



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 02:24 PM UTC

PDB ID : 9V44 / pdb_00009v44
EMDB ID : EMD-64766
Title : Coupling of polymerase-nucleoprotein-RNA in an influenza virus mini ribonucleoprotein complex
Authors : Kang, H.; Yang, Y.; Liu, Y.; Li, M.; Zhang, L.; Lin, Y.; Rao, Z.; Lou, Z.
Deposited on : 2025-05-22
Resolution : 2.97 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

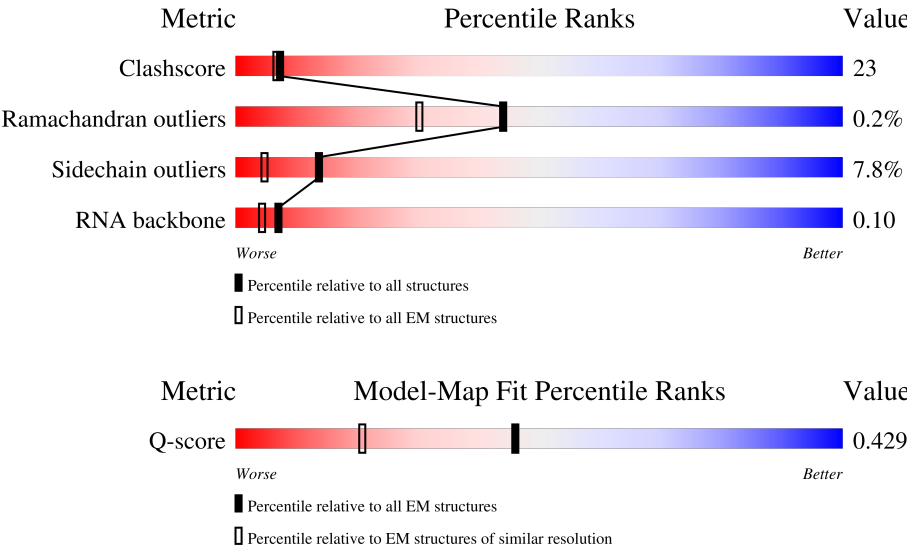
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.97 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	13205 (2.47 - 3.47)

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

Mol	Chain	Length	Quality of chain
1	A	716	
2	B	757	
3	C	759	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	498	38% 21% 45% 19% • 13%
5	E	14	29% 21% 21% 57%
6	F	24	33% 33% 33%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 17835 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Polymerase acidic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	705	Total	C	N	O	S	0	0
			5722	3628	967	1084	43		

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	736	Total	C	N	O	S	0	0
			5874	3696	1027	1107	44		

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	247	Total	C	N	O	S	0	0
			2002	1262	359	365	16		

- Molecule 4 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	434	Total	C	N	O	S	0	0
			3434	2134	635	636	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	14	Total	C	N	O	P	0	0
			288	129	42	103	14		

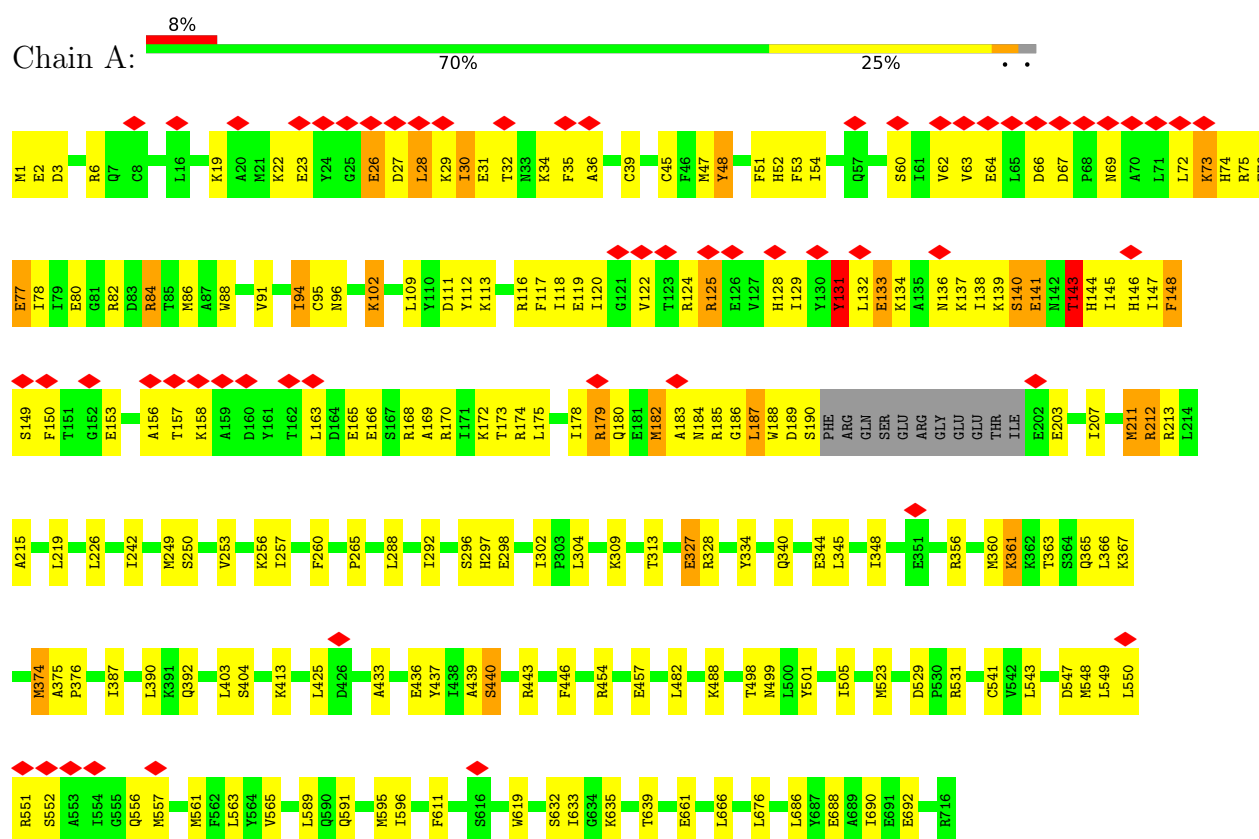
- Molecule 6 is a RNA chain called RNA (5'-R(P*AP*GP*UP*AP*GP*AP*AP*AP*CP*AP*AP*GP*GP*GP*UP*GP*UP*UP*UP*UP*UP*UP*AP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	24	Total	C	N	O	P	0	0
			515	230	91	170	24		

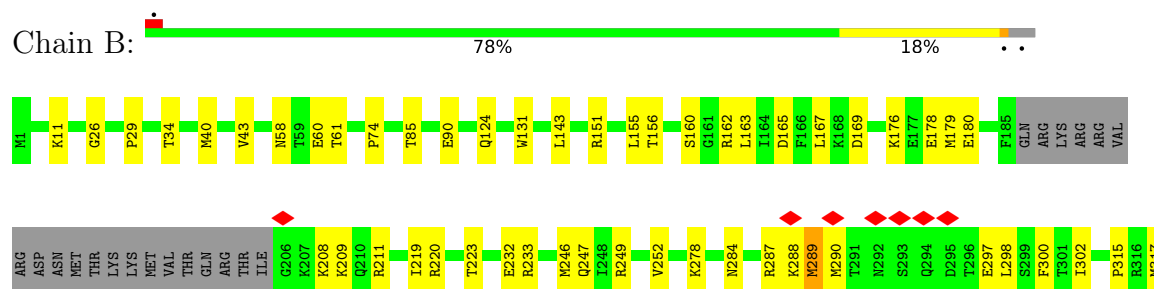
3 Residue-property plots

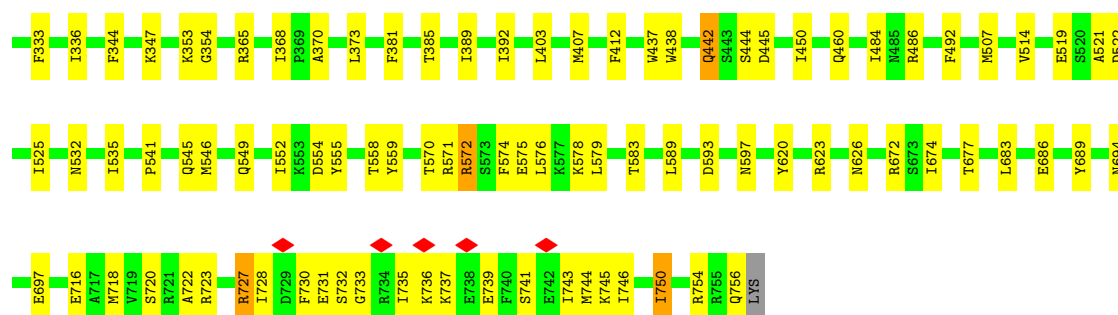
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Polymerase acidic protein



