57
4:B:364:ILE:HG22	4:B:585:VAL:HG23	1.84	0.57
4:B:802:PRO:HB3	4:B:1091:TYR:CG	2.39	0.57
5:C:208:GLU:N	5:C:208:GLU:OE1	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:139:LYS:HZ2	6:D:142:LYS:HB2	1.69	0.57
3:A:68:GLN:NE2	3:A:70:CYS:SG	2.77	0.57
4:B:185:THR:O	4:B:189:LEU:N	2.25	0.57
4:B:194:GLU:N	4:B:194:GLU:OE1	2.38	0.57
4:B:857:ARG:NH1	4:B:859:TYR:OH	2.34	0.57
3:A:12:ARG:HH21	4:B:1218:THR:HG21	1.68	0.57
3:A:440:ASP:H	3:A:460:VAL:HG12	1.70	0.57
3:A:471:ASN:OD1	3:A:472:LEU:N	2.38	0.57
3:A:781:ASP:HB2	3:A:789:LYS:HD2	1.86	0.57
3:A:865:GLN:NE2	3:A:1373:ASP:OD2	2.26	0.57
3:A:1116:LEU:HB3	3:A:1329:THR:HG23	1.87	0.57
3:A:1444:MET:HE3	8:F:135:ARG:HE	1.69	0.57
4:B:104:GLU:OE2	4:B:110:HIS:CE1	2.58	0.57
5:C:55:THR:HB	5:C:152:GLU:H	1.70	0.57
7:E:123:LEU:HD23	7:E:123:LEU:H	1.70	0.57
8:F:130:ILE:N	8:F:149:GLU:OE2	2.38	0.57
3:A:473:SER:OG	3:A:650:GLN:OE1	2.18	0.57
3:A:490:HIS:HB3	4:B:1150:ARG:HH12	1.69	0.57
5:C:179:GLU:HB2	5:C:229:TYR:HB2	1.86	0.57
3:A:243:PRO:HB2	3:A:245:PRO:HD2	1.86	0.57
3:A:557:ASP:HB3	3:A:559:VAL:HG12	1.86	0.57
4:B:918:ILE:HG22	4:B:921:ASP:HB2	1.87	0.57
8:F:84:TYR:HE2	8:F:152:ILE:HD11	1.69	0.57
3:A:806:ARG:O	4:B:728:ARG:NH2	2.38	0.57
4:B:420:LEU:HD21	4:B:456:GLY:HA3	1.86	0.57
10:H:98:TYR:OH	10:H:139:ASN:ND2	2.28	0.57
3:A:434:ARG:HD2	3:A:435:HIS:O	2.05	0.57
4:B:727:LYS:HB3	4:B:1051:THR:HG21	1.87	0.57
3:A:949:ASP:OD1	3:A:950:GLY:N	2.38	0.56
4:B:487:THR:HG22	4:B:489:SER:H	1.70	0.56
12:J:3:VAL:HG11	12:J:18:TRP:CD2	2.40	0.56
3:A:1191:TRP:HZ3	11:I:43:VAL:HG21	1.70	0.56
3:A:563:PRO:HG3	3:A:570:PRO:HB3	1.87	0.56
3:A:922:ASP:OD1	3:A:923:LEU:N	2.38	0.56
3:A:1161:THR:HG22	3:A:1163:ILE:N	2.20	0.56
3:A:1216:ILE:O	3:A:1219:THR:HG22	2.06	0.56
3:A:1363:VAL:HG23	3:A:1368:MET:HE2	1.87	0.56
4:B:1065:GLN:OE1	4:B:1068:GLY:N	2.38	0.56
5:C:114:TYR:N	5:C:117:ASP:OD2	2.35	0.56
5:C:248:ILE:HG21	13:K:102:LYS:HB2	1.87	0.56
3:A:173:THR:OG1	3:A:184:SER:OG	2.24	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1329:THR:HB	3:A:1335:ILE:HD11	1.88	0.56
5:C:76:ASP:OD2	5:C:128:ASN:N	2.38	0.56
3:A:372:LYS:NZ	13:K:2:ASN:HB2	2.20	0.56
4:B:1156:ASP:HB3	4:B:1198:TYR:H	1.71	0.56
5:C:43:THR:HG23	5:C:170:TRP:HD1	1.70	0.56
6:D:56:ARG:NH1	6:D:155:ARG:HE	2.03	0.56
8:F:84:TYR:CE2	8:F:152:ILE:HD11	2.40	0.56
13:K:8:GLU:HG2	13:K:37:LYS:HZ2	1.71	0.56
3:A:14:VAL:HG22	4:B:1216:LEU:HD21	1.87	0.56
3:A:385:ILE:O	3:A:389:THR:OG1	2.20	0.56
3:A:741:ASN:OD1	3:A:742:ASN:N	2.39	0.56
3:A:761:MET:HE1	4:B:1018:PRO:HA	1.87	0.56
4:B:323:VAL:HG13	4:B:324:ILE:HG13	1.88	0.56
4:B:1181:GLU:HG3	4:B:1188:LYS:HE3	1.88	0.56
7:E:25:ASP:OD2	7:E:187:TYR:OH	2.19	0.56
3:A:179:LEU:HD12	3:A:297:GLN:HE22	1.70	0.56
3:A:451:HIS:CD2	3:A:453:MET:HB2	2.41	0.56
3:A:1335:ILE:HG23	3:A:1339:LEU:HD12	1.88	0.56
2:O:-16:DT:H2"	2:O:-15:DA:C8	2.41	0.56
3:A:1111:MET:SD	3:A:1331:SER:OG	2.52	0.56
3:A:1149:ALA:HB1	11:I:45:ARG:HH22	1.70	0.56
4:B:874:PHE:CE1	4:B:962:LYS:HB3	2.41	0.56
11:I:27:PHE:O	11:I:36:GLU:N	2.36	0.56
4:B:82:ASP:N	4:B:83:ASN:HA	2.18	0.56
4:B:872:GLU:HG2	4:B:917:PRO:HD3	1.88	0.56
6:D:191:ALA:HA	6:D:194:LEU:HD12	1.88	0.56
5:C:166:GLU:O	13:K:6:ARG:NH2	2.26	0.55
7:E:202:SER:O	7:E:206:GLY:N	2.33	0.55
3:A:737:LEU:HD11	3:A:741:ASN:HD22	1.71	0.55
3:A:964:ILE:O	3:A:968:GLN:HG3	2.06	0.55
3:A:738:LYS:NZ	5:C:193:TYR:O	2.37	0.55
4:B:287:ARG:NH2	4:B:294:ASP:OD1	2.30	0.55
4:B:805:THR:O	4:B:1044:ALA:N	2.40	0.55
4:B:629:ASP:O	4:B:632:ARG:NH2	2.35	0.55
6:D:148:LEU:O	6:D:152:SER:OG	2.13	0.55
17:M:86:ASN:OD1	17:M:90:GLN:NE2	2.40	0.55
4:B:824:ILE:HD11	12:J:48:ARG:HD2	1.89	0.55
7:E:156:LEU:HD21	7:E:197:LYS:HB2	1.89	0.55
8:F:77:ASP:OD2	8:F:78:GLN:N	2.40	0.55
3:A:540:PHE:HB3	3:A:571:LEU:HD23	1.89	0.55
4:B:1155:SER:OG	4:B:1156:ASP:N	2.38	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:101:LEU:O	5:C:102:GLN:NE2	2.39	0.55
3:A:874:ASP:O	3:A:878:ILE:HD11	2.07	0.55
3:A:946:VAL:HG23	3:A:947:PHE:H	1.71	0.55
3:A:1192:LEU:HD11	3:A:1239:ARG:HB3	1.87	0.55
5:C:54:ASN:OD1	5:C:55:THR:N	2.39	0.55
5:C:68:GLY:HA3	14:L:69:ALA:HB1	1.88	0.55
5:C:241:ASP:N	5:C:241:ASP:OD1	2.40	0.55
11:I:44:TYR:OH	11:I:46:HIS:ND1	2.40	0.55
7:E:201:LYS:HA	7:E:206:GLY:O	2.07	0.55
9:G:13:LEU:HD12	9:G:26:LEU:HD21	1.89	0.55
15:R:14:C:O2	15:R:14:C:C2'	2.55	0.55
3:A:44:THR:N	3:A:45:GLN:HA	2.22	0.54
3:A:848:ILE:HB	3:A:1065:GLY:HA3	1.90	0.54
4:B:35:SER:HG	4:B:811:TYR:HH	1.55	0.54
3:A:337:ARG:HH21	3:A:839:ARG:CZ	2.20	0.54
3:A:1149:ALA:HB3	3:A:1196:GLU:HB3	1.89	0.54
4:B:277:LYS:HA	4:B:337:ARG:HH21	1.72	0.54
4:B:921:ASP:O	4:B:927:GLN:NE2	2.38	0.54
4:B:1156:ASP:CB	4:B:1198:TYR:H	2.19	0.54
5:C:184:ASN:ND2	5:C:189:THR:O	2.37	0.54
10:H:130:ARG:HB2	10:H:133:ASN:HB3	1.88	0.54
12:J:48:ARG:O	12:J:52:THR:HG22	2.07	0.54
13:K:9:LEU:HG	13:K:10:PHE:CD2	2.42	0.54
13:K:98:LEU:HD12	13:K:99:GLY:N	2.22	0.54
3:A:446:ARG:HD2	3:A:480:ALA:HB2	1.89	0.54
3:A:40:THR:O	3:A:50:ILE:N	2.38	0.54
3:A:535:THR:HG21	3:A:617:VAL:HG23	1.90	0.54
4:B:247:GLY:HA2	4:B:418:LYS:HE2	1.88	0.54
6:D:66:ARG:NH1	6:D:67:ARG:HH21	2.04	0.54
10:H:135:LEU:O	10:H:137:GLN:N	2.40	0.54
3:A:114:LEU:C	3:A:164:ARG:HH22	2.16	0.54
3:A:386:ASP:OD1	3:A:386:ASP:N	2.39	0.54
10:H:145:ARG:O	10:H:146:ARG:HD3	2.08	0.54
3:A:1052:GLN:HG2	3:A:1055:ARG:HH21	1.73	0.54
9:G:46:LEU:HD11	9:G:79:PHE:HB2	1.90	0.54
16:Q:377:SER:OG	17:M:67:GLN:O	2.24	0.54
3:A:918:GLU:OE1	3:A:918:GLU:N	2.35	0.54
4:B:841:MET:HE1	4:B:980:PHE:CE2	2.36	0.54
5:C:66:ARG:HH22	12:J:5:VAL:HG23	1.73	0.54
5:C:73:GLN:OE1	5:C:75:MET:N	2.36	0.54
8:F:89:GLU:OE1	8:F:89:GLU:N	2.29	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:100:PHE:HB3	11:I:109:ILE:HD11	1.90	0.54
14:L:50:ASP:OD1	14:L:51:CYS:N	2.39	0.54
4:B:620:ARG:NH1	11:I:57:GLY:HA3	2.23	0.54
4:B:863:GLU:HG2	4:B:872:GLU:HB2	1.90	0.54
3:A:530:GLY:HA3	3:A:657:LEU:HD21	1.89	0.54
3:A:682:THR:O	3:A:685:GLU:HG3	2.07	0.54
5:C:50:GLU:HB2	5:C:156:THR:HB	1.89	0.54
7:E:171:LYS:O	7:E:173:SER:N	2.39	0.54
11:I:22:ASN:HB3	11:I:24:ARG:NH1	2.23	0.54
11:I:26:LEU:HD13	11:I:37:GLU:HA	1.90	0.54
12:J:32:GLU:OE1	12:J:32:GLU:N	2.33	0.54
1:N:-5:DA:H2"	1:N:-4:DG:C8	2.42	0.54
3:A:1000:LEU:N	3:A:1011:GLN:OE1	2.36	0.54
4:B:743:ILE:HG13	4:B:744:HIS:N	2.22	0.54
3:A:833:GLU:O	3:A:837:ILE:HD12	2.07	0.53
3:A:1445:ILE:HB	9:G:61:ILE:HD11	1.90	0.53
4:B:487:THR:OG1	4:B:777:ALA:O	2.25	0.53
6:D:125:SER:O	6:D:129:LEU:HG	2.07	0.53
8:F:70:LYS:O	8:F:71:GLU:HG3	2.07	0.53
13:K:12:LEU:HA	13:K:37:LYS:HG3	1.88	0.53
3:A:537:ARG:NH1	3:A:602:ASP:OD2	2.41	0.53
3:A:1319:VAL:HG13	3:A:1322:ILE:HG13	1.89	0.53
4:B:542:MET:CE	4:B:747:MET:HB3	2.37	0.53
4:B:789:MET:HA	4:B:789:MET:HE2	1.90	0.53
4:B:957:ASN:OD1	4:B:960:GLY:N	2.41	0.53
10:H:145:ARG:C	10:H:146:ARG:HD3	2.33	0.53
16:Q:98:TYR:CD1	16:Q:100:GLU:HG2	2.43	0.53
16:Q:363:GLY:HA2	16:Q:395:PHE:HA	1.89	0.53
17:M:117:PRO:HG3	17:M:233:TYR:HA	1.91	0.53
3:A:225:ASN:O	3:A:229:SER:N	2.35	0.53
3:A:346:ASP:CG	4:B:1108:ARG:H	2.17	0.53
3:A:443:LEU:HB2	3:A:501:LEU:HD11	1.90	0.53
7:E:100:ILE:HG23	7:E:105:PHE:HB2	1.90	0.53
9:G:94:CYS:HB2	9:G:127:PRO:HB2	1.89	0.53
16:Q:28:ARG:HE	16:Q:32:LEU:HD11	1.73	0.53
17:M:67:GLN:HB2	17:M:219:CYS:SG	2.49	0.53
17:M:96:ARG:HE	17:M:105:THR:HG22	1.72	0.53
3:A:1126:ALA:HA	3:A:1304:TRP:CD1	2.42	0.53
4:B:384:ARG:HE	4:B:387:LEU:HD12	1.74	0.53
4:B:1031:LEU:HD21	4:B:1042:GLY:HA3	1.89	0.53
7:E:48:ASP:OD1	7:E:49:SER:N	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:346:ASP:OD1	3:A:347:PHE:N	2.42	0.53
3:A:1002:GLY:HA3	3:A:1007:ILE:HG21	1.91	0.53
3:A:1430:LEU:HB3	3:A:1432:GLN:NE2	2.23	0.53
10:H:95:TYR:CE2	10:H:97:MET:HG2	2.44	0.53
3:A:957:PRO:HG2	3:A:1018:PHE:CD1	2.44	0.53
4:B:245:GLU:N	4:B:246:LYS:HA	2.24	0.53
4:B:580:VAL:HG22	4:B:624:LEU:HD23	1.89	0.53
2:O:-19:DC:H2"	2:O:-18:DA:C8	2.44	0.53
3:A:1359:ASP:OD1	3:A:1359:ASP:N	2.42	0.53
11:I:17:ARG:N	11:I:26:LEU:O	2.37	0.53
3:A:851:HIS:CD2	8:F:139:PRO:HG3	2.44	0.53
4:B:696:GLU:OE1	4:B:696:GLU:N	2.41	0.53
10:H:118:PHE:O	10:H:120:GLY:N	2.42	0.53
4:B:355:ILE:O	4:B:359:GLU:HG3	2.09	0.53
4:B:705:MET:HE3	4:B:705:MET:HA	1.90	0.53
4:B:830:TYR:CZ	4:B:1000:PRO:HD3	2.44	0.53
3:A:113:LEU:O	3:A:164:ARG:NH2	2.42	0.52
3:A:851:HIS:CE1	3:A:857:ARG:HB2	2.43	0.52
3:A:857:ARG:NH1	8:F:139:PRO:HG2	2.24	0.52
3:A:1074:GLU:HG3	3:A:1075:PRO:HD3	1.91	0.52
4:B:1041:GLU:H	16:Q:23:LYS:HZ1	1.57	0.52
4:B:1041:GLU:N	16:Q:23:LYS:HZ1	2.07	0.52
7:E:3:GLN:OE1	7:E:4:GLU:HG3	2.09	0.52
3:A:619:LYS:NZ	15:R:18:A:OP2	2.42	0.52
3:A:1111:MET:C	3:A:1113:THR:H	2.17	0.52
6:D:52:LEU:HD12	6:D:148:LEU:HD23	1.92	0.52
3:A:92:HIS:HB2	3:A:236:LEU:HD23	1.92	0.52
3:A:381:THR:HG1	3:A:384:ASN:H	1.58	0.52
4:B:604:ARG:NH2	4:B:613:VAL:O	2.43	0.52
9:G:45:ILE:HG13	9:G:78:VAL:HG12	1.90	0.52
11:I:88:SER:O	11:I:91:ARG:NH1	2.38	0.52
4:B:680:THR:H	4:B:683:SER:HB2	1.74	0.52
4:B:860:MET:HB2	4:B:963:PHE:HE1	1.73	0.52
17:M:73:LEU:HD11	17:M:77:LEU:HD23	1.90	0.52
3:A:69:THR:HA	3:A:71:GLN:NE2	2.24	0.52
4:B:85:SER:O	4:B:87:LYS:N	2.42	0.52
4:B:120:ARG:HG2	4:B:955:THR:HG21	1.92	0.52
4:B:747:MET:HA	4:B:747:MET:HE2	1.92	0.52
4:B:1080:LYS:HG2	5:C:180:TYR:OH	2.10	0.52
5:C:138:GLU:OE1	5:C:138:GLU:N	2.43	0.52
9:G:21:ARG:HH12	9:G:25:TYR:H	1.57	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:20:SER:HA	12:J:23:ASN:HD21	1.74	0.52
3:A:315:LEU:HD23	3:A:315:LEU:H	1.74	0.52
3:A:336:ILE:HG22	3:A:341:MET:HE1	1.91	0.52
3:A:1166:ASP:HA	3:A:1169:ILE:HD13	1.92	0.52
4:B:546:SER:OG	4:B:631:GLY:N	2.43	0.52
4:B:745:PRO:HB2	4:B:1047:PHE:HD2	1.75	0.52
4:B:1165:ILE:HD12	4:B:1187:ASN:HD22	1.73	0.52
6:D:57:LEU:HD13	6:D:157:GLN:HG2	1.91	0.52
7:E:85:GLU:OE2	7:E:89:GLY:N	2.38	0.52
16:Q:121:PHE:HB2	17:M:131:ASN:HB3	1.92	0.52
3:A:387:ARG:HH21	3:A:437:MET:HE1	1.75	0.52
3:A:821:ARG:NH2	4:B:534:GLY:HA2	2.25	0.52
7:E:170:LEU:HD12	7:E:174:GLN:HB2	1.92	0.52
13:K:53:ASP:OD1	13:K:54:ARG:N	2.43	0.52
3:A:106:VAL:HG21	3:A:214:ILE:HD12	1.91	0.52
3:A:852:TYR:CD1	3:A:1060:PRO:HB2	2.45	0.52
7:E:180:ARG:N	7:E:215:MET:OXT	2.42	0.52
17:M:73:LEU:HD12	17:M:74:PRO:HD2	1.92	0.52
3:A:566:ILE:HB	10:H:96:VAL:HG23	1.92	0.52
4:B:102:VAL:H	4:B:112:LEU:HD23	1.74	0.52
4:B:129:PHE:HB3	4:B:166:PHE:HA	1.90	0.52
4:B:189:LEU:HD21	4:B:196:PRO:HA	1.91	0.52
5:C:255:VAL:O	5:C:258:ILE:HG22	2.10	0.52
11:I:7:CYS:HB3	11:I:10:CYS:O	2.09	0.52
16:Q:116:THR:HG22	17:M:136:THR:HG22	1.92	0.52
17:M:96:ARG:NH2	17:M:98:ASN:OD1	2.43	0.52
4:B:62:ILE:HD13	4:B:417:PHE:HD2	1.75	0.52
4:B:217:ARG:NE	4:B:407:ASP:OD2	2.35	0.52
4:B:276:ILE:O	4:B:337:ARG:NH2	2.42	0.52
7:E:182:ASP:OD2	7:E:184:VAL:HG12	2.10	0.52
3:A:768:GLN:HE21	3:A:800:VAL:HG21	1.74	0.51
3:A:903:ASN:O	3:A:907:THR:OG1	2.28	0.51
3:A:909:ASP:HB3	3:A:912:LEU:HD13	1.92	0.51
3:A:1364:ASN:OD1	3:A:1365:TYR:N	2.43	0.51
3:A:1373:ASP:HA	3:A:1376:THR:HG22	1.92	0.51
4:B:496:ARG:O	4:B:497:ARG:NH1	2.42	0.51
4:B:640:VAL:HA	4:B:651:LEU:HA	1.91	0.51
4:B:1082:MET:O	5:C:189:THR:OG1	2.20	0.51
16:Q:404:LEU:HB3	16:Q:408:GLU:OE2	2.10	0.51
3:A:1035:TYR:HB3	3:A:1037:LEU:HD23	1.91	0.51
4:B:73:GLN:HA	16:Q:330:ARG:NH2	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:33:GLN:OE1	10:H:34:ASP:N	2.43	0.51
13:K:110:ASN:HA	13:K:113:THR:HG23	1.93	0.51
17:M:106:LEU:N	17:M:120:TYR:O	2.27	0.51
3:A:589:GLN:HB3	3:A:591:PHE:CE2	2.45	0.51
4:B:29:ASP:HB3	4:B:658:ILE:HD13	1.92	0.51
9:G:116:PRO:HD3	9:G:163:ILE:HG13	1.91	0.51
1:N:17:DG:H2'	1:N:18:DT:C6	2.45	0.51
2:O:-2:DA:H2''	2:O:-1:DG:C8	2.46	0.51
3:A:172:PRO:HG3	3:A:185:TRP:CE2	2.46	0.51
3:A:590:ARG:NH1	3:A:621:THR:OG1	2.43	0.51
3:A:862:ASN:HA	7:E:174:GLN:HB3	1.92	0.51
7:E:96:PHE:CZ	7:E:100:ILE:HD11	2.45	0.51
7:E:118:PRO:HA	7:E:121:MET:HG3	1.92	0.51
3:A:1116:LEU:HD23	3:A:1311:VAL:HA	1.92	0.51
4:B:809:MET:HG3	4:B:814:PHE:HD1	1.76	0.51
4:B:922:GLU:HG2	4:B:926:GLY:HA3	1.92	0.51
7:E:87:SER:OG	7:E:88:VAL:N	2.43	0.51
9:G:10:ASN:HA	9:G:71:ASN:HA	1.91	0.51
16:Q:97:GLU:HA	17:M:99:LYS:HE3	1.92	0.51
16:Q:129:PRO:HA	16:Q:133:PHE:CD1	2.45	0.51
3:A:775:ILE:HD12	3:A:775:ILE:H	1.75	0.51
4:B:171:PRO:HG2	4:B:461:LEU:HD12	1.92	0.51
4:B:867:GLY:HA3	4:B:868:MET:O	2.10	0.51
4:B:1000:PRO:HB2	4:B:1072:MET:HE2	1.91	0.51
7:E:40:GLU:OE1	7:E:40:GLU:N	2.43	0.51
3:A:108:MET:SD	3:A:171:GLN:HG3	2.50	0.51
3:A:567:LYS:HE3	10:H:95:TYR:HD1	1.75	0.51
3:A:1215:ARG:O	3:A:1218:GLN:NE2	2.43	0.51
4:B:629:ASP:OD1	4:B:632:ARG:NE	2.36	0.51
4:B:1065:GLN:NE2	4:B:1067:ARG:H	2.08	0.51
10:H:137:GLN:OE1	10:H:139:ASN:N	2.44	0.51
6:D:59:ILE:HG13	6:D:60:LYS:HD3	1.92	0.51
3:A:348:SER:HB3	4:B:1128:LEU:HD12	1.93	0.51
3:A:993:LEU:HD21	3:A:1046:LEU:HB3	1.92	0.51
3:A:1199:ARG:HD3	3:A:1236:LEU:HD11	1.93	0.51
4:B:79:THR:CB	4:B:81:SER:H	2.24	0.51
4:B:406:LEU:HB2	4:B:545:ILE:HD11	1.93	0.51
8:F:93:ILE:HD11	8:F:132:LEU:HG	1.92	0.51
14:L:31:CYS:HB2	14:L:48:CYS:HB3	1.91	0.51
3:A:653:VAL:O	3:A:657:LEU:HD23	2.11	0.51
3:A:1426:GLU:OE2	3:A:1426:GLU:N	2.39	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:391:ASP:OD2	11:I:90:GLN:NE2	2.44	0.51
4:B:806:THR:H	4:B:809:MET:HE1	1.75	0.51
7:E:180:ARG:NH2	7:E:192:ARG:HB2	2.26	0.51
3:A:1062:GLU:OE1	3:A:1062:GLU:N	2.35	0.50
3:A:1277:GLU:N	3:A:1277:GLU:OE1	2.39	0.50
9:G:96:GLN:HA	9:G:128:PRO:HB2	1.93	0.50
16:Q:386:MET:HE3	17:M:87:LEU:HD13	1.93	0.50
4:B:216:GLU:HG2	4:B:500:THR:HB	1.92	0.50
4:B:546:SER:OG	4:B:632:ARG:N	2.33	0.50
10:H:13:SER:OG	10:H:27:GLU:OE2	2.28	0.50
3:A:1173:HIS:CE1	3:A:1227:ILE:HG23	2.47	0.50
4:B:195:CYS:HB3	4:B:782:LEU:HD22	1.94	0.50
5:C:6:PRO:HG2	13:K:101:LEU:HB2	1.94	0.50
10:H:26:ILE:N	10:H:40:LEU:O	2.38	0.50
3:A:40:THR:HB	3:A:54:ASN:HB2	1.93	0.50
3:A:542:GLU:OE1	3:A:544:ASP:N	2.33	0.50
3:A:802:ASN:ND2	3:A:806:ARG:HB2	2.17	0.50
4:B:526:GLU:OE2	4:B:752:ALA:N	2.45	0.50
7:E:43:LYS:HE3	7:E:47:CYS:HB2	1.94	0.50
7:E:141:VAL:HG13	7:E:142:VAL:HG23	1.94	0.50
10:H:37:LYS:H	10:H:126:GLU:HB2	1.77	0.50
16:Q:390:ASP:OD1	16:Q:391:LYS:N	2.44	0.50
3:A:668:ASP:OD2	3:A:742:ASN:HB2	2.11	0.50
3:A:942:PHE:HD2	3:A:943:LEU:HD22	1.75	0.50
4:B:212:LEU:HD11	4:B:409:ALA:HB2	1.94	0.50
4:B:360:PHE:HE2	4:B:374:LYS:HD2	1.76	0.50
5:C:161:LYS:O	5:C:170:TRP:NE1	2.44	0.50
6:D:31:GLN:O	6:D:34:GLN:NE2	2.44	0.50
16:Q:17:ASN:HB3	16:Q:20:PRO:HD3	1.93	0.50
4:B:35:SER:OG	4:B:811:TYR:OH	2.24	0.50
4:B:604:ARG:NH2	4:B:614:SER:HA	2.27	0.50
4:B:835:GLN:OE1	4:B:835:GLN:N	2.39	0.50
4:B:360:PHE:CE2	4:B:374:LYS:HD2	2.46	0.50
4:B:793:ALA:HB3	4:B:856:PHE:HB2	1.94	0.50
4:B:992:ILE:HD11	4:B:994:TYR:CZ	2.47	0.50
8:F:140:ASP:OD1	8:F:141:GLY:N	2.45	0.50
3:A:402:ALA:HA	3:A:434:ARG:HA	1.94	0.50
4:B:121:ASN:HA	4:B:207:GLY:HA3	1.94	0.50
4:B:247:GLY:O	4:B:249:ARG:N	2.44	0.50
4:B:604:ARG:HH22	4:B:614:SER:HA	1.77	0.50
4:B:910:VAL:HA	4:B:940:PRO:HA	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:73:GLN:OE1	5:C:74:SER:N	2.45	0.50
12:J:9:SER:HB2	12:J:45:CYS:HB2	1.94	0.50
3:A:665:GLY:O	3:A:668:ASP:HB2	2.12	0.49
4:B:582:VAL:HG22	4:B:626:ILE:HB	1.93	0.49
5:C:15:LYS:NZ	5:C:135:GLN:OE1	2.36	0.49
6:D:14:ARG:O	6:D:17:LYS:HG3	2.12	0.49
15:R:12:A:H2'	15:R:13:U:C6	2.47	0.49
3:A:325:ILE:HG13	4:B:1210:MET:CE	2.42	0.49
3:A:864:ILE:HD12	3:A:1377:THR:HG21	1.94	0.49
3:A:877:HIS:CD2	3:A:1056:SER:HA	2.47	0.49
3:A:1157:ASP:OD1	3:A:1160:SER:N	2.45	0.49
4:B:25:ILE:HG23	4:B:29:ASP:HB2	1.94	0.49
4:B:800:GLN:OE1	12:J:53:HIS:HA	2.12	0.49
4:B:900:ALA:HB1	14:L:61:THR:OG1	2.12	0.49
5:C:258:ILE:HD11	13:K:35:PHE:CZ	2.47	0.49
7:E:106:GLN:HG2	7:E:107:THR:HG23	1.93	0.49
2:O:-12:DT:OP2	3:A:332:LYS:NZ	2.45	0.49
3:A:147:VAL:HG23	3:A:170:THR:HG22	1.93	0.49
3:A:1138:ILE:HD11	3:A:1316:VAL:HG12	1.93	0.49
4:B:279:ASP:OD1	4:B:279:ASP:N	2.46	0.49
4:B:325:GLN:O	16:Q:401:TYR:OH	2.30	0.49
4:B:648:HIS:CD2	4:B:648:HIS:H	2.29	0.49
7:E:21:GLU:OE2	7:E:143:ASN:ND2	2.46	0.49
11:I:76:PRO:O	11:I:77:LYS:HD3	2.12	0.49
1:N:17:DG:H2'	1:N:18:DT:H71	1.95	0.49
3:A:35:ILE:HD12	3:A:35:ILE:H	1.77	0.49
4:B:563:MET:HE2	4:B:563:MET:HA	1.94	0.49
5:C:7:GLN:HA	13:K:104:ASN:ND2	2.27	0.49
10:H:95:TYR:HB3	10:H:144:ILE:HB	1.94	0.49
4:B:373:ARG:NE	4:B:566:LEU:HB2	2.28	0.49
11:I:54:GLU:HB2	11:I:100:PHE:CE2	2.48	0.49
3:A:66:LYS:HE2	3:A:69:THR:HG23	1.93	0.49
3:A:446:ARG:HB2	3:A:487:MET:SD	2.52	0.49
4:B:247:GLY:C	4:B:249:ARG:H	2.20	0.49
4:B:862:GLN:O	4:B:914:LYS:NZ	2.31	0.49
5:C:102:GLN:HE22	5:C:154:LYS:HA	1.78	0.49
6:D:53:SER:O	6:D:57:LEU:HG	2.12	0.49
3:A:808:LEU:O	4:B:728:ARG:NH1	2.46	0.49
4:B:336:ARG:HG3	4:B:337:ARG:H	1.78	0.49
4:B:1171:VAL:HG11	4:B:1191:ILE:HD13	1.94	0.49
4:B:1196:ILE:HD12	4:B:1197:PRO:HD2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:146:LYS:HD2	12:J:57:ILE:HD12	1.95	0.49
6:D:216:ASN:OD1	6:D:217:LEU:N	2.46	0.49
10:H:137:GLN:CD	10:H:138:GLU:H	2.20	0.49
3:A:311:GLN:CG	3:A:312:PRO:HD3	2.41	0.49
2:O:2:DC:H2"	2:O:3:DA:C8	2.48	0.49
3:A:5:GLN:HG3	4:B:1175:LEU:HD13	1.95	0.49
3:A:594:GLY:HA3	3:A:603:ASN:HD21	1.77	0.49
3:A:675:THR:HG21	3:A:736:ASN:HB2	1.95	0.49
3:A:1165:GLU:N	3:A:1165:GLU:OE1	2.44	0.49
4:B:123:THR:O	4:B:125:SER:N	2.45	0.49
4:B:327:ARG:HG3	4:B:328:GLU:OE1	2.13	0.49
5:C:35:ARG:HA	5:C:38:ILE:HG22	1.94	0.49
5:C:252:GLN:HB3	13:K:98:LEU:HD13	1.95	0.49
4:B:822:ASN:HA	4:B:1091:TYR:HA	1.94	0.49
6:D:55:ALA:HA	6:D:58:VAL:HG22	1.95	0.49
7:E:20:LYS:HD2	7:E:35:VAL:HA	1.95	0.49
3:A:171:GLN:N	3:A:171:GLN:OE1	2.44	0.48
3:A:232:GLU:OE1	3:A:232:GLU:N	2.43	0.48
3:A:766:GLY:HA2	3:A:799:PHE:HE1	1.78	0.48
3:A:1332:PHE:HA	3:A:1335:ILE:HD13	1.94	0.48
4:B:78:THR:HG23	4:B:79:THR:H	1.78	0.48
8:F:97:ARG:O	8:F:101:ILE:HG12	2.12	0.48
3:A:509:LEU:HD23	3:A:509:LEU:H	1.78	0.48
4:B:260:GLY:O	4:B:267:ARG:NH2	2.38	0.48
5:C:66:ARG:NH2	12:J:5:VAL:HG23	2.27	0.48
3:A:456:MET:HE2	3:A:478:TYR:CZ	2.49	0.48
3:A:711:ARG:CZ	11:I:97:MET:HE1	2.43	0.48
3:A:744:LYS:O	3:A:748:MET:HG3	2.13	0.48
4:B:405:ARG:NE	4:B:629:ASP:OD2	2.38	0.48
5:C:54:ASN:ND2	5:C:60:ASP:OD1	2.23	0.48
5:C:99:LEU:HD11	5:C:120:ILE:HD13	1.94	0.48
5:C:249:ASP:O	5:C:252:GLN:NE2	2.46	0.48
10:H:105:GLU:O	10:H:113:ALA:N	2.41	0.48
3:A:172:PRO:HG3	3:A:185:TRP:CZ2	2.49	0.48
3:A:261:ASP:OD1	3:A:322:VAL:HG23	2.13	0.48
3:A:960:ILE:O	3:A:963:ILE:HG22	2.14	0.48
3:A:972:HIS:O	3:A:972:HIS:ND1	2.47	0.48
3:A:1116:LEU:HG	3:A:1308:THR:HG21	1.96	0.48
4:B:256:VAL:HG21	4:B:381:MET:HE1	1.95	0.48
4:B:308:TRP:O	4:B:311:LEU:N	2.47	0.48
4:B:868:MET:O	4:B:870:ILE:N	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:87:GLN:HE22	11:I:91:ARG:NH1	2.11	0.48
13:K:24:ASP:OD1	13:K:25:THR:N	2.46	0.48
2:O:-14:DT:H4'	2:O:-14:DT:OP1	2.13	0.48
3:A:118:HIS:HA	3:A:123:ARG:NH2	2.29	0.48
3:A:120:GLU:O	3:A:123:ARG:HB2	2.13	0.48
3:A:673:GLY:O	3:A:676:MET:HG3	2.13	0.48
4:B:104:GLU:OE1	4:B:104:GLU:N	2.43	0.48
4:B:980:PHE:CE1	4:B:1094:ARG:HG3	2.46	0.48
4:B:987:LYS:HZ3	15:R:12:A:P	2.36	0.48
11:I:61:ASP:O	11:I:64:SER:OG	2.23	0.48
3:A:108:MET:C	3:A:110:CYS:H	2.21	0.48
3:A:399:HIS:O	3:A:401:GLY:N	2.45	0.48
3:A:1208:THR:H	3:A:1211:GLN:NE2	2.11	0.48
4:B:428:ILE:HA	4:B:445:LYS:HE3	1.96	0.48
4:B:530:GLY:C	4:B:532:ALA:H	2.22	0.48
5:C:167:HIS:ND1	5:C:169:LYS:HG3	2.28	0.48
9:G:49:LEU:HG	9:G:76:ALA:HA	1.96	0.48
3:A:118:HIS:HA	3:A:123:ARG:HH22	1.78	0.48
3:A:811:GLN:H	3:A:811:GLN:CD	2.19	0.48
3:A:1443:VAL:HG12	9:G:61:ILE:HD13	1.94	0.48
4:B:1072:MET:HE3	4:B:1073:TYR:H	1.79	0.48
6:D:67:ARG:NE	6:D:129:LEU:HD22	2.29	0.48
10:H:118:PHE:N	10:H:121:LEU:O	2.39	0.48
3:A:65:LEU:O	3:A:71:GLN:HA	2.13	0.48
3:A:346:ASP:OD2	4:B:1108:ARG:N	2.34	0.48
4:B:400:HIS:CE1	4:B:402:GLY:H	2.31	0.48
4:B:444:MET:SD	4:B:445:LYS:N	2.87	0.48
5:C:33:LEU:HB3	5:C:37:MET:HE1	1.96	0.48
5:C:252:GLN:HB3	13:K:98:LEU:CD1	2.44	0.48
9:G:90:THR:OG1	9:G:141:SER:OG	2.25	0.48
1:N:-6:DT:H2''	1:N:-5:DA:C8	2.48	0.48
3:A:839:ARG:NH2	3:A:1403:GLU:OE2	2.35	0.48
3:A:878:ILE:HA	3:A:956:LEU:O	2.13	0.48
3:A:1254:ALA:N	3:A:1256:GLU:OE2	2.47	0.48
4:B:706:GLN:OE1	4:B:707:PRO:HD2	2.14	0.48
17:M:239:GLN:O	17:M:243:ILE:HG12	2.13	0.48
1:N:22:DA:H2''	1:N:23:DA:OP2	2.14	0.47
3:A:871:ASP:CG	3:A:873:MET:H	2.22	0.47
3:A:1191:TRP:CZ3	11:I:43:VAL:HG21	2.49	0.47
3:A:1444:MET:HG3	9:G:58:ARG:HD2	1.96	0.47
4:B:918:ILE:HA	4:B:919:SER:C	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:61:GLU:H	5:C:61:GLU:CD	2.22	0.47
5:C:148:ARG:N	5:C:151:GLN:OE1	2.23	0.47
9:G:125:SER:HB3	9:G:128:PRO:HA	1.95	0.47
13:K:35:PHE:HD2	13:K:71:PHE:CZ	2.32	0.47
15:R:13:U:H5''	15:R:14:C:C5'	2.43	0.47
3:A:567:LYS:HE2	10:H:95:TYR:HA	1.96	0.47
4:B:124:TYR:O	4:B:172:ILE:HG22	2.14	0.47
6:D:53:SER:OG	6:D:152:SER:HB3	2.13	0.47
3:A:115:LEU:HA	3:A:164:ARG:HH12	1.78	0.47
7:E:108:GLY:N	7:E:131:THR:O	2.35	0.47
15:R:17:A:O5'	15:R:17:A:H8	1.97	0.47
3:A:121:LEU:HD12	3:A:124:GLN:NE2	2.28	0.47
3:A:528:LEU:HD22	3:A:751:SER:HB3	1.95	0.47
3:A:843:LYS:NZ	3:A:1401:SER:O	2.44	0.47
3:A:1156:PRO:HA	3:A:1190:PRO:HB2	1.96	0.47
3:A:1312:ASN:OD1	3:A:1313:LEU:N	2.47	0.47
4:B:190:TYR:CE2	4:B:196:PRO:HD3	2.43	0.47
4:B:307:ASP:CG	4:B:310:MET:HE1	2.39	0.47
4:B:522:VAL:HG21	4:B:537:LYS:HB2	1.95	0.47
6:D:64:VAL:HG23	6:D:68:ARG:NH2	2.26	0.47
1:N:2:DT:H5''	1:N:2:DT:H6	1.80	0.47
3:A:217:LYS:O	3:A:220:THR:OG1	2.28	0.47
4:B:211:VAL:HG21	4:B:483:LEU:HD13	1.95	0.47
9:G:131:GLN:HB2	9:G:136:VAL:HG22	1.96	0.47
3:A:33:ALA:HA	3:A:57:ARG:HH22	1.79	0.47
3:A:219:PHE:HB3	3:A:224:PHE:HB2	1.96	0.47
3:A:1077:THR:OG1	3:A:1078:GLN:OE1	2.29	0.47
4:B:20:ASP:OD1	4:B:22:SER:N	2.41	0.47
4:B:277:LYS:HE3	4:B:278:GLN:NE2	2.29	0.47
4:B:604:ARG:NH2	4:B:615:MET:SD	2.87	0.47
4:B:848:ARG:NH1	12:J:8:PHE:O	2.38	0.47
4:B:1106:ARG:HH22	4:B:1111:MET:HE2	1.79	0.47
7:E:185:ALA:O	7:E:189:GLY:N	2.47	0.47
11:I:69:PRO:HB2	11:I:85:PHE:CE1	2.50	0.47
16:Q:407:ASP:HB3	16:Q:411:LYS:NZ	2.30	0.47
2:O:-31:DT:H2''	2:O:-30:DT:C6	2.49	0.47
3:A:451:HIS:CD2	3:A:453:MET:HE2	2.49	0.47
3:A:1102:LYS:O	3:A:1106:ASN:CB	2.63	0.47
6:D:126:ILE:HD13	6:D:145:MET:HG3	1.96	0.47
7:E:32:GLN:O	7:E:35:VAL:HG22	2.15	0.47
8:F:97:ARG:HD2	8:F:100:GLN:NE2	2.25	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:6:ASP:HA	9:G:75:ARG:HA	1.96	0.47
1:N:-9:DC:H2"	1:N:-8:DA:C8	2.49	0.47
3:A:923:LEU:O	3:A:927:VAL:HG23	2.15	0.47
5:C:134:ILE:HG13	5:C:134:ILE:O	2.15	0.47
6:D:139:LYS:HD2	6:D:142:LYS:HD2	1.96	0.47
3:A:679:ILE:HD11	3:A:732:LEU:HB3	1.96	0.47
3:A:1417:GLU:OE1	3:A:1417:GLU:N	2.46	0.47
10:H:17:PRO:HA	10:H:24:CYS:SG	2.54	0.47
3:A:18:GLN:O	4:B:1215:ARG:N	2.48	0.46
3:A:590:ARG:HH22	3:A:620:LYS:C	2.22	0.46
3:A:807:GLY:O	4:B:728:ARG:NH1	2.49	0.46
3:A:1102:LYS:O	3:A:1106:ASN:HB3	2.13	0.46
4:B:183:GLU:N	4:B:183:GLU:OE1	2.48	0.46
6:D:56:ARG:HH12	6:D:155:ARG:HE	1.62	0.46
6:D:192:LYS:HZ2	6:D:204:ASP:HB2	1.79	0.46
8:F:108:PHE:HE1	8:F:131:PRO:HG3	1.79	0.46
10:H:41:ASP:OD2	10:H:122:LEU:N	2.44	0.46
10:H:102:TYR:CZ	10:H:115:TYR:HB3	2.50	0.46
17:M:73:LEU:HD23	17:M:78:ALA:HA	1.97	0.46
3:A:1159:ARG:HH11	3:A:1185:PHE:HB3	1.81	0.46
4:B:593:PRO:HG2	4:B:617:ARG:NH2	2.30	0.46
4:B:1100:ASP:OD1	4:B:1101:ASP:N	2.49	0.46
5:C:102:GLN:HE22	5:C:154:LYS:HG2	1.81	0.46
3:A:95:PHE:O	3:A:99:ILE:HG13	2.16	0.46
3:A:360:GLU:OE1	3:A:360:GLU:N	2.40	0.46
3:A:891:ALA:HA	3:A:894:GLU:OE2	2.15	0.46
4:B:449:ASN:O	4:B:452:THR:OG1	2.27	0.46
4:B:526:GLU:HB3	4:B:538:ASN:HD22	1.80	0.46
6:D:14:ARG:HB2	6:D:17:LYS:HE2	1.98	0.46
7:E:112:TYR:CE2	7:E:136:ASN:HB2	2.51	0.46
13:K:49:GLU:OE1	13:K:90:ALA:HB1	2.15	0.46
2:O:-19:DC:H2"	2:O:-18:DA:OP2	2.16	0.46
3:A:33:ALA:HB3	3:A:82:GLY:HA3	1.96	0.46
3:A:445:ASN:CB	3:A:455:MET:HE1	2.44	0.46
3:A:457:ALA:HB3	3:A:506:ALA:HA	1.98	0.46
3:A:722:LEU:HD12	3:A:799:PHE:CE1	2.51	0.46
4:B:304:ASP:OD2	4:B:307:ASP:N	2.45	0.46
4:B:408:LEU:HG	4:B:409:ALA:H	1.80	0.46
4:B:450:ALA:HA	4:B:453:ILE:HG22	1.96	0.46
4:B:597:MET:HE2	4:B:597:MET:HA	1.96	0.46
9:G:111:THR:HB	9:G:114:LEU:HD13	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:165:GLU:O	9:G:168:LEU:HB3	2.15	0.46
10:H:116:TYR:HB2	10:H:123:MET:SD	2.55	0.46
3:A:368:LYS:NZ	13:K:4:PRO:HD3	2.25	0.46
3:A:474:VAL:O	3:A:477:PRO:HD2	2.14	0.46
3:A:1042:PHE:O	3:A:1045:VAL:HG12	2.14	0.46
4:B:104:GLU:HG3	14:L:54:ARG:HH12	1.80	0.46
4:B:431:TYR:HD2	4:B:445:LYS:HD2	1.79	0.46
5:C:181:ASP:OD2	5:C:184:ASN:N	2.49	0.46
10:H:124:ARG:NE	10:H:126:GLU:OE1	2.48	0.46
1:N:15:DT:H2''	1:N:16:DA:C8	2.51	0.46
2:O:-15:DA:H5''	3:A:1386:ARG:HD3	1.96	0.46
3:A:252:PHE:C	3:A:254:GLU:H	2.21	0.46
3:A:928:LEU:O	3:A:931:GLU:HG3	2.16	0.46
3:A:1293:SER:N	3:A:1297:GLU:O	2.31	0.46
4:B:424:LEU:CD1	4:B:449:ASN:HB3	2.45	0.46
4:B:526:GLU:CB	4:B:538:ASN:HD22	2.28	0.46
4:B:874:PHE:HD1	4:B:962:LYS:HD3	1.81	0.46
5:C:186:LEU:HB3	5:C:188:HIS:CD2	2.51	0.46
12:J:55:ASP:O	12:J:56:LEU:HD23	2.16	0.46
3:A:62:ASP:OD1	3:A:62:ASP:N	2.49	0.46
3:A:153:PRO:HB2	3:A:156:ASP:CG	2.41	0.46
3:A:187:LYS:O	3:A:188:ASP:C	2.59	0.46
4:B:246:LYS:NZ	4:B:415:GLN:OE1	2.31	0.46