• Molecule 2: RNA-directed RNA polymerase catalytic subunit

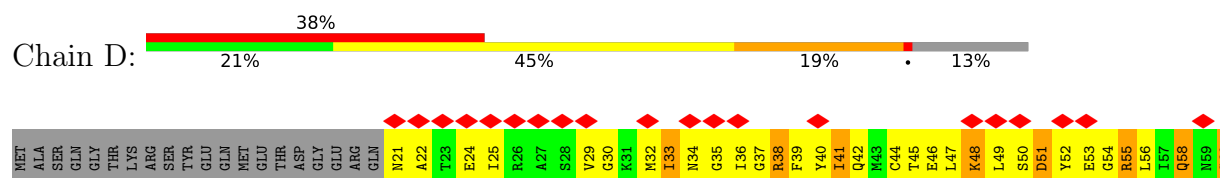


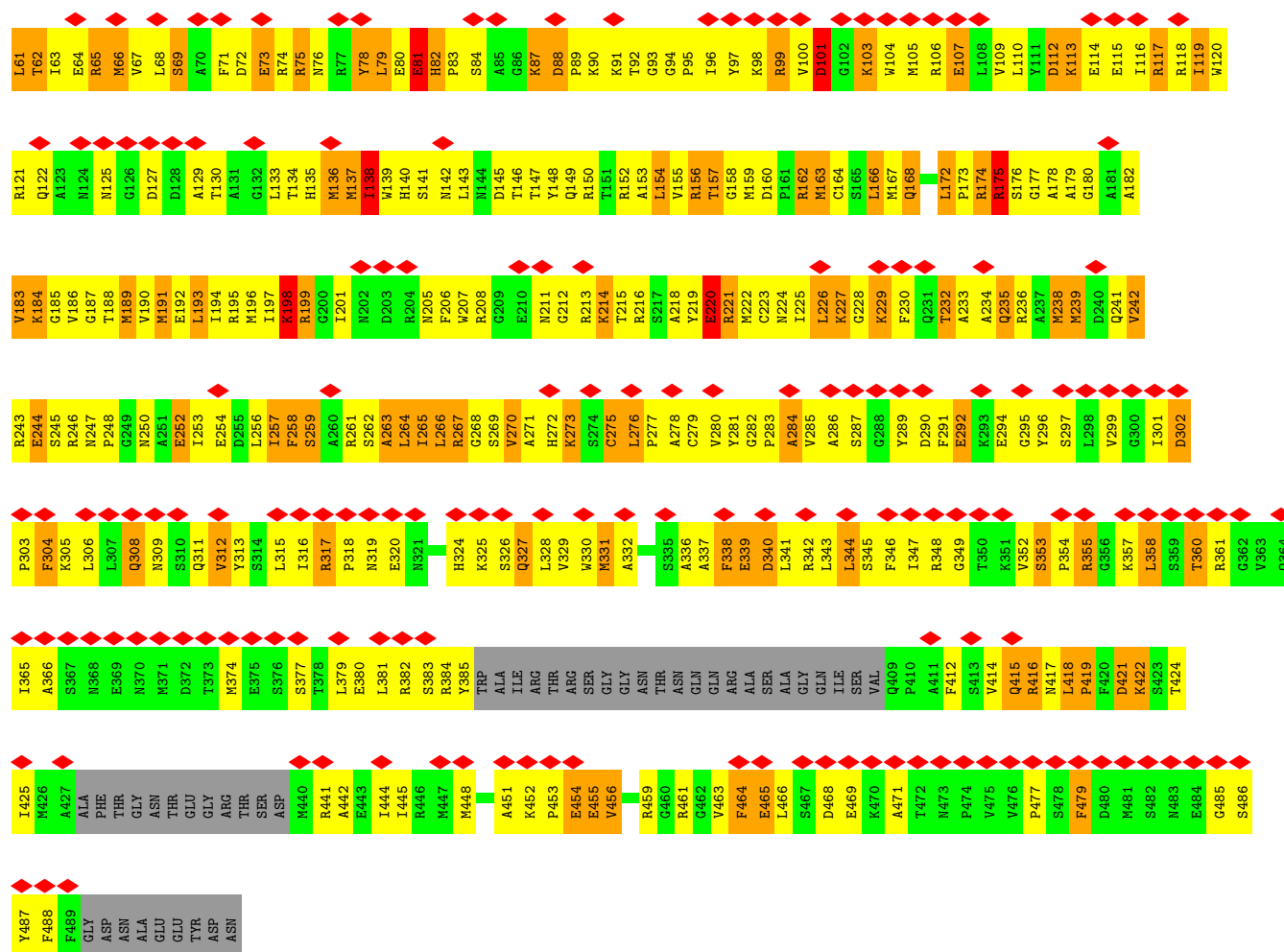


• Molecule 3: Polymerase basic protein 2



• Molecule 4: Nucleoprotein





- Molecule 5: RNA (5'-R(P*UP*UP*UP*GP*UP*CP*AP*CP*CP*CP*UP*GP*CP*U)-3')



- Molecule 6: RNA (5'-R(P*AP*GP*UP*AP*GP*AP*AP*AP*CP*AP*AP*GP*GP*GP*UP*GP*UP*UP*UP*UP*UP*AP*U)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	265200	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.957	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96000004, 0.96000004, 0.96000004	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.35	0/5843	0.56	2/7875 (0.0%)
2	B	0.29	0/5990	0.46	1/8079 (0.0%)
3	C	0.25	0/2042	0.45	0/2754
4	D	0.78	1/3493 (0.0%)	1.09	16/4689 (0.3%)
5	E	0.38	0/318	0.68	0/491
6	F	0.39	0/576	0.69	0/894
All	All	0.45	1/18262 (0.0%)	0.66	19/24782 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	65	ARG	CA-C	-5.26	1.46	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	101	ASP	N-CA-C	-11.32	101.72	114.62
2	B	572	ARG	N-CA-C	-8.48	102.49	112.92
4	D	284	ALA	N-CA-C	-6.81	103.09	111.33
4	D	258	PHE	N-CA-C	-6.41	104.22	111.14
4	D	465	GLU	N-CA-C	-6.34	98.56	108.90
4	D	101	ASP	CB-CA-C	6.28	117.64	109.28
1	A	131	TYR	N-CA-C	-6.20	104.63	111.82
4	D	138	ILE	N-CA-C	-6.09	104.41	110.62
4	D	220	GLU	N-CA-C	6.00	117.49	111.07
4	D	137	MET	N-CA-C	-5.94	104.74	112.23
4	D	263	ALA	N-CA-C	-5.87	104.29	112.45
4	D	244	GLU	N-CA-C	-5.81	105.90	112.87
4	D	198	LYS	N-CA-C	-5.74	105.17	111.82
4	D	199	ARG	N-CA-C	-5.66	105.88	112.89
1	A	143	THR	N-CA-C	-5.62	100.62	109.50
4	D	84	SER	CB-CA-C	-5.56	110.14	116.54
4	D	275	CYS	N-CA-C	5.48	118.16	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	175	ARG	N-CA-C	5.10	117.61	108.17
4	D	266	LEU	N-CA-C	5.05	117.13	108.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5722	0	5652	185	0
2	B	5874	0	5859	105	0
3	C	2002	0	2048	41	0
4	D	3434	0	3431	505	0
5	E	288	0	149	11	0
6	F	515	0	256	26	0
All	All	17835	0	17395	824	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 23.