15:R:16:C:H3'	15:R:16:C:H6	1.80	0.46
17:M:63:ARG:HH22	17:M:66:ARG:NH1	2.13	0.46
3:A:1239:ARG:HH22	3:A:1241:ARG:HH21	1.63	0.46
4:B:1222:ARG:O	4:B:1222:ARG:NE	2.48	0.46
6:D:25:ALA:HA	6:D:175:PHE:HE2	1.80	0.46
17:M:81:TRP:N	17:M:81:TRP:CD1	2.84	0.46
3:A:439:ASN:N	3:A:460:VAL:O	2.33	0.46
3:A:560:ILE:HD11	10:H:79:TRP:O	2.16	0.46
3:A:563:PRO:HA	3:A:572:TRP:NE1	2.31	0.46
4:B:803:LEU:HG	4:B:822:ASN:HD22	1.81	0.46
5:C:71:PRO:HB2	5:C:133:ILE:HD13	1.97	0.46
5:C:91:HIS:HB2	5:C:96:SER:HB2	1.98	0.46
10:H:83:GLN:OE1	13:K:54:ARG:NH2	2.48	0.46
2:O:2:DC:H2''	2:O:3:DA:H8	1.79	0.46
3:A:41:MET:HE3	3:A:47:ARG:HA	1.98	0.46
3:A:81:PHE:CE2	4:B:1208:MET:HE3	2.50	0.46
3:A:346:ASP:OD1	4:B:1107:ALA:HA	2.15	0.46
3:A:443:LEU:HD12	3:A:444:PHE:H	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:35:ARG:HE	13:K:41:THR:HB	1.81	0.46
3:A:50:ILE:HG23	3:A:52:GLY:H	1.81	0.45
3:A:999:VAL:H	3:A:1011:GLN:CD	2.25	0.45
4:B:1043:ASP:OD2	4:B:1045:SER:OG	2.30	0.45
4:B:1187:ASN:ND2	4:B:1190:ASP:HB3	2.31	0.45
5:C:146:LYS:C	5:C:147:LEU:HD12	2.40	0.45
6:D:56:ARG:HD3	6:D:149:THR:HA	1.97	0.45
11:I:113:ASP:OD1	11:I:115:LYS:NZ	2.40	0.45
3:A:372:LYS:HD2	13:K:2:ASN:HB3	1.99	0.45
3:A:530:GLY:CA	3:A:657:LEU:HD21	2.45	0.45
3:A:563:PRO:HD2	10:H:79:TRP:CD1	2.51	0.45
3:A:1121:GLU:CD	3:A:1122:PRO:HD2	2.42	0.45
4:B:345:LYS:N	4:B:348:ARG:HH21	2.14	0.45
4:B:839:MET:HG2	4:B:1010:LEU:HD12	1.97	0.45
4:B:901:PRO:HA	4:B:949:VAL:HG12	1.97	0.45
5:C:56:THR:HG23	5:C:58:LEU:H	1.80	0.45
9:G:21:ARG:NH1	9:G:24:GLN:HB2	2.31	0.45
16:Q:109:GLU:CD	16:Q:109:GLU:H	2.24	0.45
3:A:85:ASP:O	3:A:273:ASN:ND2	2.47	0.45
3:A:98:LYS:O	3:A:102:VAL:HG23	2.16	0.45
4:B:1065:GLN:HE22	4:B:1067:ARG:HB2	1.82	0.45
5:C:11:ARG:HD3	5:C:19:ASP:HB3	1.98	0.45
5:C:104:PHE:HA	5:C:152:GLU:OE1	2.16	0.45
3:A:1282:VAL:HG12	3:A:1308:THR:HA	1.98	0.45
4:B:778:MET:HE1	4:B:1094:ARG:HH11	1.81	0.45
9:G:62:LEU:HD12	9:G:63:PRO:HD2	1.97	0.45
3:A:570:PRO:C	3:A:571:LEU:HD12	2.42	0.45
3:A:727:ASP:OD1	3:A:728:LYS:N	2.50	0.45
3:A:737:LEU:HD11	3:A:741:ASN:ND2	2.31	0.45
3:A:826:ASP:HA	4:B:508:LEU:HD11	1.99	0.45
3:A:1116:LEU:H	3:A:1308:THR:HG22	1.82	0.45
3:A:1198:ASP:HB3	3:A:1201:ALA:HB3	1.99	0.45
3:A:1209:MET:HE1	3:A:1228:TRP:HB2	1.98	0.45
4:B:976:ILE:O	4:B:990:ILE:HB	2.17	0.45
3:A:1143:LEU:O	3:A:1147:THR:N	2.50	0.45
3:A:1390:ASN:ND2	3:A:1402:PHE:HB3	2.32	0.45
3:A:1399:ARG:NH1	3:A:1408:ILE:HD11	2.32	0.45
4:B:216:GLU:CG	4:B:500:THR:HB	2.46	0.45
4:B:278:GLN:OE1	4:B:335:GLY:HA2	2.17	0.45
4:B:281:PRO:HD2	4:B:284:ILE:HD12	1.99	0.45
4:B:637:LEU:HD12	4:B:693:ILE:HG13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1073:TYR:CE1	4:B:1080:LYS:HD2	2.52	0.45
6:D:152:SER:O	6:D:221:TYR:OH	2.31	0.45
7:E:55:ARG:HB2	7:E:84:ASP:OD1	2.16	0.45
9:G:56:ILE:HG22	9:G:72:VAL:HG22	1.98	0.45
11:I:21:GLU:HG2	11:I:22:ASN:N	2.32	0.45
11:I:28:GLU:HB3	11:I:35:VAL:HG23	1.97	0.45
16:Q:118:LEU:HB3	16:Q:392:VAL:HG22	1.99	0.45
3:A:1330:ASN:OD1	3:A:1331:SER:N	2.50	0.45
4:B:259:TYR:O	4:B:267:ARG:NH2	2.50	0.45
4:B:438:GLU:HA	4:B:439:ALA:HA	1.68	0.45
9:G:110:VAL:HG11	9:G:163:ILE:HG12	1.98	0.45
10:H:18:GLY:O	10:H:19:ARG:HG2	2.17	0.45
3:A:1112:LYS:HD2	3:A:1112:LYS:HA	1.85	0.45
4:B:810:GLU:HG3	16:Q:24:ARG:HH22	1.82	0.45
7:E:72:PHE:HB2	7:E:75:MET:HE1	1.99	0.45
10:H:108:SER:C	10:H:110:ASP:H	2.25	0.45
3:A:821:ARG:HH21	4:B:534:GLY:HA2	1.81	0.45
4:B:363:HIS:HD2	4:B:364:ILE:HG23	1.80	0.45
4:B:441:ASP:CG	4:B:444:MET:H	2.24	0.45
5:C:11:ARG:NH2	5:C:209:TYR:OH	2.40	0.45
13:K:60:ALA:O	13:K:73:LEU:HD12	2.16	0.45
17:M:200:ARG:HD2	17:M:201:TYR:N	2.32	0.45
1:N:16:DA:H2'	1:N:17:DG:C8	2.52	0.45
3:A:1361:SER:HA	3:A:1362:TYR:HA	1.63	0.45
4:B:1106:ARG:HH22	4:B:1111:MET:CE	2.30	0.45
7:E:92:THR:O	7:E:95:THR:OG1	2.29	0.45
9:G:21:ARG:NH2	9:G:25:TYR:HB2	2.26	0.45
12:J:16:ASP:OD1	12:J:17:LYS:N	2.50	0.45
14:L:31:CYS:HA	14:L:56:LEU:HD23	1.99	0.45
1:N:24:DA:H2''	1:N:25:DA:C8	2.52	0.44
3:A:770:VAL:HG12	3:A:771:GLU:CD	2.43	0.44
3:A:1329:THR:HG22	3:A:1331:SER:H	1.82	0.44
6:D:54:GLU:HA	6:D:57:LEU:HD12	2.00	0.44
14:L:30:ILE:HA	14:L:36:SER:O	2.16	0.44
16:Q:100:GLU:OE1	17:M:94:LYS:HB3	2.17	0.44
3:A:791:ASP:OD1	3:A:792:TYR:N	2.51	0.44
3:A:868:TYR:CD1	3:A:1058:VAL:HG21	2.45	0.44
4:B:89:GLU:HG3	4:B:159:ASP:OD1	2.17	0.44
4:B:139:ALA:N	4:B:150:GLU:O	2.50	0.44
4:B:995:ARG:HB2	4:B:997:GLU:OE2	2.18	0.44
4:B:1106:ARG:HD2	4:B:1126:GLY:C	2.43	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:180:ARG:HH21	7:E:192:ARG:HB2	1.81	0.44
10:H:7:ASP:OD1	10:H:8:ASP:N	2.51	0.44
10:H:12:VAL:HG21	10:H:26:ILE:HD11	1.99	0.44
12:J:19:GLU:OE1	12:J:19:GLU:N	2.40	0.44
17:M:98:ASN:OD1	17:M:103:LYS:HB3	2.16	0.44
3:A:455:MET:HG3	4:B:1137:CYS:SG	2.58	0.44
4:B:843:GLN:NE2	4:B:847:ASP:OD1	2.50	0.44
5:C:6:PRO:HA	5:C:24:ASN:HB2	1.98	0.44
5:C:142:VAL:HG21	12:J:5:VAL:HG22	1.99	0.44
5:C:148:ARG:HG2	12:J:61:LEU:HG	1.98	0.44
9:G:3:PHE:HE2	9:G:82:PHE:HE2	1.64	0.44
9:G:14:HIS:CG	9:G:15:PRO:HD2	2.52	0.44
12:J:18:TRP:CZ2	12:J:22:LEU:HD21	2.52	0.44
3:A:33:ALA:C	3:A:34:LYS:HD3	2.42	0.44
3:A:678:GLU:HA	3:A:681:GLU:HG3	1.99	0.44
3:A:764:CYS:SG	3:A:765:VAL:N	2.90	0.44
4:B:68:THR:HG21	16:Q:334:VAL:HB	2.00	0.44
4:B:1010:LEU:HD11	4:B:1092:TYR:CE2	2.49	0.44
4:B:1032:SER:OG	4:B:1089:PRO:HG2	2.17	0.44
5:C:40:GLU:N	5:C:40:GLU:OE1	2.51	0.44
5:C:62:PHE:O	5:C:66:ARG:HG3	2.17	0.44
6:D:72:ARG:HB3	6:D:76:LYS:NZ	2.32	0.44
10:H:109:LYS:O	10:H:109:LYS:HD3	2.17	0.44
3:A:368:LYS:NZ	13:K:2:ASN:O	2.49	0.44
3:A:928:LEU:HD13	3:A:987:VAL:HG11	2.00	0.44
4:B:1163:CYS:HB3	4:B:1166:CYS:HB2	1.89	0.44
7:E:121:MET:HA	7:E:124:VAL:HG23	1.99	0.44
7:E:169:ARG:NH2	8:F:140:ASP:OD2	2.50	0.44
10:H:135:LEU:HD22	10:H:137:GLN:HB2	1.99	0.44
16:Q:23:LYS:HA	16:Q:23:LYS:HD3	1.87	0.44
3:A:545:GLN:O	3:A:549:MET:HG2	2.17	0.44
3:A:965:GLN:HA	3:A:968:GLN:OE1	2.17	0.44
3:A:1063:MET:SD	3:A:1436:ILE:HD12	2.58	0.44
3:A:1259:MET:SD	3:A:1260:LEU:N	2.91	0.44
4:B:174:LEU:HA	4:B:174:LEU:HD23	1.73	0.44
4:B:237:VAL:HG12	4:B:257:LYS:HG2	2.00	0.44
4:B:343:ILE:HD12	4:B:343:ILE:H	1.83	0.44
4:B:953:LEU:HD21	4:B:965:LYS:HB2	1.99	0.44
6:D:209:ARG:HA	6:D:212:LYS:NZ	2.33	0.44
7:E:22:MET:HE2	7:E:187:TYR:CD1	2.53	0.44
9:G:116:PRO:HA	9:G:164:LYS:NZ	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:4:DA:H5'	1:N:5:DA:H5'	1.99	0.44
2:O:-28:DG:H2'	2:O:-27:DT:H71	2.00	0.44
3:A:890:ASP:O	3:A:893:PHE:HB3	2.18	0.44
4:B:43:LEU:O	4:B:496:ARG:NH2	2.51	0.44
4:B:344:LYS:HA	4:B:348:ARG:HE	1.82	0.44
4:B:803:LEU:HG	4:B:822:ASN:ND2	2.33	0.44
4:B:929:THR:HG23	4:B:931:TYR:HB2	1.99	0.44
5:C:162:GLY:HA3	5:C:170:TRP:CD2	2.53	0.44
7:E:13:TRP:CE3	7:E:39:LEU:HD12	2.52	0.44
7:E:48:ASP:OD1	7:E:52:ARG:HB2	2.18	0.44
7:E:153:HIS:CD2	7:E:184:VAL:HG21	2.52	0.44
7:E:154:ILE:CG2	7:E:197:LYS:HB3	2.48	0.44
14:L:51:CYS:HB3	14:L:53:HIS:ND1	2.33	0.44
16:Q:120:LYS:HB3	16:Q:394:LYS:HA	1.99	0.44
3:A:311:GLN:HG2	3:A:312:PRO:CD	2.46	0.44
3:A:946:VAL:HG23	3:A:947:PHE:N	2.32	0.44
4:B:57:TYR:C	4:B:59:LEU:H	2.24	0.44
4:B:102:VAL:HB	4:B:112:LEU:HD21	2.00	0.44
4:B:223:VAL:HG22	4:B:240:ILE:HD11	2.00	0.44
4:B:350:GLN:HA	4:B:353:LYS:HG2	1.99	0.44
4:B:689:LEU:HD23	4:B:689:LEU:HA	1.87	0.44
4:B:996:ARG:HG3	4:B:1007:VAL:HG11	2.00	0.44
7:E:23:VAL:HG13	7:E:78:LEU:HD21	1.99	0.44
7:E:47:CYS:C	7:E:54:GLN:HE22	2.26	0.44
9:G:7:LEU:HD22	9:G:74:TYR:OH	2.18	0.44
9:G:165:GLU:HB3	9:G:168:LEU:HD23	2.00	0.44
16:Q:119:LEU:HD21	16:Q:121:PHE:CE1	2.52	0.44
3:A:42:ASP:HB3	3:A:45:GLN:C	2.43	0.44
3:A:67:CYS:C	3:A:68:GLN:HG3	2.43	0.44
3:A:337:ARG:HE	3:A:839:ARG:HH22	1.66	0.44
3:A:353:ILE:HG22	3:A:468:PHE:HB2	1.99	0.44
3:A:1207:LEU:CD1	3:A:1211:GLN:HE21	2.31	0.44
3:A:1326:ARG:HA	7:E:148:GLU:OE2	2.18	0.44
4:B:328:GLU:HA	4:B:331:LEU:HD12	2.00	0.44
4:B:882:THR:HB	4:B:885:MET:HB3	2.00	0.44
5:C:148:ARG:HG3	5:C:148:ARG:O	2.17	0.44
6:D:52:LEU:HG	6:D:148:LEU:HA	1.98	0.44
17:M:86:ASN:CG	17:M:87:LEU:H	2.25	0.44
17:M:105:THR:HA	17:M:121:ASP:HA	1.99	0.44
2:O:-3:DA:C2	3:A:252:PHE:CD2	3.06	0.43
3:A:314:ALA:O	3:A:322:VAL:HG12	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:543:LEU:HD22	3:A:572:TRP:HZ3	1.83	0.43
3:A:1444:MET:HE3	8:F:135:ARG:NE	2.33	0.43
4:B:67:SER:HG	4:B:92:PHE:H	1.64	0.43
4:B:431:TYR:HA	4:B:434:ARG:HB3	2.00	0.43
4:B:573:GLN:N	4:B:573:GLN:OE1	2.51	0.43
6:D:63:LEU:O	6:D:66:ARG:HG3	2.17	0.43
6:D:123:LEU:HA	6:D:145:MET:HE1	1.99	0.43
17:M:225:MET:SD	17:M:226:PRO:HD2	2.58	0.43
3:A:513:SER:HB3	3:A:520:CYS:HB3	1.99	0.43
3:A:1293:SER:HB3	3:A:1297:GLU:H	1.83	0.43
4:B:128:LEU:HD11	4:B:170:LEU:HG	2.00	0.43
5:C:187:LYS:HB2	5:C:219:PHE:HE1	1.82	0.43
7:E:88:VAL:HG11	7:E:116:ILE:HG23	1.99	0.43
10:H:96:VAL:HG12	10:H:143:LEU:HD22	2.00	0.43
16:Q:128:ASN:HB3	16:Q:131:THR:OG1	2.18	0.43
16:Q:326:ARG:HD3	16:Q:326:ARG:HA	1.80	0.43
2:O:-2:DA:H2''	2:O:-1:DG:N7	2.33	0.43
3:A:449:SER:O	4:B:1133:MET:HE2	2.18	0.43
3:A:956:LEU:HD23	3:A:956:LEU:HA	1.87	0.43
4:B:51:PHE:CG	4:B:173:MET:HB2	2.53	0.43
5:C:235:VAL:HG13	5:C:237:SER:H	1.82	0.43
7:E:126:SER:OG	7:E:127:ILE:N	2.51	0.43
9:G:142:ARG:HG3	9:G:171:ILE:HD13	2.00	0.43
12:J:24:LEU:O	12:J:28:ASP:HB2	2.18	0.43
14:L:63:ARG:NH1	14:L:64:LEU:H	2.17	0.43
1:N:25:DA:H2''	1:N:26:DA:H8	1.83	0.43
3:A:332:LYS:HD2	3:A:332:LYS:HA	1.79	0.43
3:A:368:LYS:HZ3	13:K:3:ALA:HA	1.83	0.43
3:A:399:HIS:HB3	3:A:400:PRO:HD3	1.99	0.43
3:A:557:ASP:C	13:K:26:LYS:HE3	2.43	0.43
3:A:1042:PHE:O	3:A:1046:LEU:HG	2.18	0.43
5:C:239:PRO:O	5:C:242:GLN:HB2	2.18	0.43
17:M:233:TYR:C	17:M:235:LYS:H	2.26	0.43
3:A:115:LEU:N	3:A:164:ARG:HH22	2.15	0.43
3:A:230:ARG:HB3	3:A:232:GLU:OE1	2.19	0.43
3:A:476:SER:OG	3:A:477:PRO:HD3	2.19	0.43
3:A:957:PRO:HG2	3:A:1018:PHE:HD1	1.82	0.43
4:B:198:ASP:OD2	4:B:202:TYR:OH	2.28	0.43
4:B:412:LEU:HB3	4:B:466:TRP:HZ2	1.83	0.43
4:B:651:LEU:HD23	4:B:651:LEU:H	1.84	0.43
4:B:862:GLN:HB3	4:B:963:PHE:HD1	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:912:ILE:HG13	4:B:939:THR:HB	1.99	0.43
5:C:16:ASP:OD1	5:C:16:ASP:N	2.46	0.43
3:A:116:ASP:HB3	3:A:164:ARG:CZ	2.49	0.43
3:A:778:GLY:HA3	4:B:516:ASN:HB2	2.00	0.43
4:B:203:PHE:N	4:B:210:LYS:O	2.50	0.43
13:K:39:ASP:OD1	13:K:41:THR:HG22	2.19	0.43
3:A:12:ARG:HH21	4:B:1218:THR:CG2	2.31	0.43
3:A:390:GLN:NE2	3:A:390:GLN:O	2.51	0.43
3:A:445:ASN:OD1	3:A:446:ARG:N	2.50	0.43
3:A:943:LEU:HA	3:A:946:VAL:HG22	2.00	0.43
3:A:1400:CYS:HB2	3:A:1405:THR:HG23	2.00	0.43
4:B:69:LEU:HD12	4:B:69:LEU:HA	1.84	0.43
4:B:213:ILE:O	4:B:215:GLN:NE2	2.52	0.43
4:B:709:ASP:OD1	4:B:710:LEU:N	2.48	0.43
6:D:123:LEU:HA	6:D:145:MET:CE	2.48	0.43
3:A:453:MET:C	3:A:455:MET:H	2.27	0.43
3:A:666:ILE:CG1	4:B:1026:LEU:HB3	2.48	0.43
3:A:807:GLY:HA3	4:B:728:ARG:HH22	1.84	0.43
3:A:1063:MET:HG3	4:B:1139:ILE:HG22	2.01	0.43
4:B:424:LEU:O	4:B:428:ILE:HG13	2.19	0.43
4:B:595:ARG:O	4:B:598:GLU:HG3	2.18	0.43
4:B:836:GLU:OE1	4:B:836:GLU:N	2.52	0.43
4:B:862:GLN:HB3	4:B:963:PHE:CD1	2.53	0.43
5:C:45:ALA:HA	5:C:72:LEU:HD13	2.00	0.43
6:D:55:ALA:O	6:D:59:ILE:HG23	2.18	0.43
8:F:79:ARG:NH1	8:F:150:GLU:OE1	2.38	0.43
3:A:81:PHE:CZ	4:B:1208:MET:HE3	2.54	0.43
3:A:844:ALA:HB3	3:A:845:LEU:HD12	2.01	0.43
4:B:658:ILE:O	4:B:662:MET:HG2	2.19	0.43
4:B:979:LYS:O	4:B:1095:LEU:HB2	2.19	0.43
5:C:249:ASP:O	5:C:252:GLN:HG3	2.19	0.43
9:G:91:VAL:HG11	9:G:137:ILE:HG12	2.01	0.43
12:J:17:LYS:HB3	12:J:39:LEU:HD21	2.01	0.43
13:K:8:GLU:HG2	13:K:37:LYS:NZ	2.33	0.43
13:K:81:TYR:CE2	13:K:86:ALA:HB2	2.54	0.43
3:A:146:MET:HB3	3:A:171:GLN:O	2.18	0.43
3:A:842:VAL:O	3:A:846:GLU:HG3	2.19	0.43
3:A:889:SER:HA	3:A:1297:GLU:HG3	2.00	0.43
3:A:1104:ILE:HD12	3:A:1352:VAL:HG22	2.01	0.43
3:A:1171:GLN:O	3:A:1175:SER:OG	2.36	0.43
5:C:32:SER:O	5:C:36:VAL:HG13	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:147:HIS:CE1	7:E:149:LEU:HB2	2.54	0.43
16:Q:140:HIS:HB2	16:Q:142:LYS:HZ2	1.84	0.43
3:A:302:THR:HA	3:A:305:ASP:O	2.19	0.42
3:A:857:ARG:HB3	3:A:861:GLY:HA2	1.99	0.42
3:A:1207:LEU:HD21	3:A:1274:ARG:HH21	1.83	0.42
6:D:177:VAL:HA	6:D:180:LEU:HB2	2.01	0.42
3:A:354:SER:OG	3:A:469:ARG:NE	2.52	0.42
3:A:538:ASP:OD1	10:H:22:LYS:HB2	2.18	0.42
3:A:1173:HIS:CD2	3:A:1227:ILE:HG23	2.54	0.42
4:B:499:ASN:OD1	4:B:500:THR:N	2.51	0.42
4:B:923:GLU:HG3	4:B:924:GLU:OE1	2.19	0.42
4:B:1152:MET:HE3	4:B:1152:MET:HA	2.01	0.42
5:C:101:LEU:HB3	5:C:155:LEU:HB2	2.00	0.42
6:D:63:LEU:HD13	6:D:126:ILE:HG22	2.00	0.42
10:H:18:GLY:C	10:H:19:ARG:HG2	2.44	0.42
10:H:42:ILE:HD12	10:H:42:ILE:HA	1.87	0.42
12:J:23:ASN:HB2	12:J:27:GLU:OE2	2.19	0.42
15:R:16:C:C6	15:R:16:C:O5'	2.72	0.42
17:M:108:LEU:HB3	17:M:118:HIS:HA	2.00	0.42
3:A:849:MET:HG3	3:A:1063:MET:HE1	2.00	0.42
3:A:902:LEU:H	3:A:902:LEU:HD23	1.84	0.42
3:A:1225:PHE:CE2	3:A:1227:ILE:HD11	2.55	0.42
4:B:282:ILE:HD12	4:B:382:ILE:HD13	2.01	0.42
4:B:828:ALA:O	4:B:834:ASN:ND2	2.53	0.42
4:B:919:SER:HA	4:B:920:PRO:HA	1.74	0.42
4:B:954:VAL:O	14:L:56:LEU:HB2	2.19	0.42
16:Q:105:ALA:O	17:M:89:GLY:HA2	2.17	0.42
16:Q:428:LEU:O	16:Q:432:GLY:N	2.52	0.42
3:A:343:LYS:HE3	4:B:1117:GLN:HE21	1.84	0.42
3:A:446:ARG:CD	3:A:480:ALA:HB2	2.49	0.42
3:A:589:GLN:HG3	3:A:606:LEU:HD13	2.01	0.42
3:A:1004:ASN:HD21	3:A:1007:ILE:HG12	1.84	0.42
3:A:1263:ILE:O	3:A:1267:MET:HG2	2.18	0.42
4:B:21:GLU:N	4:B:21:GLU:OE1	2.52	0.42
4:B:839:MET:HE1	4:B:988:GLY:C	2.45	0.42
5:C:11:ARG:HG2	5:C:11:ARG:HH11	1.84	0.42
7:E:198:ILE:HB	7:E:210:SER:OG	2.20	0.42
10:H:5:LEU:HB2	10:H:59:ILE:HG21	2.01	0.42
10:H:118:PHE:HB2	10:H:121:LEU:HB2	2.01	0.42
12:J:4:PRO:HD3	12:J:53:HIS:HD2	1.84	0.42
17:M:133:TYR:HB3	17:M:214:ILE:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:5:DT:H2"	2:O:6:DA:C8	2.54	0.42
3:A:207:ILE:HD12	3:A:207:ILE:H	1.85	0.42
3:A:274:ILE:O	3:A:277:GLU:HG3	2.19	0.42
3:A:543:LEU:HD21	3:A:570:PRO:HB2	2.00	0.42
3:A:672:ASP:OD2	3:A:674:PRO:HG2	2.20	0.42
3:A:756:ILE:HD12	3:A:756:ILE:H	1.85	0.42
3:A:914:GLU:OE1	3:A:978:PRO:HB2	2.20	0.42
4:B:51:PHE:CD1	4:B:173:MET:HB2	2.55	0.42
4:B:297:ILE:H	4:B:297:ILE:HD12	1.84	0.42
4:B:839:MET:N	4:B:989:THR:O	2.52	0.42
4:B:1153:GLU:OE1	4:B:1153:GLU:N	2.53	0.42
7:E:4:GLU:HA	7:E:7:ARG:HG2	2.00	0.42
7:E:112:TYR:CD1	7:E:116:ILE:HD11	2.54	0.42
1:N:-3:DT:H2"	1:N:-2:DG:H8	1.84	0.42
2:O:-13:DA:C8	3:A:832:ALA:HA	2.55	0.42
3:A:177:ASP:OD1	3:A:177:ASP:N	2.52	0.42
3:A:1244:ARG:HA	3:A:1245:PRO:HD3	1.92	0.42
6:D:173:HIS:CD2	6:D:175:PHE:HB3	2.54	0.42
7:E:171:LYS:C	7:E:173:SER:H	2.28	0.42
9:G:138:THR:O	9:G:141:SER:HB3	2.20	0.42
11:I:113:ASP:OD2	11:I:115:LYS:HB2	2.19	0.42
14:L:27:LEU:HD11	14:L:62:LYS:NZ	2.35	0.42
3:A:88:LYS:HB3	3:A:293:GLU:OE2	2.19	0.42
3:A:90:VAL:HG21	3:A:300:VAL:HG11	2.01	0.42
3:A:92:HIS:NE2	3:A:304:MET:HE2	2.35	0.42
3:A:344:ARG:CZ	4:B:1129:ARG:HB2	2.50	0.42
3:A:415:LEU:HA	3:A:418:SER:HB2	2.00	0.42
4:B:954:VAL:HG23	4:B:964:VAL:HG22	2.02	0.42
5:C:183:TRP:CE3	5:C:213:PRO:HD3	2.55	0.42
9:G:115:MET:HG2	9:G:163:ILE:HD11	2.01	0.42
10:H:130:ARG:H	10:H:130:ARG:CD	2.32	0.42
3:A:32:VAL:N	3:A:81:PHE:O	2.51	0.42
3:A:50:ILE:HG13	3:A:51:GLY:H	1.85	0.42
3:A:439:ASN:HA	3:A:460:VAL:H	1.85	0.42
3:A:635:ARG:HA	3:A:635:ARG:HD3	1.89	0.42
3:A:843:LYS:HD3	3:A:846:GLU:CD	2.44	0.42
3:A:1044:TRP:CD2	3:A:1048:ASN:ND2	2.88	0.42
4:B:75:ALA:C	4:B:77:HIS:H	2.25	0.42
4:B:144:GLY:HA2	4:B:145:ARG:HA	1.79	0.42
4:B:760:ASP:OD1	4:B:761:HIS:N	2.53	0.42
4:B:772:ALA:HA	4:B:775:LYS:HZ1	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:48:ASP:CG	7:E:52:ARG:HB2	2.44	0.42
8:F:70:LYS:C	8:F:72:LYS:H	2.28	0.42
11:I:28:GLU:HA	11:I:35:VAL:HA	2.02	0.42
15:R:16:C:C6	15:R:16:C:C3'	3.03	0.42
2:O:-3:DA:H2	3:A:252:PHE:CD2	2.37	0.42
3:A:151:ASP:OD1	3:A:163:SER:HA	2.20	0.42
3:A:362:ASP:O	3:A:459:ARG:N	2.46	0.42
4:B:603:LEU:HB3	4:B:609:ILE:CD1	2.49	0.42
5:C:229:TYR:O	5:C:230:MET:HE2	2.19	0.42
5:C:257:SER:O	5:C:260:LEU:HG	2.19	0.42
6:D:14:ARG:HE	6:D:17:LYS:NZ	2.18	0.42
7:E:106:GLN:OE1	7:E:106:GLN:N	2.43	0.42
8:F:94:LEU:HD21	8:F:125:LEU:HD22	2.02	0.42
9:G:24:GLN:O	9:G:28:THR:HG23	2.20	0.42
17:M:86:ASN:HA	17:M:88:HIS:CE1	2.55	0.42
1:N:30:DA:H2''	1:N:31:DA:C8	2.55	0.42
3:A:252:PHE:HE1	15:R:4:C:N1	2.17	0.42
3:A:444:PHE:CZ	3:A:487:MET:HG2	2.55	0.42
3:A:851:HIS:CG	8:F:139:PRO:HG3	2.55	0.42
3:A:858:ASN:OD1	3:A:862:ASN:N	2.49	0.42
3:A:1202:MET:HE3	3:A:1207:LEU:HB3	2.01	0.42
4:B:445:LYS:HE2	4:B:445:LYS:HB2	1.85	0.42
4:B:847:ASP:HB3	5:C:167:HIS:CE1	2.55	0.42
4:B:1036:ALA:O	12:J:47:ARG:HD3	2.19	0.42
5:C:33:LEU:HA	5:C:36:VAL:HG22	2.01	0.42
11:I:19:ASP:CG	11:I:22:ASN:HB2	2.45	0.42
17:M:68:VAL:N	17:M:217:THR:O	2.53	0.42
2:O:-20:DG:H2''	2:O:-19:DC:C6	2.54	0.41
3:A:1195:LEU:O	3:A:1237:ILE:HA	2.20	0.41
3:A:1315:GLU:OE1	3:A:1315:GLU:N	2.53	0.41
3:A:1384:VAL:O	3:A:1384:VAL:HG23	2.20	0.41
4:B:326:ASP:O	4:B:329:THR:OG1	2.35	0.41
4:B:526:GLU:HG2	4:B:771:SER:OG	2.20	0.41
4:B:638:PHE:CD2	4:B:743:ILE:HG22	2.55	0.41
9:G:121:PHE:HB2	9:G:130:TYR:CD2	2.55	0.41
10:H:58:THR:HB	10:H:143:LEU:HB2	2.02	0.41
11:I:65:ASP:OD2	11:I:67:THR:OG1	2.33	0.41
17:M:70:LEU:HD12	17:M:70:LEU:HA	1.92	0.41
3:A:351:THR:HG22	4:B:1103:ILE:HG13	2.01	0.41
3:A:367:PRO:HA	3:A:463:ILE:O	2.19	0.41
3:A:1173:HIS:NE2	3:A:1227:ILE:HG23	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:998:ASP:HB2	4:B:1076:HIS:CD2	2.55	0.41
5:C:39:ALA:O	5:C:164:ALA:HB3	2.20	0.41
5:C:148:ARG:NH1	12:J:63:TYR:O	2.54	0.41
5:C:148:ARG:HD3	12:J:61:LEU:O	2.20	0.41
7:E:26:ARG:NH1	7:E:189:GLY:HA3	2.36	0.41
7:E:60:PHE:O	7:E:80:VAL:HG22	2.20	0.41
7:E:171:LYS:O	7:E:171:LYS:HG3	2.20	0.41
13:K:18:LYS:HA	13:K:18:LYS:HD2	1.89	0.41
3:A:1199:ARG:NH1	3:A:1231:ASP:OD1	2.53	0.41
4:B:190:TYR:CE1	12:J:62:ARG:HG3	2.55	0.41
4:B:487:THR:HG22	4:B:489:SER:N	2.34	0.41
4:B:662:MET:HE3	4:B:662:MET:HB3	1.82	0.41
4:B:737:THR:HG22	11:I:66:PRO:HB3	2.02	0.41
4:B:1115:THR:HG23	4:B:1117:GLN:H	1.85	0.41
6:D:50:LEU:HD12	6:D:50:LEU:HA	1.91	0.41
8:F:72:LYS:HD3	8:F:72:LYS:HA	1.81	0.41
3:A:41:MET:HA	3:A:49:LYS:HA	2.01	0.41
3:A:332:LYS:HA	3:A:337:ARG:NH1	2.36	0.41
3:A:929:LEU:O	3:A:932:GLU:HG3	2.20	0.41
4:B:289:LEU:HD22	4:B:375:ALA:HB2	2.03	0.41
4:B:1134:GLU:HA	4:B:1137:CYS:SG	2.60	0.41
7:E:136:ASN:ND2	7:E:138:ALA:HB3	2.33	0.41
9:G:56:ILE:C	9:G:57:GLN:OE1	2.63	0.41
10:H:26:ILE:HG22	10:H:40:LEU:HB3	2.02	0.41
10:H:54:SER:O	10:H:146:ARG:NH1	2.53	0.41
12:J:3:VAL:HA	12:J:53:HIS:CD2	2.56	0.41
1:N:-3:DT:OP1	4:B:868:MET:N	2.53	0.41
3:A:57:ARG:O	3:A:68:GLN:HB3	2.20	0.41
3:A:1079:MET:HE2	3:A:1098:VAL:HG23	2.03	0.41
3:A:1121:GLU:HG3	3:A:1123:GLY:H	1.85	0.41
3:A:1217:LYS:HE3	3:A:1221:LYS:HD2	2.02	0.41
4:B:274:PRO:HA	4:B:275:TYR:HA	1.67	0.41
4:B:441:ASP:OD1	4:B:444:MET:HG3	2.21	0.41
5:C:54:ASN:OD1	5:C:56:THR:HG22	2.20	0.41
5:C:101:LEU:HD13	5:C:118:LEU:HB3	2.02	0.41
5:C:191:TYR:HB3	5:C:201:TRP:NE1	2.35	0.41
6:D:65:GLU:HA	6:D:68:ARG:CZ	2.51	0.41
7:E:43:LYS:HD2	7:E:43:LYS:HA	1.67	0.41
10:H:101:ALA:HB2	10:H:116:TYR:CE1	2.55	0.41
14:L:31:CYS:SG	14:L:48:CYS:CB	3.08	0.41
3:A:13:THR:OG1	3:A:1432:GLN:HG2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:364:VAL:HG12	3:A:459:ARG:O	2.21	0.41
3:A:370:ILE:O	3:A:374:LEU:N	2.50	0.41
3:A:407:ARG:HG2	3:A:430:TRP:CE2	2.55	0.41
3:A:534:LEU:HD13	3:A:656:TRP:CD2	2.55	0.41
3:A:1063:MET:CE	3:A:1436:ILE:HG23	2.50	0.41
4:B:251:ILE:H	4:B:251:ILE:HD12	1.84	0.41
4:B:919:SER:H	4:B:923:GLU:HA	1.86	0.41
6:D:126:ILE:HG13	6:D:127:ASP:N	2.34	0.41
6:D:152:SER:HB2	6:D:155:ARG:NH2	2.30	0.41
8:F:130:ILE:HB	8:F:148:VAL:HG11	2.01	0.41
17:M:120:TYR:HD2	17:M:226:PRO:HA	1.85	0.41
3:A:451:HIS:HD2	3:A:453:MET:H	1.69	0.41
3:A:926:GLN:HE21	3:A:930:ASP:CG	2.29	0.41
3:A:1147:THR:HA	3:A:1197:LEU:HD23	2.03	0.41
4:B:295:GLY:O	4:B:299:GLU:HG2	2.21	0.41
4:B:364:ILE:CG2	4:B:585:VAL:HG23	2.48	0.41
4:B:445:LYS:NZ	4:B:449:ASN:OD1	2.37	0.41
4:B:513:GLN:H	4:B:513:GLN:HG3	1.70	0.41
6:D:192:LYS:HG2	6:D:199:ASN:HA	2.02	0.41
7:E:156:LEU:HB2	7:E:195:VAL:O	2.21	0.41
8:F:82:THR:HA	8:F:83:PRO:HD3	1.88	0.41
9:G:99:PHE:H	9:G:115:MET:HE1	1.85	0.41
11:I:62:ILE:HD13	11:I:62:ILE:HA	1.96	0.41
17:M:67:GLN:OE1	17:M:67:GLN:N	2.50	0.41
17:M:121:ASP:OD1	17:M:225:MET:HB3	2.21	0.41
3:A:525:GLN:CD	4:B:1013:ASN:HD21	2.28	0.41
3:A:549:MET:SD	3:A:577:ILE:HD13	2.60	0.41
4:B:408:LEU:HA	4:B:408:LEU:HD12	1.87	0.41
4:B:757:PRO:HD3	4:B:983:ARG:NE	2.32	0.41
4:B:992:ILE:HD11	4:B:994:TYR:CE2	2.56	0.41
4:B:1164:GLY:N	4:B:1190:ASP:OD1	2.54	0.41
4:B:1202:LEU:HA	4:B:1205:GLN:OE1	2.20	0.41
10:H:12:VAL:CG1	10:H:53:ASP:H	2.32	0.41
11:I:103:CYS:HB3	11:I:106:CYS:SG	2.61	0.41
13:K:40:HIS:H	13:K:40:HIS:CD2	2.38	0.41
1:N:16:DA:H3'	1:N:17:DG:H8	1.86	0.41
2:O:-17:DC:H2'	2:O:-16:DT:H72	2.03	0.41
3:A:67:CYS:O	3:A:68:GLN:HG3	2.20	0.41
3:A:96:ILE:HD13	3:A:96:ILE:HA	1.93	0.41
3:A:129:LYS:O	3:A:129:LYS:HG3	2.21	0.41
3:A:737:LEU:HD21	3:A:741:ASN:HD22	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1435:PRO:HA	3:A:1439:GLY:O	2.21	0.41
3:A:1438:THR:OG1	8:F:92:ARG:HD3	2.20	0.41
4:B:247:GLY:O	4:B:250:PHE:CD2	2.74	0.41
4:B:590:HIS:HD2	4:B:592:ASN:N	2.19	0.41
4:B:975:GLN:HG2	4:B:976:ILE:H	1.85	0.41
4:B:1027:ILE:H	4:B:1027:ILE:HD12	1.85	0.41
5:C:254:LYS:O	5:C:257:SER:OG	2.32	0.41
11:I:73:ARG:O	11:I:83:ASN:ND2	2.54	0.41
11:I:76:PRO:HD2	11:I:77:LYS:NZ	2.36	0.41
12:J:31:ASP:OD1	12:J:34:THR:OG1	2.34	0.41
13:K:84:LYS:O	13:K:87:LEU:HG	2.20	0.41
16:Q:376:LEU:HA	16:Q:385:THR:O	2.21	0.41
17:M:105:THR:OG1	17:M:120:TYR:O	2.34	0.41
3:A:376:TYR:CD1	3:A:377:PRO:HD2	2.56	0.41
3:A:890:ASP:O	3:A:893:PHE:N	2.54	0.41
3:A:956:LEU:HD22	3:A:957:PRO:HD2	2.02	0.41
3:A:1104:ILE:HG13	3:A:1105:LEU:N	2.36	0.41
4:B:59:LEU:O	4:B:62:ILE:HG22	2.21	0.41
4:B:101:MET:HE3	4:B:109:THR:HG22	2.02	0.41
4:B:431:TYR:CD2	4:B:445:LYS:HD2	2.56	0.41
4:B:821:GLN:NE2	4:B:851:PHE:H	2.19	0.41
4:B:829:CYS:C	4:B:831:SER:H	2.29	0.41
4:B:963:PHE:CZ	4:B:965:LYS:HD3	2.55	0.41
5:C:10:ILE:HB	13:K:108:GLU:CD	2.45	0.41
5:C:259:LEU:HD13	13:K:91:CYS:HB2	2.03	0.41
6:D:195:ILE:HG13	9:G:86:VAL:HG23	2.02	0.41
7:E:29:PHE:N	7:E:65:THR:HG22	2.36	0.41
9:G:91:VAL:HB	9:G:141:SER:HB2	2.03	0.41
16:Q:432:GLY:C	17:M:198:ARG:HH21	2.29	0.41
3:A:150:THR:O	3:A:165:GLY:N	2.45	0.40
3:A:407:ARG:HG2	3:A:430:TRP:CD2	2.56	0.40
3:A:543:LEU:HA	3:A:546:VAL:HG22	2.02	0.40
4:B:497:ARG:HD3	4:B:497:ARG:HA	1.74	0.40
4:B:758:PHE:CE2	4:B:1044:ALA:HA	2.56	0.40
4:B:950:ASP:OD1	4:B:951:GLN:N	2.55	0.40
16:Q:104:ARG:H	16:Q:383:SER:HB3	1.86	0.40
16:Q:408:GLU:HA	16:Q:411:LYS:HE2	2.03	0.40
17:M:71:VAL:HG22	17:M:222:CYS:SG	2.61	0.40
3:A:272:ALA:O	3:A:296:LEU:HD11	2.21	0.40
3:A:407:ARG:HB2	3:A:411:ASP:HB2	2.04	0.40
3:A:1425:SER:O	3:A:1429:ILE:HG12	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:69:LEU:HB3	4:B:90:ILE:HG13	2.04	0.40
4:B:558:LEU:HD21	4:B:580:VAL:HG11	2.04	0.40
7:E:60:PHE:H	7:E:80:VAL:CG2	2.34	0.40
9:G:38:CYS:HA	9:G:44:TYR:HA	2.02	0.40
17:M:112:ASP:OD1	17:M:118:HIS:NE2	2.54	0.40
3:A:122:MET:HA	3:A:125:ALA:HB3	2.04	0.40
3:A:566:ILE:HD12	10:H:97:MET:HA	2.03	0.40
3:A:1229:SER:OG	3:A:1230:GLU:N	2.55	0.40
4:B:344:LYS:HZ2	4:B:348:ARG:H	1.69	0.40
4:B:824:ILE:N	4:B:1009:ASP:OD2	2.40	0.40
4:B:889:THR:C	4:B:891:ASP:H	2.30	0.40
6:D:39:ASN:HB2	6:D:45:GLU:HB2	2.02	0.40
7:E:106:GLN:O	7:E:131:THR:N	2.47	0.40
9:G:13:LEU:HD21	9:G:17:PHE:O	2.20	0.40
17:M:85:ASN:O	17:M:88:HIS:NE2	2.54	0.40
1:N:22:DA:H2"	1:N:23:DA:C8	2.57	0.40
3:A:156:ASP:OD1	3:A:157:ASP:N	2.51	0.40
3:A:831:THR:HG23	3:A:832:ALA:N	2.36	0.40
3:A:934:LYS:O	3:A:937:VAL:HG12	2.21	0.40
3:A:1135:ARG:HG3	3:A:1282:VAL:HG23	2.02	0.40
3:A:1163:ILE:H	3:A:1163:ILE:HD12	1.86	0.40
14:L:40:LEU:CD1	14:L:44:ASP:HB2	2.51	0.40
3:A:315:LEU:HB2	3:A:321:PRO:HA	2.04	0.40
3:A:800:VAL:HA	3:A:812:GLU:CD	2.46	0.40
4:B:552:MET:HA	4:B:555:ILE:HG22	2.03	0.40
4:B:592:ASN:O	4:B:596:LEU:HD13	2.21	0.40
4:B:916:THR:OG1	4:B:935:ARG:HB3	2.22	0.40
5:C:36:VAL:HG11	5:C:251:LEU:HD12	2.04	0.40
5:C:100:THR:OG1	5:C:121:VAL:HG21	2.22	0.40
13:K:8:GLU:OE1	13:K:69:ALA:N	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	1417/1733 (82%)	1266 (89%)	148 (10%)	3 (0%)	43	73
4	B	1150/1224 (94%)	1001 (87%)	147 (13%)	2 (0%)	43	73
5	C	263/318 (83%)	231 (88%)	32 (12%)	0	100	100
6	D	164/221 (74%)	159 (97%)	5 (3%)	0	100	100
7	E	212/215 (99%)	196 (92%)	16 (8%)	0	100	100
8	F	85/155 (55%)	77 (91%)	8 (9%)	0	100	100
9	G	169/171 (99%)	155 (92%)	14 (8%)	0	100	100
10	H	129/146 (88%)	110 (85%)	19 (15%)	0	100	100
11	I	112/122 (92%)	102 (91%)	10 (9%)	0	100	100
12	J	64/70 (91%)	54 (84%)	10 (16%)	0	100	100
13	K	113/120 (94%)	108 (96%)	5 (4%)	0	100	100
14	L	42/70 (60%)	30 (71%)	12 (29%)	0	100	100
16	Q	208/735 (28%)	202 (97%)	6 (3%)	0	100	100
17	M	131/400 (33%)	123 (94%)	8 (6%)	0	100	100
All	All	4259/5700 (75%)	3814 (90%)	440 (10%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	188	ASP
4	B	364	ILE
3	A	195	ASP
3	A	253	ASN
4	B	363	HIS