All (824) 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:D:330:TRP:CH2	4:D:344:LEU:HD22	1.51	1.41
4:D:91:LYS:CG	4:D:112:ASP:HA	1.64	1.26
4:D:110:LEU:HD12	4:D:110:LEU:O	1.31	1.23
4:D:330:TRP:CZ3	4:D:344:LEU:HD22	1.78	1.18
4:D:143:LEU:HA	4:D:332:ALA:HB1	1.25	1.17
4:D:316:ILE:HG12	4:D:325:LYS:CD	1.76	1.15
1:A:165:GLU:CG	1:A:168:ARG:HG3	1.75	1.14
1:A:165:GLU:HG3	1:A:168:ARG:CG	1.79	1.10
4:D:355:ARG:HE	4:D:355:ARG:HA	1.21	1.06
4:D:91:LYS:HG2	4:D:112:ASP:HA	1.07	1.05
4:D:347:ILE:HG21	4:D:461:ARG:NH1	1.76	1.00
4:D:330:TRP:CH2	4:D:344:LEU:CD2	2.45	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:417:ASN:HB3	4:D:453:PRO:O	1.61	0.98
4:D:316:ILE:CD1	4:D:325:LYS:HD3	1.93	0.98
1:A:165:GLU:HG3	1:A:168:ARG:HG3	0.98	0.98
4:D:114:GLU:HA	4:D:117:ARG:HD2	1.47	0.97
4:D:316:ILE:HD11	4:D:325:LYS:HD3	1.45	0.96
4:D:91:LYS:HD3	4:D:112:ASP:HB3	1.49	0.95
4:D:329:VAL:HG21	4:D:379:LEU:HD21	1.45	0.95
4:D:445:ILE:HD13	4:D:448:MET:CE	1.97	0.95
4:D:30:GLY:CA	4:D:295:GLY:HA2	1.96	0.94
4:D:110:LEU:O	4:D:110:LEU:CD1	2.15	0.94
4:D:316:ILE:HG12	4:D:325:LYS:HD2	1.48	0.94
4:D:267:ARG:HH22	4:D:453:PRO:HA	1.30	0.94
4:D:279:CYS:O	4:D:283:PRO:HD3	1.67	0.93
4:D:91:LYS:CD	4:D:112:ASP:HA	1.98	0.93
4:D:330:TRP:HH2	4:D:344:LEU:HD22	1.12	0.93
4:D:91:LYS:HG2	4:D:112:ASP:CA	1.97	0.93
4:D:143:LEU:O	4:D:146:THR:HG22	1.69	0.93
4:D:347:ILE:CG2	4:D:463:VAL:HG21	2.00	0.91
4:D:419:PRO:HG2	4:D:453:PRO:HG2	1.48	0.91
4:D:64:GLU:HG3	4:D:140:HIS:HE1	1.33	0.91
4:D:72:ASP:HB3	4:D:75:ARG:HB3	1.53	0.90
4:D:385:TYR:HD1	4:D:465:GLU:HA	1.36	0.90
4:D:143:LEU:HA	4:D:332:ALA:CB	2.01	0.90
4:D:195:ARG:HA	4:D:198:LYS:HE2	1.52	0.89
4:D:91:LYS:HE3	4:D:110:LEU:CD1	2.03	0.89
4:D:99:ARG:HA	4:D:104:TRP:HA	1.54	0.88
4:D:149:GLN:HB2	6:F:23:A:H1'	1.55	0.88
4:D:316:ILE:CG1	4:D:325:LYS:CD	2.51	0.88
4:D:385:TYR:HB3	4:D:464:PHE:O	1.73	0.88
4:D:137:MET:SD	4:D:173:PRO:HD2	2.13	0.87
1:A:29:LYS:HG2	1:A:30:ILE:HG13	1.54	0.87
4:D:347:ILE:HG13	4:D:461:ARG:HH12	1.40	0.87
4:D:338:PHE:HB3	4:D:487:TYR:HB3	1.54	0.87
4:D:40:TYR:HD2	4:D:282:GLY:HA3	1.40	0.86
4:D:30:GLY:HA3	4:D:295:GLY:HA2	1.55	0.86
4:D:355:ARG:HA	4:D:355:ARG:NE	1.91	0.85
2:B:750:ILE:HD11	3:C:8:ARG:HA	1.57	0.85
6:F:20:U:H4'	6:F:20:U:OP1	1.76	0.84
4:D:317:ARG:HD3	4:D:361:ARG:NH2	1.93	0.84
4:D:21:ASN:O	4:D:24:GLU:HG2	1.77	0.84
4:D:267:ARG:NH1	4:D:454:GLU:HB2	1.92	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:445:ILE:HA	4:D:448:MET:HE3	1.58	0.84
4:D:118:ARG:HA	4:D:121:ARG:HD2	1.61	0.83
4:D:88:ASP:HB3	4:D:110:LEU:HD22	1.61	0.83
4:D:40:TYR:CD2	4:D:282:GLY:HA3	2.14	0.81
4:D:347:ILE:HD12	4:D:463:VAL:HG11	1.60	0.81
4:D:486:SER:OG	4:D:488:PHE:CE2	2.32	0.81
4:D:173:PRO:HG2	4:D:175:ARG:HH21	1.46	0.81
1:A:146:HIS:CD2	1:A:156:ALA:HB2	2.16	0.81
4:D:262:SER:O	4:D:266:LEU:HG	1.81	0.81
4:D:347:ILE:HG21	4:D:461:ARG:HH11	1.41	0.80
4:D:340:ASP:HA	4:D:485:GLY:O	1.81	0.80
4:D:330:TRP:HH2	4:D:344:LEU:CD2	1.86	0.79
4:D:349:GLY:HA3	4:D:384:ARG:HH21	1.46	0.79
4:D:49:LEU:HD22	4:D:53:GLU:HG2	1.64	0.79
4:D:91:LYS:CD	4:D:112:ASP:CA	2.60	0.79
4:D:316:ILE:CG1	4:D:325:LYS:HD3	2.11	0.79
4:D:91:LYS:HD3	4:D:112:ASP:CB	2.12	0.79
4:D:330:TRP:HZ3	4:D:344:LEU:HD13	1.48	0.79
4:D:60:SER:HB2	4:D:279:CYS:HB2	1.63	0.79
4:D:60:SER:CB	4:D:279:CYS:HB2	2.12	0.79
4:D:78:TYR:HB2	5:E:231:U:C4	2.17	0.78
4:D:196:MET:SD	4:D:222:MET:SD	2.82	0.78
4:D:486:SER:OG	4:D:488:PHE:CD2	2.37	0.78
4:D:65:ARG:CZ	6:F:20:U:H1'	2.14	0.77
4:D:330:TRP:CZ3	4:D:344:LEU:CD2	2.66	0.77
1:A:207:ILE:HB	1:A:212:ARG:HH21	1.50	0.77
4:D:168:GLN:HB3	4:D:183:VAL:HG12	1.66	0.77
4:D:445:ILE:HD13	4:D:448:MET:HE1	1.64	0.77
4:D:64:GLU:HG3	4:D:140:HIS:CE1	2.19	0.76
1:A:141:GLU:HG2	1:A:143:THR:HG23	1.66	0.76
4:D:347:ILE:HD12	4:D:463:VAL:CG1	2.15	0.76
4:D:316:ILE:HG12	4:D:325:LYS:CE	2.14	0.76
1:A:119:GLU:HB2	1:A:145:ILE:HG13	1.68	0.76
6:F:13:G:H5''	6:F:13:G:H8	1.51	0.76
4:D:157:THR:HG22	4:D:159:MET:H	1.51	0.75
1:A:124:ARG:HD2	1:A:189:ASP:HA	1.69	0.75
4:D:148:TYR:CE1	6:F:22:U:OP1	2.40	0.75
4:D:299:VAL:HG12	4:D:299:VAL:O	1.86	0.75
4:D:60:SER:O	4:D:64:GLU:HG2	1.87	0.75
4:D:71:PHE:HD2	4:D:133:LEU:HD11	1.51	0.75
4:D:418:LEU:N	4:D:419:PRO:HD3	2.01	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:267:ARG:NH2	4:D:453:PRO:HA	2.02	0.74
1:A:375:ALA:HB3	4:D:208:ARG:HH22	1.53	0.74
4:D:383:SER:O	4:D:466:LEU:HD11	1.87	0.74
4:D:419:PRO:HG2	4:D:453:PRO:CG	2.16	0.74
4:D:445:ILE:HD13	4:D:448:MET:HE3	1.69	0.74
1:A:96:ASN:ND2	3:C:170:ASN:OD1	2.21	0.73
4:D:253:ILE:O	4:D:257:ILE:HG12	1.88	0.73
6:F:22:U:H4'	6:F:23:A:H5'	1.71	0.73
4:D:113:LYS:CG	4:D:117:ARG:HH21	2.00	0.73
4:D:347:ILE:HG21	4:D:463:VAL:HG21	1.70	0.72
4:D:147:THR:HG22	4:D:328:LEU:HD21	1.70	0.72