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	1235/1520 (81%)	1231 (100%)	4 (0%)	86	83
4	B	1000/1061 (94%)	997 (100%)	3 (0%)	86	83
5	C	233/274 (85%)	233 (100%)	0	100	100
6	D	146/200 (73%)	146 (100%)	0	100	100
7	E	196/197 (100%)	196 (100%)	0	100	100
8	F	77/137 (56%)	77 (100%)	0	100	100
9	G	151/152 (99%)	151 (100%)	0	100	100
10	H	118/128 (92%)	118 (100%)	0	100	100
11	I	108/116 (93%)	108 (100%)	0	100	100
12	J	61/65 (94%)	61 (100%)	0	100	100
13	K	99/102 (97%)	99 (100%)	0	100	100
14	L	39/57 (68%)	39 (100%)	0	100	100
16	Q	147/641 (23%)	147 (100%)	0	100	100
17	M	125/363 (34%)	125 (100%)	0	100	100
All	All	3735/5013 (74%)	3728 (100%)	7 (0%)	85	85

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	189	ARG
3	A	191	THR
3	A	193	ASP
3	A	195	ASP
4	B	264	SER
4	B	265	SER
4	B	1183	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	71	GLN
3	A	253	ASN
3	A	399	HIS
3	A	451	HIS
3	A	458	HIS
3	A	545	GLN
3	A	576	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	768	GLN
3	A	802	ASN
3	A	851	HIS
3	A	935	GLN
3	A	965	GLN
3	A	994	GLN
3	A	1009	ASN
3	A	1173	HIS
3	A	1427	ASN
4	B	73	GLN
4	B	110	HIS
4	B	538	ASN
4	B	572	HIS
4	B	590	HIS
4	B	834	ASN
4	B	842	ASN
4	B	1187	ASN
5	C	102	GLN
5	C	203	GLN
6	D	39	ASN
6	D	41	GLN
6	D	150	ASN
7	E	114	ASN
8	F	100	GLN
9	G	24	GLN
9	G	117	GLN
10	H	52	GLN
11	I	22	ASN
11	I	87	GLN
11	I	89	GLN
13	K	40	HIS
16	Q	30	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	R	14/15 (93%)	8 (57%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	R	5	C
15	R	8	A
15	R	9	C
15	R	10	A
15	R	11	A
15	R	13	U
15	R	15	C
15	R	18	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

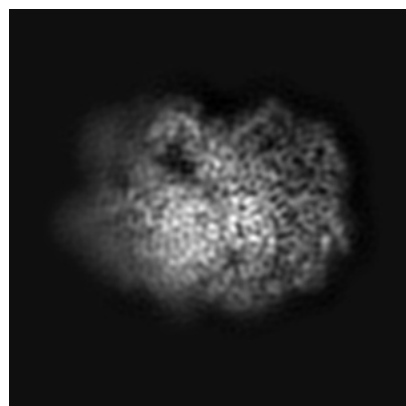
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23887. These allow visual inspection of the internal detail of the map and identification of artifacts.

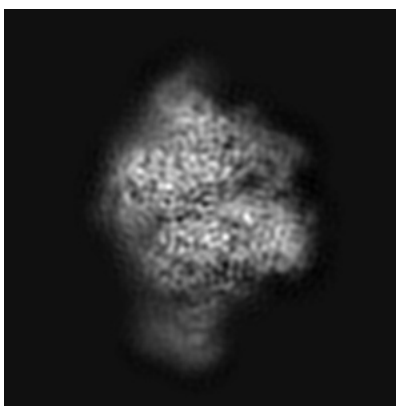
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

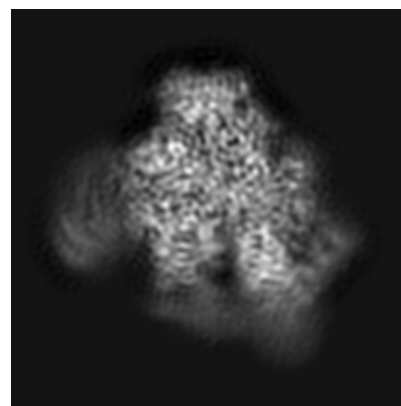
6.1.1 Primary map



X

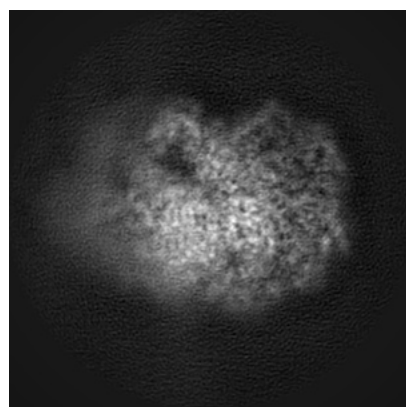


Y

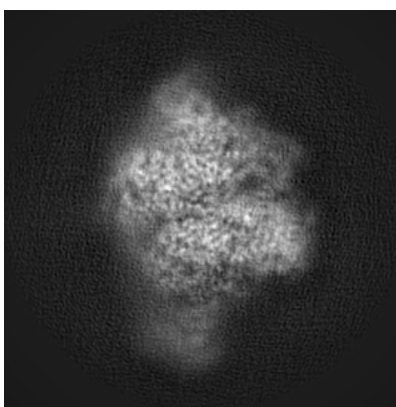


Z

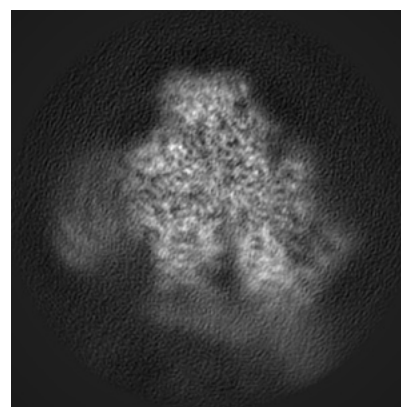
6.1.2 Raw map



X



Y

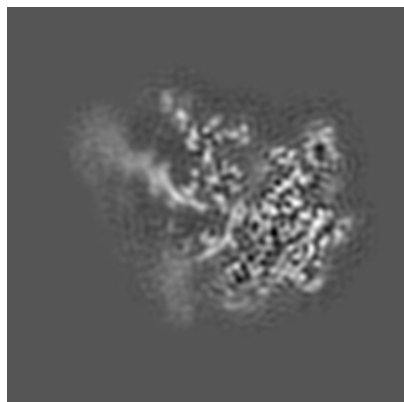


Z

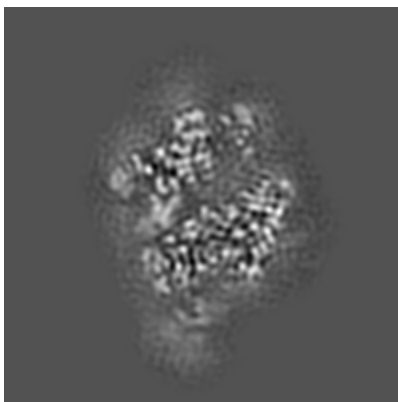
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

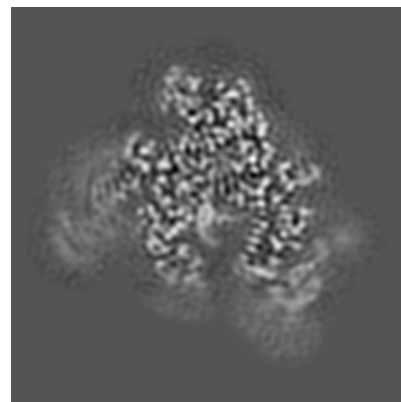
6.2.1 Primary map



X Index: 110

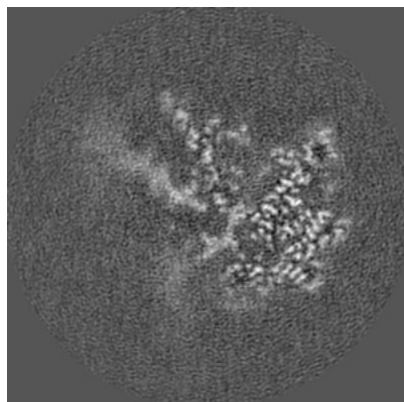


Y Index: 110

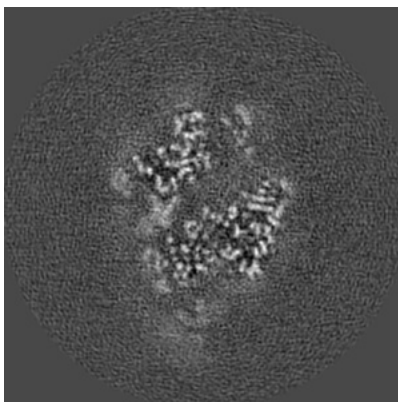


Z Index: 110

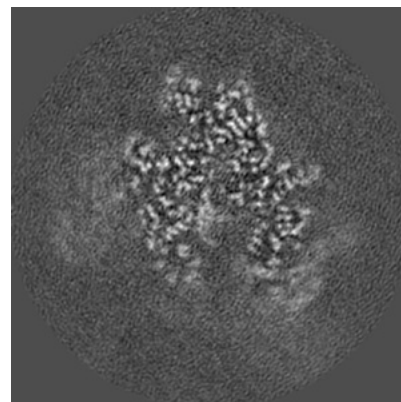
6.2.2 Raw map



X Index: 110



Y Index: 110

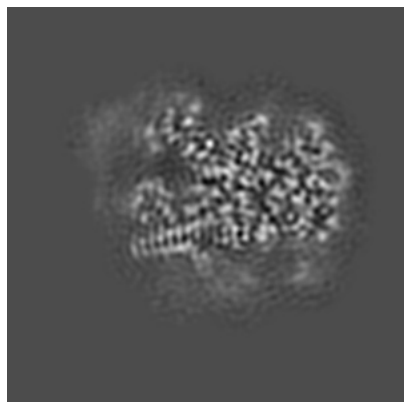


Z Index: 110

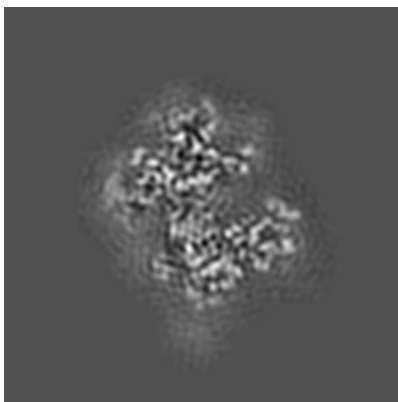
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

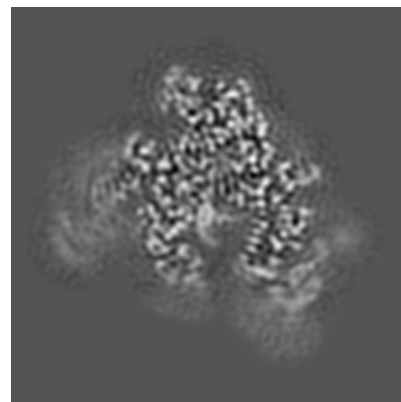
6.3.1 Primary map



X Index: 96

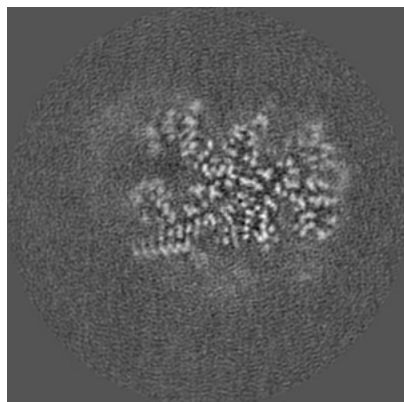


Y Index: 131

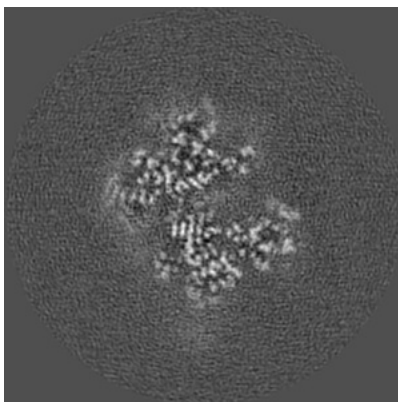


Z Index: 110

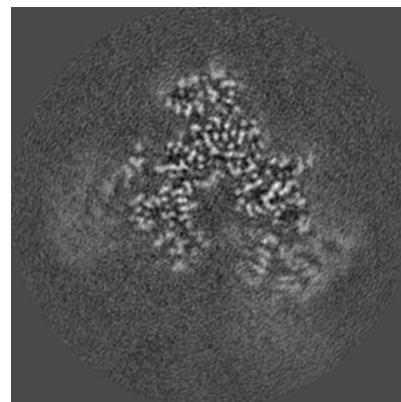
6.3.2 Raw map



X Index: 95



Y Index: 131

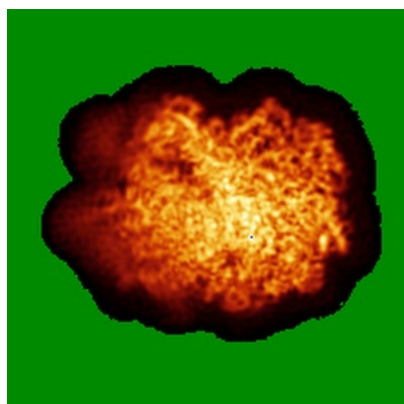


Z Index: 101

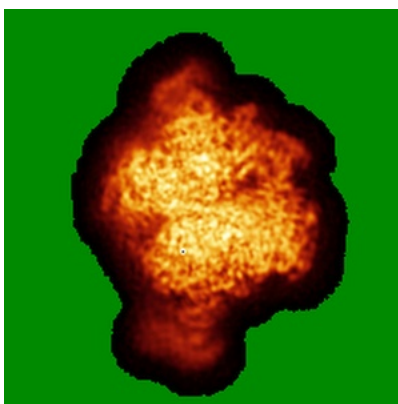
The images above show the largest variance slices of the map in three orthogonal directions.