4:D:198:LYS:HA	4:D:201:ILE:HD12	1.71	0.72
4:D:320:GLU:HG2	4:D:360:THR:HA	1.71	0.72
4:D:100:VAL:HG13	4:D:101:ASP:H	1.54	0.72
4:D:354:PRO:HB2	4:D:357:LYS:HG3	1.69	0.72
4:D:30:GLY:HA2	4:D:295:GLY:HA2	1.70	0.72
2:B:302:ILE:HG12	2:B:484:ILE:HD13	1.72	0.72
4:D:385:TYR:CD1	4:D:465:GLU:HA	2.24	0.72
1:A:117:PHE:H	1:A:143:THR:HB	1.55	0.71
4:D:445:ILE:HA	4:D:448:MET:CE	2.19	0.71
2:B:178:GLU:HB3	2:B:211:ARG:HD2	1.71	0.70
4:D:280:VAL:O	4:D:283:PRO:HD2	1.92	0.70
2:B:131:TRP:HE1	2:B:247:GLN:HE22	1.39	0.69
4:D:252:GLU:O	4:D:256:LEU:HG	1.92	0.69
4:D:91:LYS:HE3	4:D:110:LEU:HD13	1.73	0.69
4:D:143:LEU:CA	4:D:332:ALA:HB1	2.15	0.69
5:E:232:G:H4'	5:E:233:U:OP1	1.93	0.69
4:D:271:ALA:HB2	4:D:459:ARG:NH1	2.07	0.69
4:D:78:TYR:HB2	5:E:231:U:N3	2.08	0.69
1:A:84:ARG:HB2	1:A:84:ARG:CZ	2.23	0.69
2:B:252:VAL:HG13	2:B:412:PHE:HE1	1.58	0.69
4:D:30:GLY:HA3	4:D:295:GLY:CA	2.22	0.69
4:D:90:LYS:O	4:D:113:LYS:HB2	1.93	0.69
4:D:91:LYS:CD	4:D:112:ASP:CB	2.71	0.69
4:D:176:SER:HB3	4:D:180:GLY:H	1.57	0.68
4:D:96:ILE:HD11	4:D:107:GLU:HG3	1.75	0.68
4:D:149:GLN:HB2	6:F:23:A:C1'	2.23	0.68
4:D:146:THR:CG2	4:D:332:ALA:HB2	2.22	0.68
1:A:146:HIS:HD2	1:A:156:ALA:HB2	1.58	0.68
2:B:85:THR:HG22	2:B:317:MET:HE1	1.74	0.68
4:D:47:LEU:O	4:D:48:LYS:HB2	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:GLU:O	1:A:165:GLU:HG2	1.92	0.68
4:D:71:PHE:CD2	4:D:133:LEU:HD11	2.28	0.68
4:D:136:MET:O	4:D:139:TRP:HB3	1.92	0.68
4:D:329:VAL:HG11	4:D:379:LEU:CD2	2.24	0.68
1:A:134:LYS:HZ3	1:A:147:ILE:HB	1.57	0.68
4:D:271:ALA:HB2	4:D:459:ARG:CZ	2.25	0.67
2:B:208:LYS:HG2	2:B:209:LYS:H	1.60	0.67
3:C:18:GLU:O	3:C:22:LYS:HB2	1.95	0.67
4:D:134:THR:HA	4:D:137:MET:HE3	1.76	0.67
1:A:168:ARG:O	1:A:172:LYS:HG2	1.95	0.67
1:A:443:ARG:HD3	2:B:545:GLN:HB2	1.75	0.67
4:D:42:GLN:HB2	4:D:119:ILE:HD11	1.77	0.66
4:D:353:SER:OG	4:D:358:LEU:HD11	1.95	0.66
1:A:117:PHE:N	1:A:143:THR:HB	2.09	0.66
1:A:360:MET:HE3	1:A:482:LEU:HB2	1.76	0.66
4:D:139:TRP:CE2	4:D:277:PRO:HB3	2.30	0.66
3:C:156:ALA:O	3:C:160:GLN:NE2	2.29	0.66
4:D:267:ARG:H	4:D:267:ARG:HE	1.43	0.66
1:A:117:PHE:HB2	1:A:143:THR:CB	2.25	0.66
4:D:95:PRO:HB3	4:D:106:ARG:CZ	2.26	0.66
4:D:296:TYR:HD1	4:D:302:ASP:HB3	1.61	0.65
4:D:64:GLU:HB3	4:D:136:MET:HE1	1.79	0.65
1:A:133:GLU:HA	1:A:136:ASN:HD21	1.60	0.65
4:D:30:GLY:CA	4:D:295:GLY:CA	2.73	0.65
4:D:174:ARG:HH22	5:E:230:U:H2'	1.61	0.65
4:D:315:LEU:HD22	4:D:374:MET:HB3	1.77	0.65
4:D:176:SER:HB3	4:D:180:GLY:N	2.11	0.65
4:D:192:GLU:O	4:D:196:MET:HG3	1.97	0.65
1:A:387:ILE:HD11	1:A:390:LEU:HD13	1.77	0.65
4:D:417:ASN:HB2	4:D:419:PRO:HD3	1.77	0.65
4:D:316:ILE:HD12	4:D:377:SER:OG	1.97	0.65
1:A:133:GLU:HA	1:A:136:ASN:ND2	2.11	0.65
4:D:29:VAL:O	4:D:33:ILE:HD12	1.96	0.65
4:D:139:TRP:CZ3	4:D:143:LEU:HD11	2.32	0.65
4:D:239:MET:O	4:D:242:VAL:HG12	1.97	0.65
4:D:316:ILE:HG12	4:D:325:LYS:HE2	1.79	0.65
4:D:383:SER:O	4:D:466:LEU:CD1	2.45	0.64
1:A:257:ILE:H	2:B:460:GLN:HE22	1.43	0.64
4:D:385:TYR:C	4:D:466:LEU:HG	2.22	0.64
4:D:39:PHE:CE2	4:D:119:ILE:HG23	2.33	0.64
4:D:417:ASN:C	4:D:419:PRO:HD3	2.22	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:GLU:OE2	2:B:211:ARG:NE	2.31	0.64
4:D:93:GLY:HA3	4:D:109:VAL:O	1.98	0.64
4:D:29:VAL:O	4:D:32:MET:HG3	1.98	0.64
4:D:142:ASN:HA	4:D:145:ASP:OD2	1.97	0.64
4:D:250:ASN:HA	4:D:253:ILE:HD12	1.80	0.63
4:D:232:THR:CB	4:D:266:LEU:HD13	2.28	0.63
1:A:26:GLU:O	1:A:31:GLU:HG2	1.99	0.63
2:B:370:ALA:HA	2:B:373:LEU:HD13	1.80	0.63
4:D:72:ASP:CB	4:D:75:ARG:HB3	2.27	0.63
1:A:78:ILE:O	1:A:82:ARG:NH1	2.32	0.63
1:A:552:SER:OG	1:A:557:MET:SD	2.57	0.63
2:B:40:MET:HE1	2:B:389:ILE:HG12	1.81	0.63
4:D:137:MET:SD	4:D:172:LEU:HG	2.38	0.63
1:A:131:TYR:HD1	1:A:132:LEU:N	1.97	0.63
4:D:253:ILE:HA	4:D:256:LEU:HD12	1.81	0.63
4:D:347:ILE:CG2	4:D:463:VAL:CG2	2.77	0.63
4:D:113:LYS:HG2	4:D:117:ARG:HH21	1.63	0.63
4:D:138:ILE:HA	4:D:172:LEU:HD11	1.79	0.63
4:D:194:ILE:O	4:D:198:LYS:HB2	1.99	0.62
1:A:184:ASN:HB3	1:A:185:ARG:HH11	1.64	0.62
1:A:182:MET:O	1:A:186:GLY:N	2.33	0.62
4:D:232:THR:HB	4:D:266:LEU:HD13	1.81	0.62
1:A:27:ASP:OD1	1:A:35:PHE:HE2	1.83	0.62
4:D:69:SER:O	4:D:75:ARG:HD2	1.99	0.62
4:D:112:ASP:O	4:D:116:ILE:HD12	2.00	0.62
1:A:124:ARG:HA	1:A:150:PHE:CD2	2.35	0.62
3:C:166:VAL:HG13	3:C:167:VAL:HG23	1.80	0.62
1:A:76:PHE:HB3	1:A:109:LEU:HD22	1.81	0.62
4:D:146:THR:OG1	4:D:328:LEU:HD12	1.99	0.61
1:A:73:LYS:HB2	2:B:727:ARG:NH2	2.15	0.61
1:A:178:ILE:HG23	1:A:182:MET:HE2	1.82	0.61
2:B:289:MET:HE2	2:B:437:TRP:HE3	1.65	0.61
4:D:53:GLU:HA	4:D:56:LEU:HB2	1.82	0.61
4:D:91:LYS:HD2	4:D:112:ASP:CA	2.29	0.61
4:D:139:TRP:CZ2	4:D:143:LEU:HD21	2.35	0.61
4:D:95:PRO:CG	4:D:106:ARG:NH2	2.63	0.61
1:A:298:GLU:HA	1:A:488:LYS:HD2	1.82	0.61
5:E:233:U:H1'	5:E:234:C:O4'	2.01	0.61