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

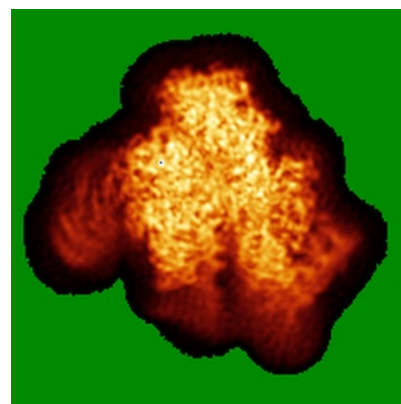
6.4.1 Primary map



X

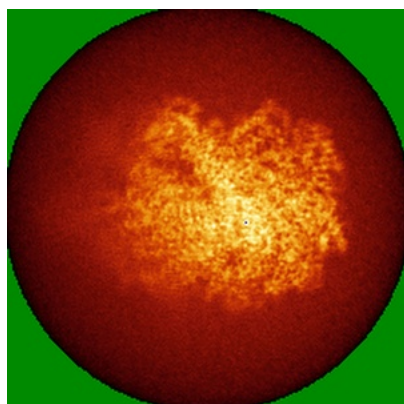


Y

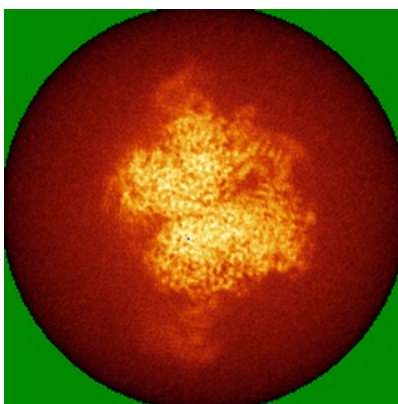


Z

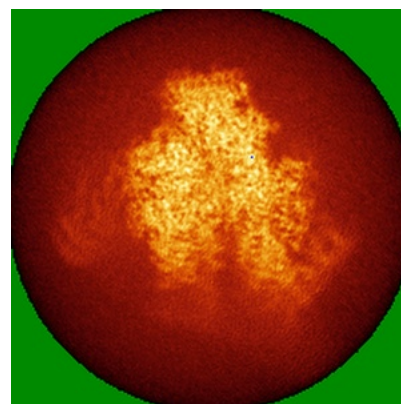
6.4.2 Raw map



X



Y

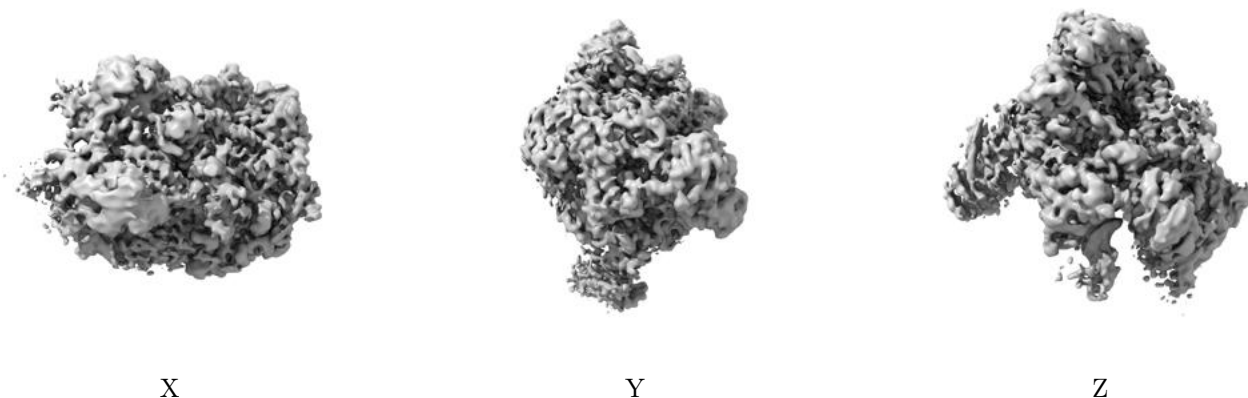


Z

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

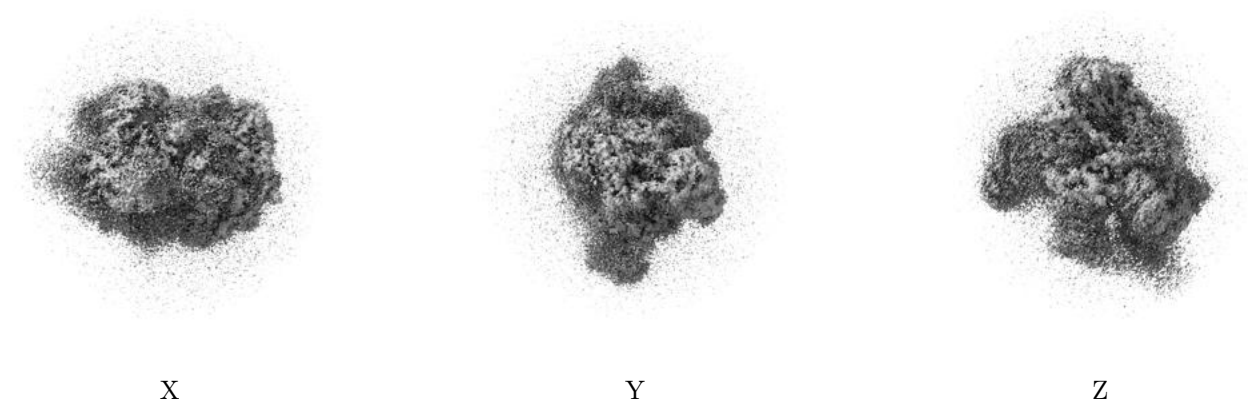
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0084. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

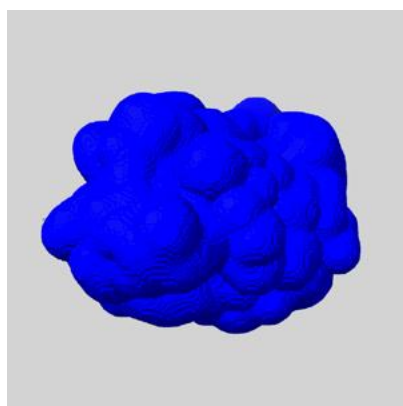
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

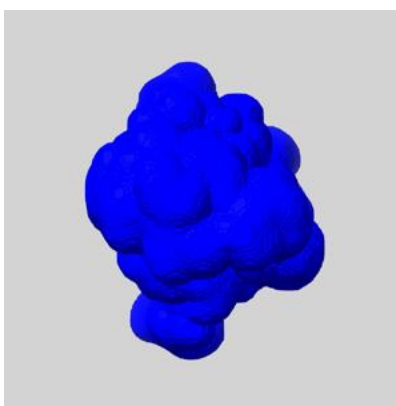
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

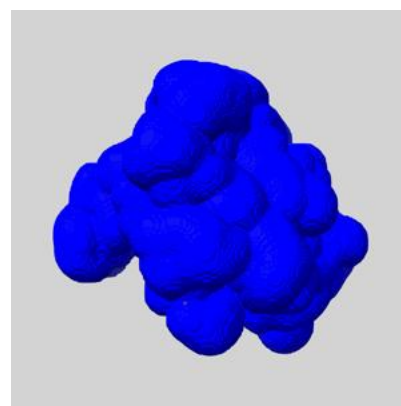
6.6.1 emd_23887_msk_1.map [i](#)



X



Y

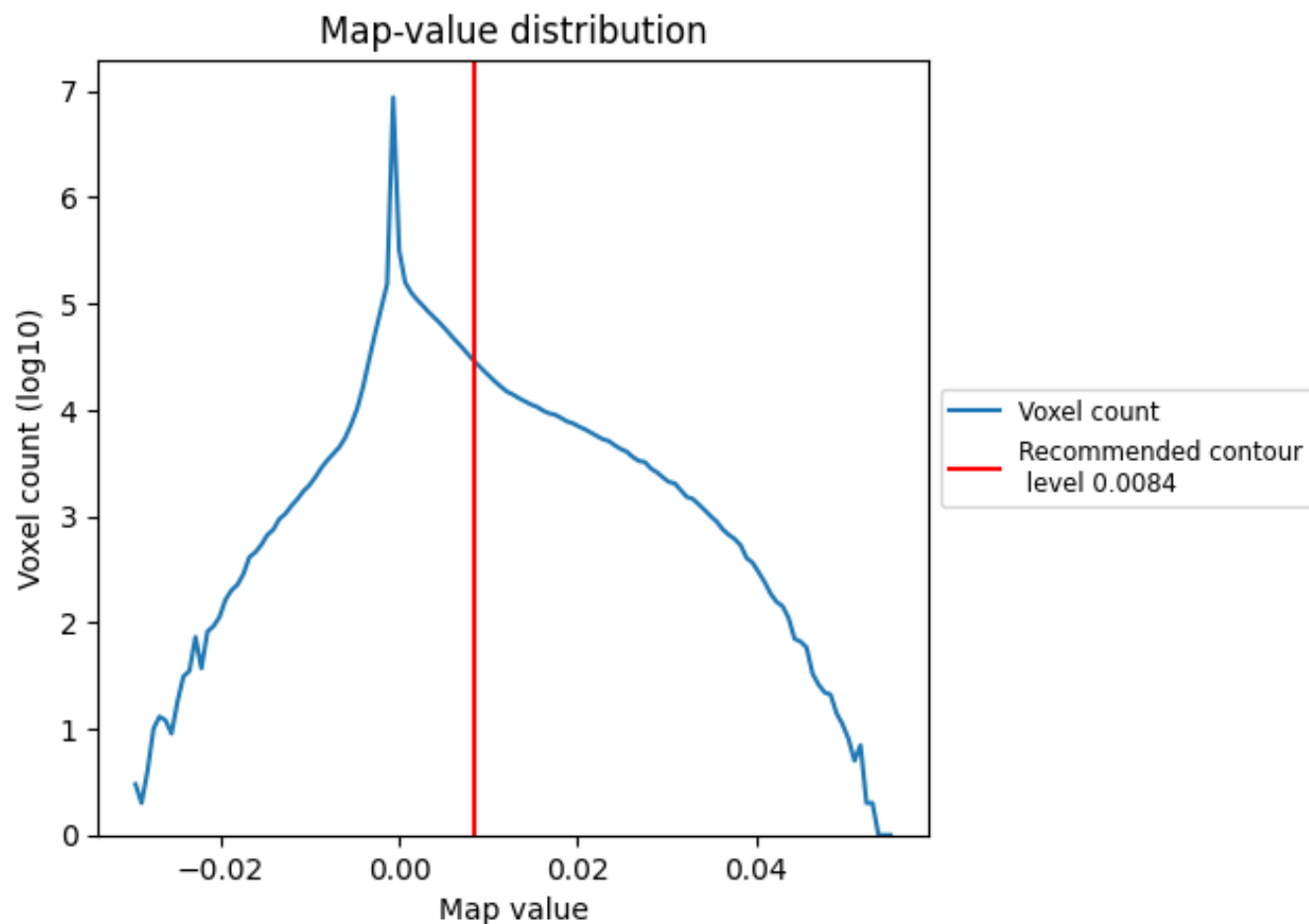


Z

7 Map analysis [i](#)

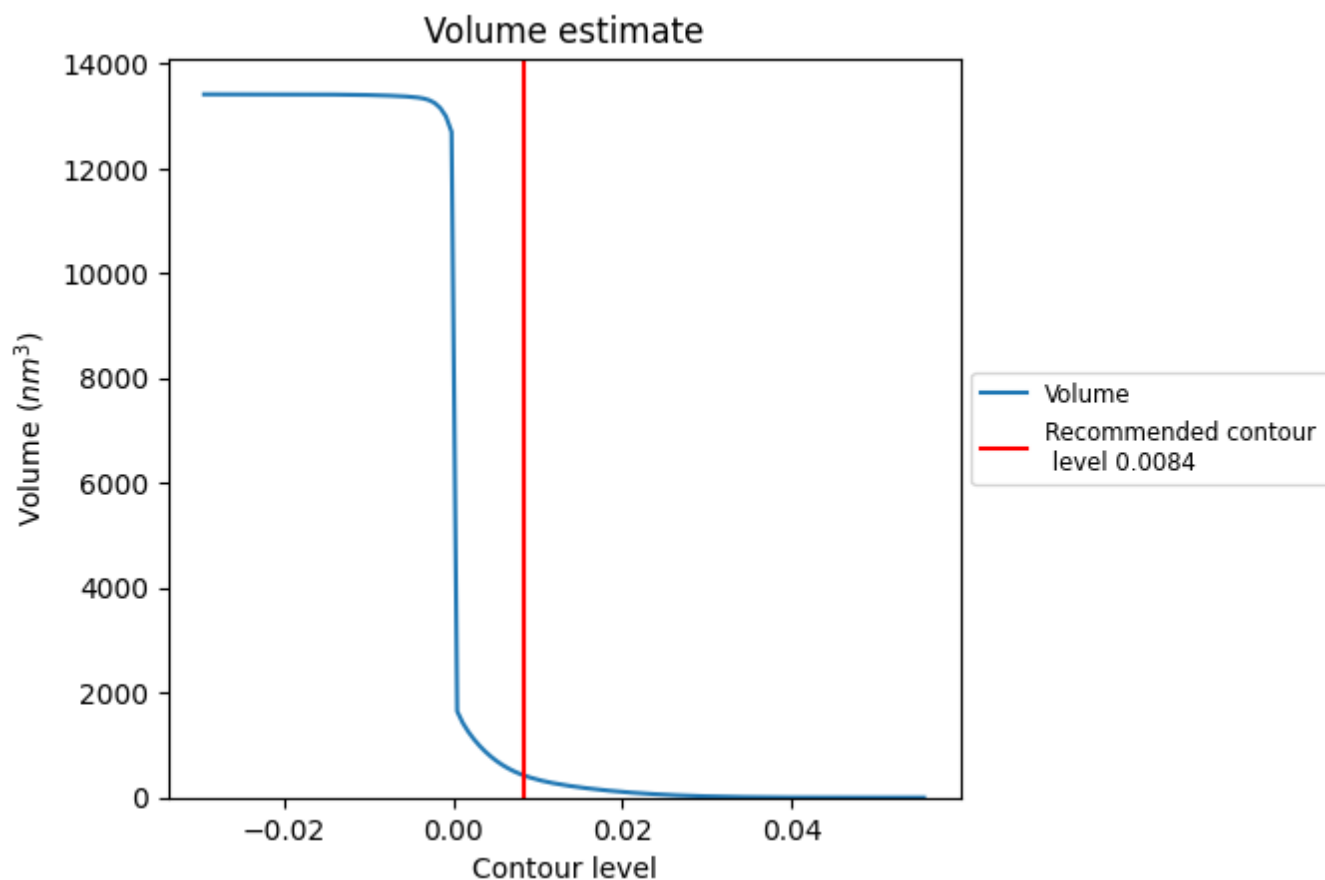
This section contains the results of statistical analysis of the map.

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.