4:D:139:TRP:O	4:D:143:LEU:HD13	1.99	0.60
1:A:150:PHE:O	1:A:179:ARG:HD2	2.01	0.60
4:D:176:SER:O	4:D:177:GLY:C	2.43	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:754:ARG:NH2	2:B:756:GLN:OE1	2.34	0.60
4:D:40:TYR:CZ	4:D:279:CYS:HA	2.36	0.60
4:D:63:ILE:O	4:D:67:VAL:HG23	2.00	0.60
1:A:183:ALA:HB2	1:A:188:TRP:CD1	2.35	0.60
4:D:338:PHE:CB	4:D:487:TYR:HB3	2.27	0.60
4:D:63:ILE:HA	4:D:66:MET:HE2	1.84	0.60
4:D:184:LYS:HG2	4:D:188:THR:HG21	1.82	0.60
6:F:22:U:C4'	6:F:23:A:H5'	2.32	0.60
4:D:276:LEU:HD21	4:D:303:PRO:HB2	1.84	0.59
4:D:254:GLU:HB3	4:D:258:PHE:CZ	2.37	0.59
4:D:130:THR:HA	4:D:133:LEU:HB2	1.85	0.59
4:D:308:GLN:HG2	4:D:382:ARG:HA	1.82	0.59
4:D:342:ARG:HB2	4:D:479:PHE:HB3	1.85	0.59
4:D:384:ARG:O	4:D:466:LEU:HD12	2.03	0.59
4:D:87:LYS:HA	4:D:87:LYS:CE	2.33	0.59
4:D:146:THR:HG21	4:D:332:ALA:HB2	1.85	0.59
1:A:179:ARG:O	1:A:182:MET:N	2.35	0.59
2:B:623:ARG:NH1	3:C:101:ARG:O	2.35	0.59
2:B:731:GLU:CD	2:B:737:LYS:HD3	2.27	0.59
3:C:119:PHE:O	3:C:123:GLU:HG2	2.03	0.59
2:B:514:VAL:HG11	2:B:558:THR:HG21	1.84	0.59
1:A:27:ASP:OD1	1:A:35:PHE:CE2	2.56	0.59
2:B:34:THR:HG22	2:B:353:LYS:HB3	1.85	0.58
2:B:297:GLU:HG3	2:B:298:LEU:H	1.68	0.58
4:D:425:ILE:CG2	4:D:448:MET:SD	2.91	0.58
4:D:116:ILE:O	4:D:119:ILE:HG22	2.01	0.58
4:D:296:TYR:HD1	4:D:302:ASP:CB	2.16	0.58
4:D:444:ILE:O	4:D:448:MET:HG3	2.02	0.58
1:A:52:HIS:HD2	1:A:76:PHE:HE2	1.51	0.58
4:D:91:LYS:HE3	4:D:110:LEU:HD11	1.85	0.58
4:D:329:VAL:CG2	4:D:379:LEU:HD21	2.26	0.58
1:A:19:LYS:HA	1:A:22:LYS:HD2	1.85	0.58
4:D:159:MET:HE1	4:D:191:MET:HB2	1.84	0.58
4:D:64:GLU:HB3	4:D:136:MET:CE	2.32	0.58
2:B:176:LYS:HD2	2:B:179:MET:HE2	1.85	0.58
4:D:168:GLN:HB2	4:D:272:HIS:CE1	2.38	0.58
2:B:178:GLU:OE1	2:B:211:ARG:NH1	2.37	0.58
2:B:694:ASN:O	2:B:697:GLU:HB3	2.03	0.58
4:D:263:ALA:O	4:D:264:LEU:C	2.44	0.58
1:A:29:LYS:HG2	1:A:30:ILE:CG1	2.29	0.58
2:B:575:GLU:OE2	3:C:71:ASN:ND2	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:735:ILE:HG22	2:B:736:LYS:H	1.68	0.58
1:A:661:GLU:HG3	1:A:690:ILE:HG12	1.85	0.57
2:B:300:PHE:HB3	2:B:484:ILE:HD11	1.85	0.57
4:D:278:ALA:O	4:D:279:CYS:C	2.45	0.57
1:A:179:ARG:O	1:A:180:GLN:C	2.47	0.57
2:B:40:MET:HE2	2:B:392:ILE:HG21	1.86	0.57
4:D:232:THR:OG1	4:D:266:LEU:HD13	2.05	0.57
4:D:37:GLY:CA	4:D:281:TYR:HB3	2.35	0.57
4:D:197:ILE:HG23	4:D:248:PRO:HB2	1.86	0.57
4:D:216:ARG:O	4:D:220:GLU:HG2	2.04	0.57
4:D:263:ALA:O	4:D:266:LEU:N	2.37	0.57
4:D:347:ILE:CG1	4:D:461:ARG:HH12	2.15	0.57
1:A:32:THR:HA	1:A:35:PHE:HB2	1.86	0.57
1:A:51:PHE:CE1	1:A:52:HIS:HE1	2.22	0.57
4:D:91:LYS:CD	4:D:112:ASP:HB3	2.29	0.57
4:D:139:TRP:NE1	4:D:277:PRO:HB3	2.19	0.57
2:B:43:VAL:HG22	2:B:403:LEU:HD12	1.86	0.57
4:D:87:LYS:CD	4:D:110:LEU:HB3	2.34	0.57
4:D:94:GLY:O	4:D:96:ILE:HG23	2.04	0.57
4:D:96:ILE:HD11	4:D:107:GLU:CG	2.34	0.57
4:D:180:GLY:O	4:D:184:LYS:HB2	2.03	0.57
1:A:133:GLU:O	1:A:137:LYS:HG3	2.05	0.57
4:D:87:LYS:CG	4:D:110:LEU:HB3	2.34	0.57
4:D:262:SER:HB2	4:D:444:ILE:HD11	1.87	0.57
4:D:79:LEU:O	4:D:83:PRO:HD3	2.05	0.57
4:D:341:LEU:HD23	4:D:352:VAL:O	2.04	0.57
4:D:461:ARG:HD2	4:D:463:VAL:HB	1.87	0.57
4:D:73:GLU:HA	4:D:76:ASN:HD22	1.69	0.57
4:D:172:LEU:HG	4:D:173:PRO:HD2	1.86	0.57
2:B:287:ARG:HA	2:B:290:MET:HB2	1.86	0.57
3:C:135:PHE:CE1	3:C:240:TRP:HB3	2.40	0.56
2:B:672:ARG:HH22	3:C:81:MET:HE2	1.70	0.56
4:D:120:TRP:CZ2	4:D:129:ALA:HB3	2.41	0.56
4:D:135:HIS:CE1	4:D:276:LEU:H	2.23	0.56
2:B:160:SER:OG	2:B:165:ASP:OD2	2.23	0.56
2:B:746:ILE:HG23	3:C:8:ARG:HD3	1.86	0.56
4:D:226:LEU:O	4:D:229:LYS:HB2	2.06	0.56
4:D:330:TRP:HZ3	4:D:344:LEU:CD1	2.17	0.56
2:B:208:LYS:HG2	2:B:209:LYS:N	2.20	0.56
4:D:22:ALA:HA	4:D:25:ILE:HD12	1.87	0.56
2:B:26:GLY:O	2:B:233:ARG:NH2	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:54:GLY:C	4:D:55:ARG:HD3	2.30	0.56
4:D:33:ILE:HG21	4:D:296:TYR:HD2	1.70	0.56
2:B:723:ARG:HD3	2:B:744:MET:HE1	1.87	0.56
4:D:95:PRO:HB3	4:D:106:ARG:NE	2.21	0.56
4:D:302:ASP:N	4:D:303:PRO:HD2	2.20	0.56
2:B:579:LEU:O	2:B:583:THR:OG1	2.23	0.56
4:D:62:THR:HG23	4:D:94:GLY:HA3	1.87	0.56
4:D:355:ARG:HD2	4:D:487:TYR:OH	2.06	0.56
2:B:315:PRO:HG3	2:B:407:MET:HE2	1.87	0.56
4:D:235:GLN:NE2	4:D:444:ILE:HD13	2.21	0.56
4:D:425:ILE:HG21	4:D:448:MET:SD	2.46	0.56
1:A:124:ARG:HA	1:A:150:PHE:HB2	1.86	0.55
2:B:347:LYS:HE2	2:B:403:LEU:HD22	1.87	0.55
4:D:227:LYS:HB2	4:D:239:MET:HE2	1.88	0.55
3:C:114:VAL:HG21	3:C:198:ILE:HD12	1.88	0.55
3:C:186:THR:O	3:C:190:LYS:HG2	2.06	0.55
2:B:626:ASN:HD22	3:C:99:TRP:HZ2	1.53	0.55
4:D:33:ILE:HG22	4:D:291:PHE:HB3	1.89	0.55
4:D:299:VAL:O	4:D:299:VAL:CG1	2.55	0.55
1:A:523:MET:HG2	1:A:565:VAL:HG12	1.87	0.55
4:D:119:ILE:O	4:D:119:ILE:HD13	2.05	0.55
4:D:272:HIS:CD2	4:D:337:ALA:HB2	2.42	0.55
4:D:329:VAL:HG11	4:D:379:LEU:HD23	1.88	0.55