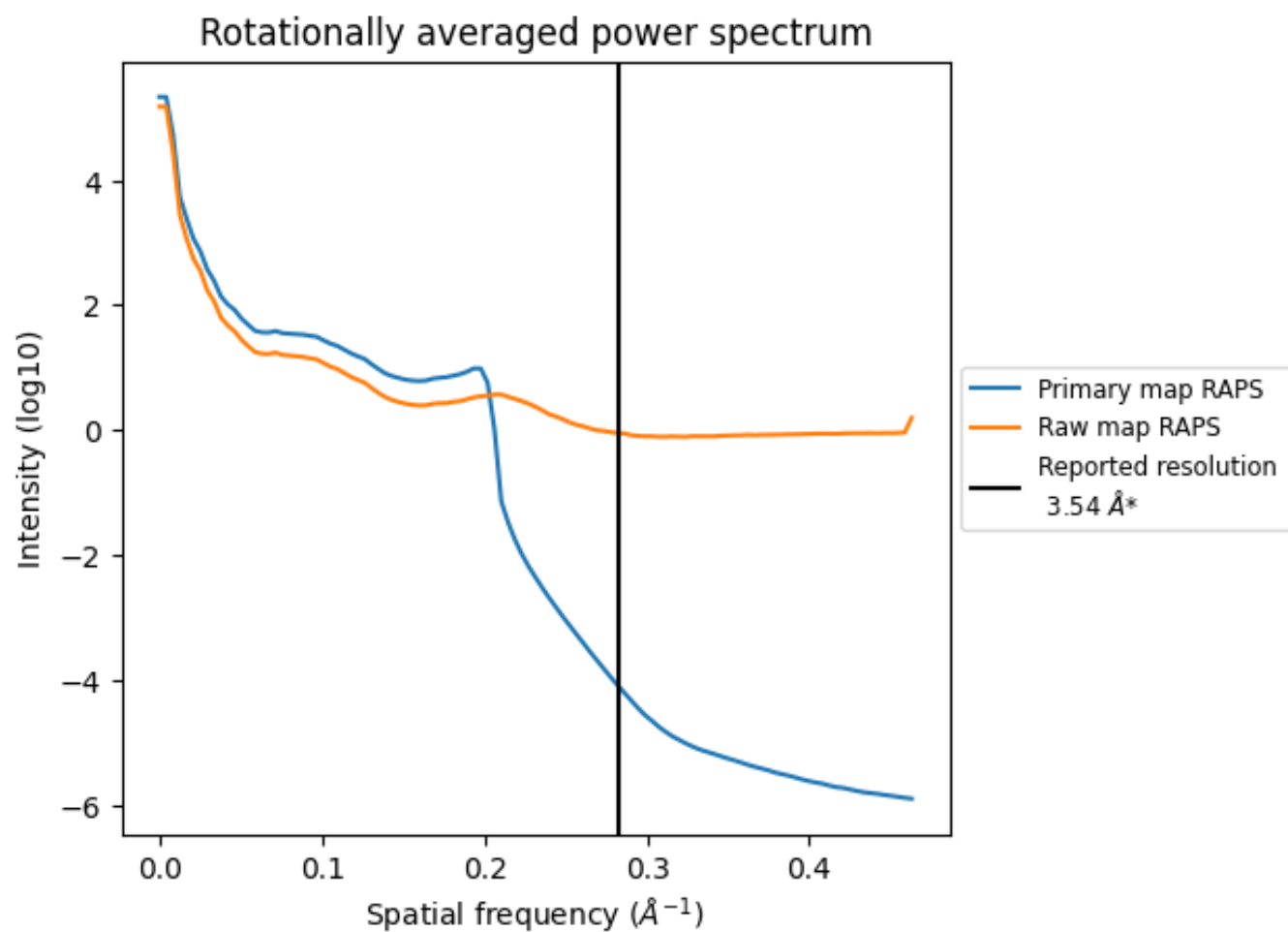
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 420 nm³; this corresponds to an approximate mass of 379 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 ⓘ

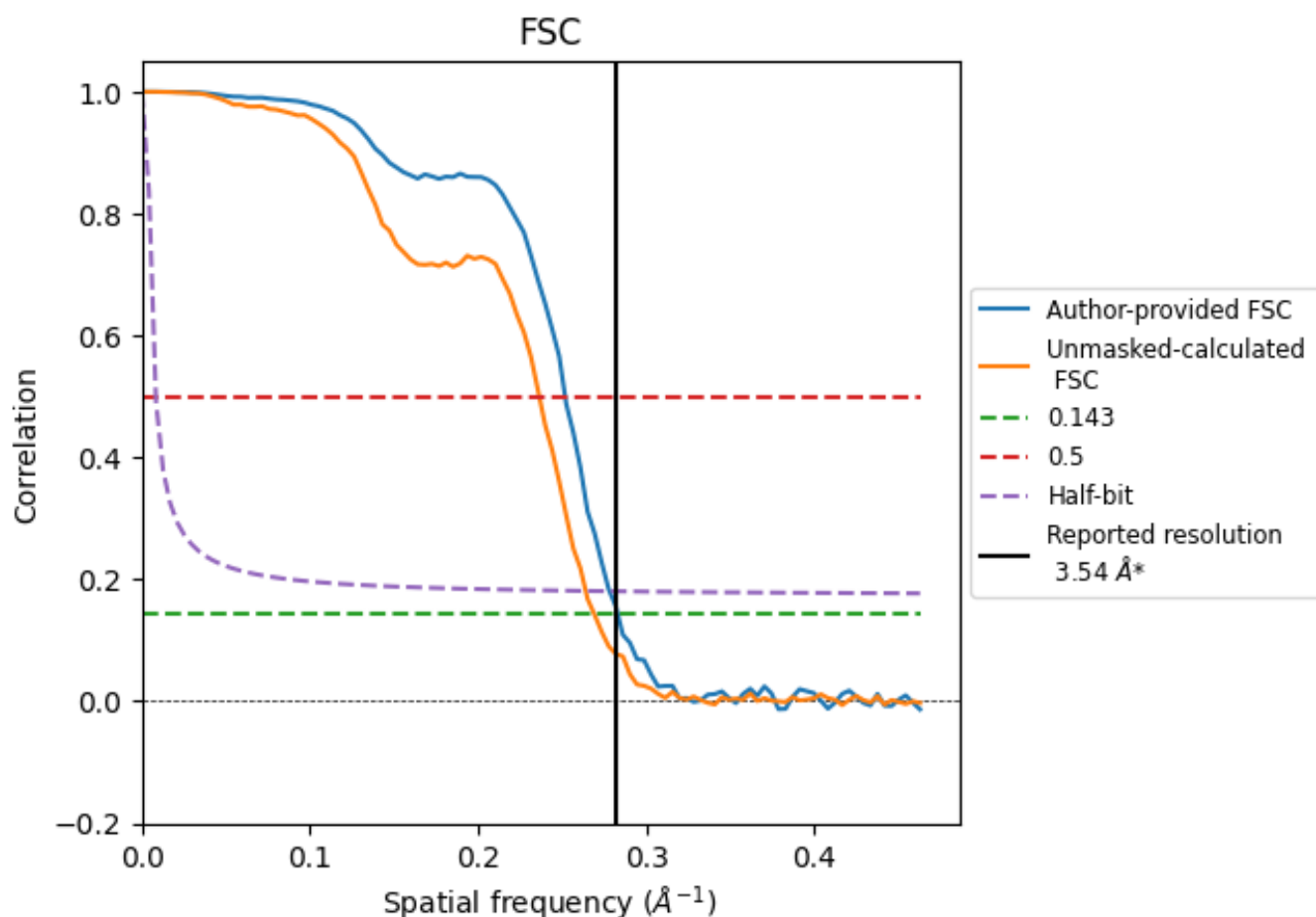


*Reported resolution corresponds to spatial frequency of 0.282 Å⁻¹

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 0.282 Å⁻¹

8.2 Resolution estimates [i](#)

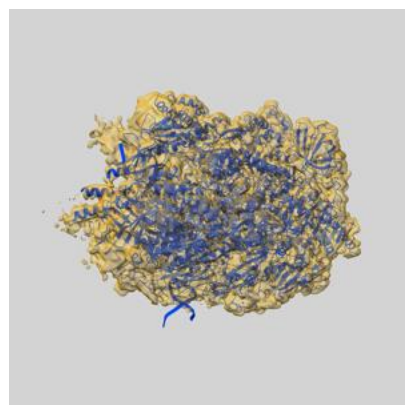
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.54	-	-
Author-provided FSC curve	3.53	3.97	3.59
Unmasked-calculated*	3.72	4.23	3.79

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

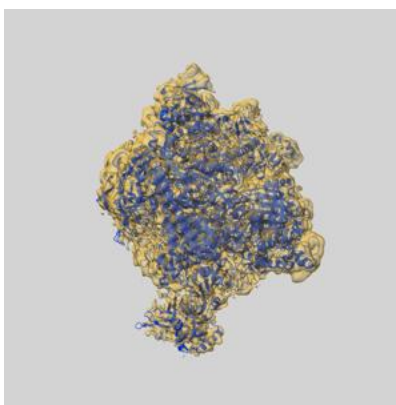
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23887 and PDB model 7MK9. Per-residue inclusion information can be found in section [3](#) on page [8](#).

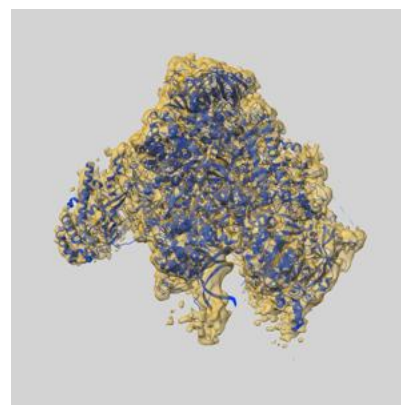
9.1 Map-model overlay [i](#)



X



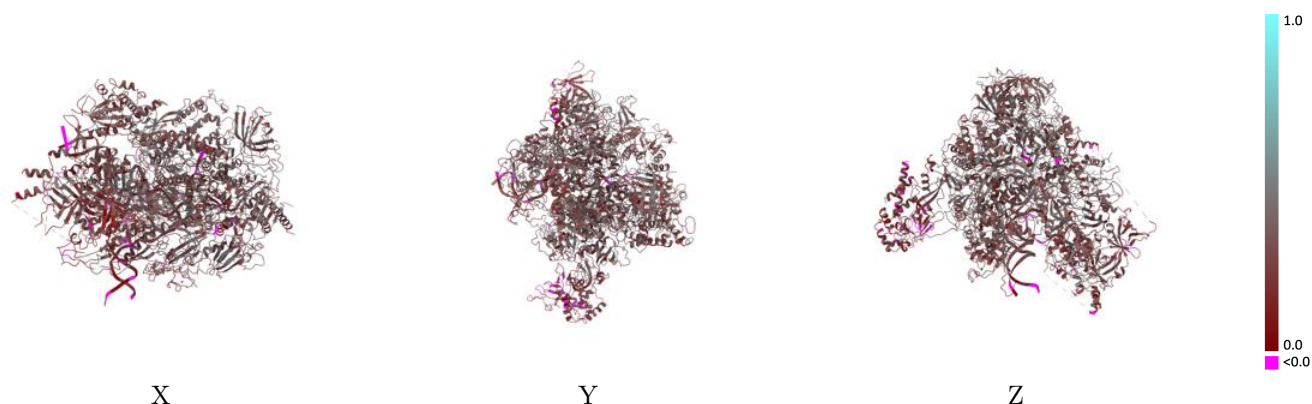
Y



Z

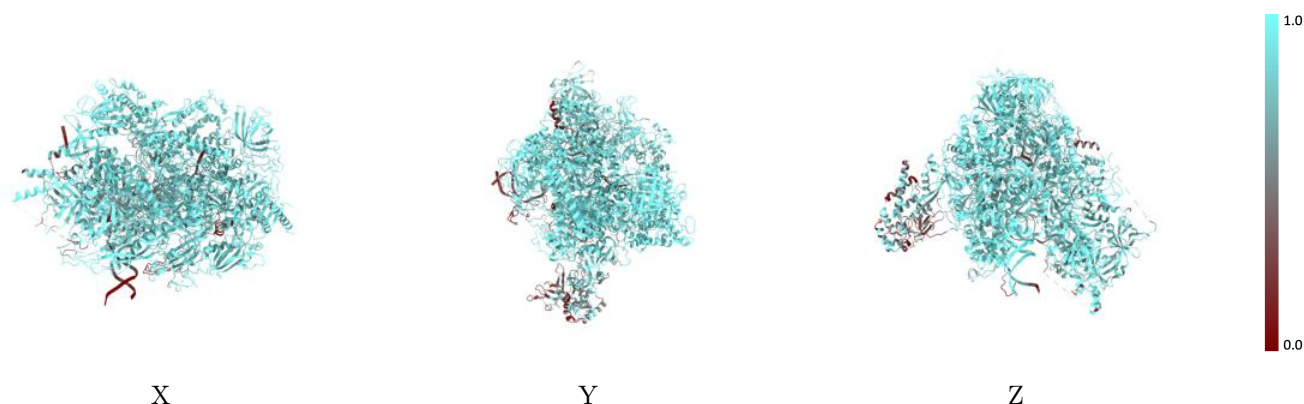
The images above show the 3D surface view of the map at the recommended contour level 0.0084 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



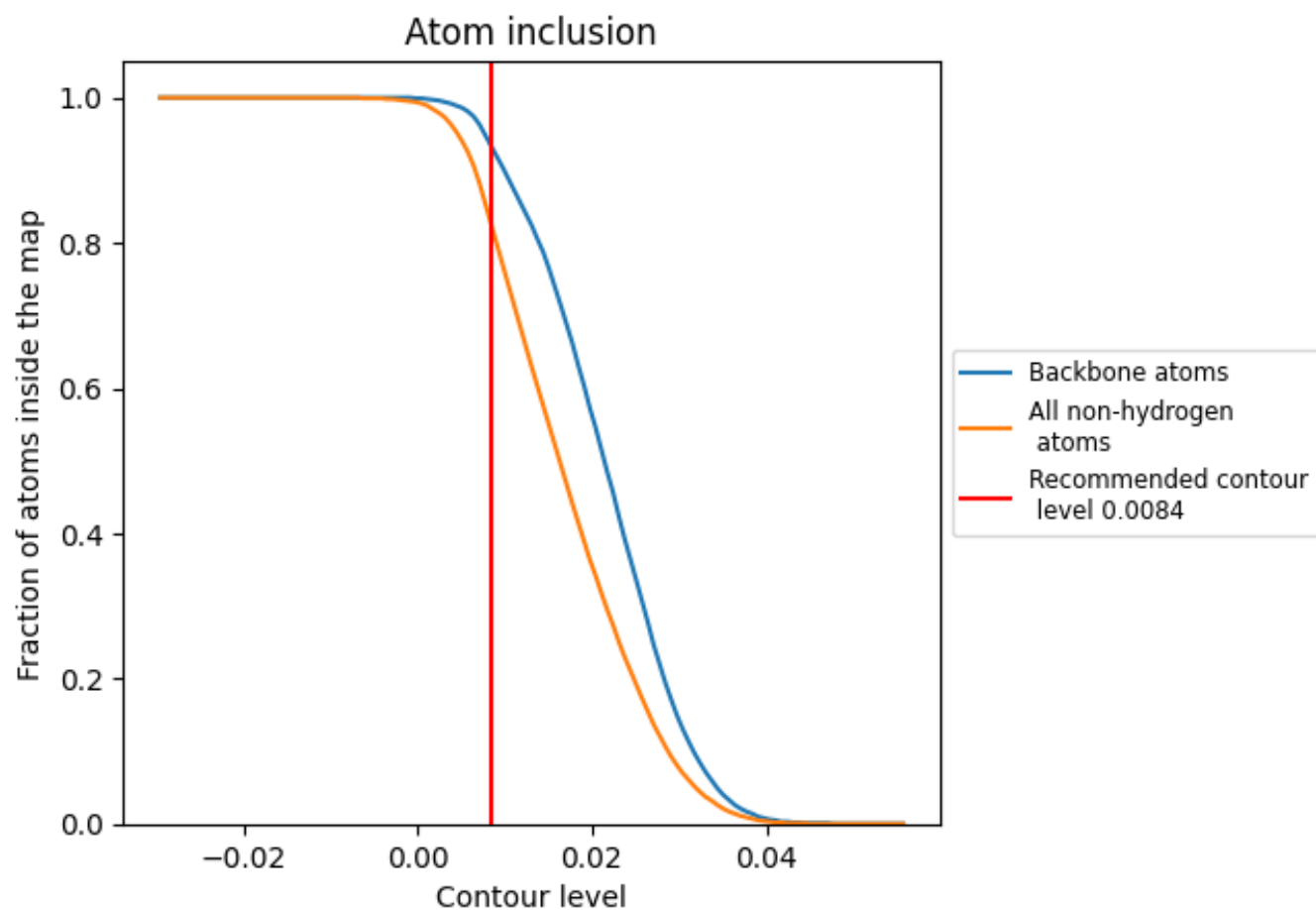
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0084).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 83% 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 (0.0084) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8270	 0.3170
A	 0.8810	 0.3470
B	 0.8380	 0.3360
C	 0.9000	 0.3600
D	 0.5130	 0.1930
E	 0.9050	 0.3440
F	 0.8750	 0.3580
G	 0.5470	 0.1910
H	 0.9300	 0.3400
I	 0.8800	 0.3390
J	 0.9290	 0.3570
K	 0.8330	 0.3200
L	 0.9000	 0.3260
M	 0.7830	 0.2340
N	 0.5910	 0.1750
O	 0.7400	 0.2100
Q	 0.7520	 0.2700
R	 0.7440	 0.2300