4:D:235:GLN:O	4:D:238:MET:N	2.40	0.55
1:A:446:PHE:CZ	1:A:589:LEU:HB3	2.42	0.55
4:D:37:GLY:HA2	4:D:281:TYR:HB3	1.88	0.55
4:D:232:THR:CG2	4:D:235:GLN:HG2	2.35	0.55
3:C:108:THR:HG23	3:C:111:TYR:CD1	2.42	0.55
3:C:182:GLN:O	3:C:186:THR:OG1	2.23	0.55
1:A:179:ARG:HA	1:A:182:MET:HB2	1.88	0.54
4:D:38:ARG:HD2	4:D:285:VAL:HG11	1.88	0.54
4:D:95:PRO:CG	4:D:106:ARG:HH21	2.19	0.54
4:D:95:PRO:HG3	4:D:106:ARG:NH2	2.22	0.54
4:D:157:THR:HG23	4:D:194:ILE:HG21	1.89	0.54
4:D:95:PRO:HB3	4:D:106:ARG:NH2	2.22	0.54
4:D:415:GLN:HG3	4:D:454:GLU:HG3	1.89	0.54
6:F:4:A:N6	6:F:5:G:O6	2.41	0.54
4:D:75:ARG:HD3	4:D:76:ASN:N	2.22	0.54
1:A:166:GLU:N	1:A:166:GLU:OE1	2.40	0.54
4:D:146:THR:HG23	4:D:328:LEU:HD11	1.89	0.54
4:D:316:ILE:CG1	4:D:325:LYS:HE2	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:HIS:CD2	1:A:158:LYS:HE3	2.43	0.54
1:A:292:ILE:HG22	1:A:313:THR:HG21	1.89	0.54
4:D:284:ALA:C	4:D:291:PHE:HZ	2.15	0.54
3:C:158:GLU:HA	3:C:161:ASP:HB2	1.90	0.54
4:D:25:ILE:O	4:D:29:VAL:HG23	2.07	0.54
4:D:347:ILE:HG21	4:D:461:ARG:HH12	1.67	0.54
4:D:451:ALA:O	4:D:453:PRO:HD3	2.08	0.54
4:D:113:LYS:HA	4:D:116:ILE:HD13	1.90	0.54
5:E:237:C:H5''	5:E:237:C:H6	1.73	0.54
1:A:45:CYS:SG	1:A:120:ILE:HG21	2.48	0.54
1:A:73:LYS:HB2	2:B:727:ARG:HH21	1.73	0.54
1:A:242:ILE:HG13	2:B:90:GLU:OE1	2.08	0.54
4:D:182:ALA:O	4:D:270:VAL:HG23	2.08	0.54
4:D:232:THR:O	4:D:236:ARG:HG3	2.08	0.54
1:A:67:ASP:HB2	1:A:69:ASN:ND2	2.23	0.53
4:D:153:ALA:HA	4:D:156:ARG:HE	1.72	0.53
4:D:421:ASP:HB3	4:D:424:THR:OG1	2.08	0.53
1:A:134:LYS:NZ	1:A:147:ILE:HB	2.24	0.53
2:B:730:PHE:CD1	2:B:735:ILE:HD12	2.43	0.53
4:D:55:ARG:HH12	4:D:311:GLN:H	1.56	0.53
4:D:190:VAL:O	4:D:194:ILE:HG12	2.09	0.53
4:D:301:ILE:HG23	4:D:305:LYS:HD2	1.89	0.53
4:D:355:ARG:HD2	4:D:487:TYR:CZ	2.44	0.53
6:F:18:U:H3'	6:F:18:U:H6	1.72	0.53
2:B:124:GLN:O	2:B:249:ARG:NH2	2.42	0.53
2:B:578:LYS:HB2	3:C:101:ARG:HD2	1.90	0.53
4:D:205:ASN:O	4:D:206:PHE:C	2.50	0.53
4:D:261:ARG:O	4:D:265:ILE:HG12	2.09	0.53
4:D:338:PHE:HA	4:D:487:TYR:CD2	2.44	0.53
4:D:419:PRO:HG2	4:D:453:PRO:HB2	1.91	0.53
1:A:117:PHE:CA	1:A:143:THR:HB	2.39	0.53
4:D:194:ILE:HG22	4:D:198:LYS:HD3	1.91	0.53
1:A:31:GLU:HG3	1:A:34:LYS:HE3	1.91	0.53
4:D:317:ARG:HD3	4:D:361:ARG:HH21	1.70	0.53
4:D:317:ARG:HB3	4:D:318:PRO:HD2	1.90	0.53
4:D:441:ARG:HG2	4:D:442:ALA:N	2.24	0.53
1:A:1:MET:HG2	1:A:32:THR:HG21	1.90	0.52
4:D:62:THR:O	4:D:65:ARG:HB3	2.08	0.52
1:A:73:LYS:HD3	1:A:112:TYR:CD2	2.44	0.52
1:A:30:ILE:O	1:A:34:LYS:HE2	2.09	0.52
4:D:34:ASN:HD22	4:D:292:GLU:H	1.56	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:118:ARG:O	4:D:122:GLN:HG2	2.09	0.52
1:A:175:LEU:HG	1:A:179:ARG:HD3	1.90	0.52
4:D:419:PRO:HG2	4:D:453:PRO:CB	2.39	0.52
1:A:179:ARG:O	1:A:182:MET:HB2	2.09	0.52
2:B:143:LEU:HD13	2:B:246:MET:HE2	1.90	0.52
4:D:87:LYS:HG3	4:D:110:LEU:HB3	1.92	0.52
4:D:88:ASP:HB3	4:D:110:LEU:CD2	2.35	0.52
4:D:243:ARG:C	4:D:245:SER:N	2.66	0.52
4:D:263:ALA:C	4:D:265:ILE:N	2.59	0.52
1:A:2:GLU:H	1:A:32:THR:HB	1.75	0.52
4:D:61:LEU:HA	4:D:140:HIS:CE1	2.45	0.52
4:D:365:ILE:HG22	4:D:366:ALA:O	2.10	0.52
1:A:392:GLN:HE21	2:B:381:PHE:HD1	1.57	0.52
4:D:113:LYS:HB3	4:D:117:ARG:HE	1.75	0.52
4:D:296:TYR:CD1	4:D:302:ASP:HB3	2.42	0.52
4:D:417:ASN:ND2	4:D:452:LYS:HG3	2.24	0.52
2:B:58:ASN:HD22	2:B:61:THR:H	1.57	0.51
4:D:175:ARG:HD2	4:D:175:ARG:O	2.09	0.51
1:A:117:PHE:HB2	1:A:143:THR:HB	1.92	0.51
2:B:532:ASN:HA	2:B:535:ILE:HG22	1.91	0.51
4:D:355:ARG:HH11	4:D:358:LEU:CD2	2.23	0.51
1:A:3:ASP:OD1	1:A:6:ARG:NH2	2.40	0.51
1:A:122:VAL:HG13	1:A:148:PHE:HB3	1.91	0.51
2:B:718:MET:HE2	3:C:7:LEU:HD12	1.93	0.51
4:D:21:ASN:HA	4:D:24:GLU:OE2	2.09	0.51
4:D:342:ARG:HD3	4:D:416:ARG:HD2	1.93	0.51
4:D:417:ASN:O	4:D:418:LEU:HD13	2.11	0.51
1:A:334:TYR:HB3	1:A:565:VAL:HG21	1.91	0.51
4:D:211:ASN:O	4:D:214:LYS:HG2	2.10	0.51
4:D:258:PHE:HA	4:D:261:ARG:HG3	1.92	0.51
4:D:141:SER:CB	4:D:172:LEU:HD12	2.41	0.51
1:A:147:ILE:HG12	1:A:148:PHE:H	1.75	0.51
4:D:148:TYR:CD1	6:F:22:U:OP1	2.63	0.51
4:D:214:LYS:HB2	5:E:229:U:H5''	1.92	0.51
4:D:347:ILE:HG23	4:D:463:VAL:CG2	2.41	0.51
1:A:302:ILE:HG12	1:A:356:ARG:HH21	1.76	0.51
4:D:316:ILE:CD1	4:D:325:LYS:CD	2.73	0.51
1:A:125:ARG:NH2	1:A:129:ILE:HD11	2.25	0.51
1:A:249:MET:HE2	1:A:253:VAL:HG21	1.93	0.51
1:A:304:LEU:HD13	1:A:348:ILE:HD12	1.93	0.51
4:D:230:PHE:HZ	4:D:239:MET:HG3	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ILE:HG12	1:A:498:THR:HG22	1.93	0.51
1:A:661:GLU:CD	1:A:690:ILE:HA	2.36	0.51
4:D:119:ILE:HD13	4:D:119:ILE:C	2.36	0.51
4:D:297:SER:O	4:D:303:PRO:HD3	2.10	0.51
4:D:341:LEU:HD12	4:D:341:LEU:H	1.76	0.51
1:A:635:LYS:O	1:A:639:THR:HG23	2.11	0.50
4:D:35:GLY:HA2	4:D:38:ARG:NH1	2.26	0.50
4:D:96:ILE:CD1	4:D:107:GLU:CG	2.89	0.50
4:D:39:PHE:HD2	4:D:120:TRP:HA	1.76	0.50
4:D:218:ALA:O	4:D:219:TYR:C	2.54	0.50
4:D:304:PHE:CE2	4:D:463:VAL:HG23	2.46	0.50
6:F:4:A:C5	6:F:5:G:C6	2.99	0.50
1:A:53:PHE:HD1	1:A:63:VAL:HG21	1.76	0.50
4:D:455:GLU:HB2	4:D:456:VAL:HG22	1.93	0.50
6:F:13:G:H5'	6:F:13:G:C8	2.40	0.50
2:B:219:ILE:O	2:B:223:THR:OG1	2.27	0.50
4:D:32:MET:O	4:D:36:ILE:HG12	2.12	0.50
4:D:166:LEU:HD12	4:D:187:GLY:H	1.77	0.50
4:D:247:ASN:N	4:D:248:PRO:HD3	2.27	0.50
4:D:337:ALA:O	4:D:338:PHE:C	2.53	0.50
1:A:457:GLU:OE2	1:A:501:TYR:OH	2.24	0.50
4:D:193:LEU:HA	4:D:196:MET:SD	2.52	0.50
4:D:83:PRO:HG3	4:D:89:PRO:HG3	1.93	0.50
4:D:250:ASN:O	4:D:253:ILE:HB	2.10	0.50
1:A:36:ALA:HA	1:A:39:CYS:SG	2.51	0.50
4:D:221:ARG:CZ	4:D:221:ARG:HB3	2.41	0.50
4:D:224:ASN:HA	4:D:227:LYS:HZ1	1.75	0.50
4:D:243:ARG:C	4:D:245:SER:H	2.20	0.50
4:D:355:ARG:NH1	4:D:358:LEU:HB2	2.26	0.50
1:A:184:ASN:HB3	1:A:185:ARG:NH1	2.26	0.50
4:D:137:MET:HE2	4:D:175:ARG:NH2	2.27	0.50
4:D:228:GLY:HA2	4:D:236:ARG:NH2	2.27	0.50
4:D:417:ASN:CB	4:D:419:PRO:HD3	2.42	0.50
1:A:165:GLU:CG	1:A:165:GLU:O	2.61	0.49
2:B:574:PHE:CE1	2:B:578:LYS:HE2	2.48	0.49
4:D:21:ASN:O	4:D:24:GLU:CG	2.56	0.49
4:D:100:VAL:HG13	4:D:101:ASP:N	2.24	0.49
4:D:464:PHE:CD2	4:D:471:ALA:HA	2.46	0.49
5:E:233:U:H1'	5:E:234:C:C1'	2.42	0.49
2:B:284:ASN:O	2:B:288:LYS:HG3	2.12	0.49
3:C:189:LYS:O	3:C:193:LEU:HB2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:PHE:C	1:A:175:LEU:HD21	2.37	0.49
4:D:65:ARG:NH2	6:F:20:U:H1'	2.27	0.49
4:D:212:GLY:HA2	4:D:215:THR:OG1	2.12	0.49
4:D:326:SER:OG	4:D:380:GLU:HB2	2.13	0.49
1:A:260:PHE:CZ	1:A:265:PRO:HG3	2.47	0.49
4:D:441:ARG:H	4:D:441:ARG:HD3	1.76	0.49
4:D:185:GLY:O	4:D:186:VAL:C	2.54	0.49
4:D:283:PRO:O	4:D:287:SER:HB2	2.12	0.49
4:D:99:ARG:HG3	4:D:104:TRP:CD1	2.47	0.49
1:A:116:ARG:HB3	1:A:143:THR:HA	1.95	0.49
4:D:113:LYS:HA	4:D:116:ILE:CD1	2.41	0.49
4:D:205:ASN:C	4:D:207:TRP:N	2.68	0.49
4:D:384:ARG:C	4:D:466:LEU:HD12	2.37	0.49
4:D:88:ASP:H	4:D:110:LEU:HD22	1.77	0.49
4:D:147:THR:HB	6:F:22:U:N3	2.27	0.49
4:D:167:MET:HG2	4:D:187:GLY:HA3	1.94	0.49
1:A:75:ARG:O	1:A:111:ASP:HA	2.12	0.49
1:A:345:LEU:HD23	1:A:348:ILE:HD11	1.94	0.49
1:A:551:ARG:NH1	1:A:556:GLN:HB3	2.28	0.49
4:D:196:MET:CE	4:D:222:MET:SD	3.01	0.49
4:D:281:TYR:O	4:D:285:VAL:HG23	2.12	0.49
4:D:417:ASN:CG	4:D:453:PRO:HD2	2.38	0.49
1:A:26:GLU:CD	1:A:27:ASP:H	2.21	0.49
4:D:263:ALA:C	4:D:266:LEU:H	2.20	0.49
4:D:341:LEU:HD12	4:D:341:LEU:N	2.28	0.49
4:D:343:LEU:O	4:D:347:ILE:HG12	2.13	0.49
1:A:174:ARG:O	1:A:178:ILE:HG12	2.13	0.48
1:A:86:MET:HE3	2:B:720:SER:HB3	1.95	0.48
4:D:80:GLU:O	4:D:81:GLU:C	2.56	0.48
2:B:593:ASP:OD2	2:B:620:TYR:OH	2.30	0.48
4:D:120:TRP:HZ2	4:D:129:ALA:HB3	1.78	0.48
4:D:242:VAL:HG23	4:D:252:GLU:OE2	2.12	0.48
6:F:18:U:C3'	6:F:18:U:C6	2.96	0.48
1:A:482:LEU:HD12	1:A:505:ILE:HG12	1.94	0.48
4:D:214:LYS:HG3	5:E:229:U:H4'	1.96	0.48
1:A:124:ARG:HG2	1:A:189:ASP:OD1	2.14	0.48
1:A:134:LYS:HE2	1:A:134:LYS:HB3	1.48	0.48
2:B:151:ARG:HD2	2:B:156:THR:HG22	1.94	0.48
2:B:552:ILE:HG13	2:B:597:ASN:ND2	2.28	0.48
4:D:41:ILE:HD11	4:D:286:ALA:N	2.28	0.48
4:D:92:THR:HG22	4:D:113:LYS:CE	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:100:VAL:HG12	4:D:103:LYS:O	2.14	0.48
1:A:169:ALA:O	1:A:173:THR:HG23	2.12	0.48
1:A:128:HIS:HA	1:A:131:TYR:CE2	2.48	0.48
4:D:185:GLY:HA2	4:D:270:VAL:HG11	1.95	0.48
4:D:235:GLN:O	4:D:236:ARG:C	2.56	0.48
4:D:261:ARG:O	4:D:264:LEU:HB3	2.14	0.48
4:D:258:PHE:O	4:D:261:ARG:N	2.46	0.48
4:D:289:TYR:CE2	4:D:291:PHE:HA	2.48	0.48
4:D:338:PHE:HA	4:D:487:TYR:CB	2.44	0.48
1:A:125:ARG:HH22	1:A:129:ILE:HD11	1.78	0.47
2:B:739:GLU:O	2:B:743:ILE:HG12	2.14	0.47
4:D:152:ARG:O	4:D:153:ALA:C	2.56	0.47
4:D:155:VAL:O	4:D:156:ARG:C	2.57	0.47
4:D:329:VAL:HG11	4:D:379:LEU:HD21	1.94	0.47
4:D:331:MET:SD	4:D:336:ALA:HB3	2.54	0.47
4:D:355:ARG:HH11	4:D:358:LEU:HD23	1.79	0.47
4:D:417:ASN:OD1	4:D:453:PRO:HD2	2.14	0.47
4:D:421:ASP:HB3	4:D:424:THR:HG1	1.77	0.47
1:A:95:CYS:SG	1:A:102:LYS:HB3	2.55	0.47
4:D:232:THR:HG22	4:D:235:GLN:H	1.78	0.47
1:A:48:TYR:CZ	1:A:163:LEU:HD21	2.49	0.47
1:A:139:LYS:O	1:A:140:SER:C	2.57	0.47
1:A:203:GLU:OE2	2:B:162:ARG:NH2	2.29	0.47
4:D:159:MET:HE2	4:D:159:MET:HB2	1.74	0.47
4:D:301:ILE:HD13	4:D:469:GLU:HG3	1.96	0.47
4:D:327:GLN:C	4:D:327:GLN:CD	2.81	0.47
4:D:366:ALA:CB	6:F:21:U:H3	2.27	0.47
1:A:632:SER:OG	1:A:633:ILE:N	2.47	0.47
4:D:78:TYR:O	4:D:81:GLU:HB3	2.14	0.47
4:D:79:LEU:O	4:D:80:GLU:C	2.57	0.47
4:D:347:ILE:CG2	4:D:461:ARG:NH1	2.65	0.47
4:D:417:ASN:HB2	4:D:419:PRO:CD	2.44	0.47
4:D:421:ASP:O	4:D:425:ILE:HG12	2.14	0.47
1:A:309:LYS:O	1:A:313:THR:HG23	2.15	0.47
4:D:273:LYS:HE3	4:D:273:LYS:HB3	1.45	0.47
1:A:376:PRO:HB2	2:B:365:ARG:HG2	1.97	0.47
4:D:34:ASN:ND2	4:D:292:GLU:H	2.12	0.47
4:D:117:ARG:HB3	4:D:121:ARG:CZ	2.44	0.47
4:D:304:PHE:CZ	4:D:463:VAL:HG23	2.50	0.47
4:D:134:THR:O	4:D:138:ILE:HG13	2.14	0.47
4:D:345:SER:O	4:D:348:ARG:O	2.33	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:355:ARG:NH1	4:D:358:LEU:HD23	2.30	0.47
1:A:375:ALA:HB2	6:F:10:A:H3'	1.97	0.47
4:D:138:ILE:HD11	4:D:179:ALA:HB1	1.96	0.47
4:D:139:TRP:CH2	4:D:143:LEU:HD21	2.50	0.47
4:D:162:ARG:HH22	4:D:261:ARG:HG2	1.80	0.47
2:B:289:MET:HE2	2:B:437:TRP:CE3	2.47	0.46
2:B:674:ILE:O	2:B:677:THR:OG1	2.32	0.46
4:D:477:PRO:HG2	4:D:479:PHE:CZ	2.50	0.46
1:A:77:GLU:O	1:A:109:LEU:HD23	2.15	0.46
2:B:208:LYS:CG	2:B:209:LYS:H	2.26	0.46
2:B:438:TRP:HA	2:B:450:ILE:O	2.15	0.46
2:B:578:LYS:CB	3:C:101:ARG:HD2	2.45	0.46
4:D:159:MET:O	4:D:160:ASP:HB2	2.15	0.46
4:D:193:LEU:HD11	4:D:222:MET:HB3	1.98	0.46
4:D:234:ALA:HB3	4:D:235:GLN:HE21	1.80	0.46
4:D:276:LEU:HD21	4:D:303:PRO:CB	2.44	0.46
4:D:163:MET:HB2	4:D:488:PHE:HE1	1.80	0.46
4:D:214:LYS:HG2	4:D:215:THR:N	2.30	0.46
4:D:229:LYS:HZ2	4:D:270:VAL:HB	1.80	0.46
4:D:353:SER:CB	4:D:358:LEU:HD11	2.46	0.46
1:A:131:TYR:CD1	1:A:132:LEU:N	2.80	0.46
2:B:741:SER:O	2:B:745:LYS:HG2	2.16	0.46
4:D:272:HIS:HD2	4:D:337:ALA:CB	2.28	0.46
1:A:340:GLN:NE2	1:A:344:GLU:OE2	2.47	0.46
3:C:36:SER:O	3:C:36:SER:OG	2.30	0.46
4:D:308:GLN:CD	4:D:382:ARG:HG2	2.40	0.46
4:D:312:VAL:HG11	4:D:381:LEU:HD12	1.97	0.46
4:D:346:PHE:O	4:D:347:ILE:C	2.56	0.46
1:A:439:ALA:HB2	2:B:541:PRO:HB2	1.98	0.46
3:C:102:ASN:OD1	3:C:102:ASN:N	2.48	0.46
3:C:147:ILE:HD13	3:C:216:ARG:HG3	1.97	0.46
4:D:33:ILE:HG21	4:D:296:TYR:CD2	2.50	0.46
4:D:37:GLY:HA3	4:D:285:VAL:CG2	2.46	0.46
4:D:139:TRP:HB2	4:D:275:CYS:HB3	1.97	0.46
4:D:465:GLU:O	4:D:468:ASP:N	2.48	0.46
1:A:54:ILE:CG2	1:A:73:LYS:HD2	2.46	0.46
1:A:117:PHE:HB2	1:A:143:THR:HG21	1.98	0.46
1:A:118:ILE:HA	1:A:144:HIS:O	2.16	0.46
1:A:541:CYS:O	1:A:565:VAL:HG22	2.16	0.46
2:B:278:LYS:HD3	2:B:492:PHE:HE2	1.81	0.46
4:D:139:TRP:CE3	4:D:143:LEU:HD11	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:O	1:A:179:ARG:HD3	2.16	0.46
2:B:728:ILE:O	2:B:732:SER:HB3	2.16	0.46
4:D:113:LYS:HG2	4:D:117:ARG:NH2	2.31	0.46
4:D:113:LYS:C	4:D:117:ARG:HE	2.25	0.46
1:A:529:ASP:OD2	1:A:531:ARG:NH2	2.46	0.45
3:C:113:LYS:HA	3:C:113:LYS:HD3	1.78	0.45
4:D:41:ILE:O	4:D:45:THR:HG23	2.16	0.45
4:D:188:THR:O	4:D:192:GLU:HG2	2.15	0.45
4:D:232:THR:O	4:D:233:ALA:C	2.58	0.45
4:D:316:ILE:CG1	4:D:325:LYS:HD2	2.33	0.45
4:D:130:THR:HA	4:D:133:LEU:HD12	1.99	0.45
1:A:184:ASN:C	1:A:185:ARG:HD2	2.42	0.45
3:C:60:ASP:O	3:C:63:ILE:HG12	2.16	0.45
3:C:225:SER:O	3:C:229:ILE:HG12	2.17	0.45
4:D:117:ARG:HB3	4:D:121:ARG:NH2	2.31	0.45
1:A:179:ARG:HB3	1:A:188:TRP:CE3	2.51	0.45
2:B:381:PHE:HB3	2:B:385:THR:HB	1.98	0.45
2:B:572:ARG:O	2:B:576:LEU:HG	2.16	0.45
3:C:79:SER:OG	3:C:80:LYS:N	2.48	0.45
3:C:150:GLY:HA3	3:C:213:ARG:CZ	2.47	0.45
4:D:44:CYS:O	4:D:45:THR:C	2.59	0.45
4:D:222:MET:O	4:D:223:CYS:C	2.58	0.45
4:D:268:GLY:O	4:D:269:SER:C	2.59	0.45
2:B:442:GLN:HE21	2:B:442:GLN:HB3	1.54	0.45
4:D:113:LYS:CB	4:D:117:ARG:HH21	2.30	0.45
4:D:137:MET:SD	4:D:137:MET:C	2.99	0.45
4:D:139:TRP:CG	4:D:140:HIS:N	2.85	0.45
4:D:147:THR:HB	6:F:22:U:H3	1.80	0.45
4:D:157:THR:HG21	4:D:159:MET:HE2	1.97	0.45
4:D:345:SER:HB3	4:D:352:VAL:H	1.82	0.45
1:A:76:PHE:CB	1:A:109:LEU:HD22	2.45	0.45
3:C:87:ASP:OD1	3:C:87:ASP:N	2.41	0.45
4:D:52:TYR:CD1	4:D:56:LEU:HG	2.52	0.45
4:D:291:PHE:CD1	4:D:291:PHE:N	2.83	0.45
1:A:215:ALA:HB1	1:A:226:LEU:HD22	1.99	0.45
1:A:288:LEU:HD23	1:A:561:MET:HE3	1.98	0.45
4:D:58:GLN:HB2	4:D:97:TYR:CE1	2.51	0.45
1:A:117:PHE:CB	1:A:143:THR:HB	2.47	0.45
4:D:87:LYS:HD3	4:D:110:LEU:HD23	1.99	0.45
4:D:358:LEU:HD12	4:D:358:LEU:HA	1.78	0.45
4:D:418:LEU:N	4:D:418:LEU:HD22	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:18:U:H3'	6:F:18:U:C6	2.52	0.45
1:A:88:TRP:HA	1:A:91:VAL:HG12	1.99	0.45
1:A:296:SER:OG	1:A:297:HIS:N	2.50	0.45
4:D:146:THR:HG23	4:D:328:LEU:CD1	2.46	0.45
4:D:328:LEU:HD13	4:D:355:ARG:NH2	2.32	0.45
4:D:79:LEU:HG	4:D:80:GLU:N	2.27	0.44
4:D:272:HIS:CD2	4:D:337:ALA:CB	3.00	0.44
1:A:124:ARG:O	1:A:150:PHE:HB2	2.17	0.44
2:B:519:GLU:OE2	2:B:572:ARG:NH1	2.44	0.44
4:D:91:LYS:HD2	4:D:112:ASP:N	2.32	0.44
4:D:148:TYR:CG	4:D:149:GLN:N	2.85	0.44
4:D:180:GLY:CA	4:D:184:LYS:HD2	2.48	0.44
4:D:347:ILE:HG23	4:D:463:VAL:CG1	2.46	0.44
1:A:60:SER:H	1:A:75:ARG:CZ	2.31	0.44
4:D:95:PRO:CB	4:D:106:ARG:NH2	2.80	0.44
4:D:136:MET:C	4:D:139:TRP:HB3	2.42	0.44
4:D:188:THR:HA	4:D:191:MET:HE3	1.99	0.44
2:B:344:PHE:CD2	2:B:407:MET:HE1	2.53	0.44
2:B:733:GLY:O	2:B:735:ILE:N	2.49	0.44
1:A:51:PHE:CE1	1:A:52:HIS:CE1	3.04	0.44
1:A:249:MET:HE3	2:B:74:PRO:HG2	2.00	0.44
4:D:155:VAL:O	4:D:158:GLY:N	2.49	0.44
4:D:205:ASN:HA	4:D:208:ARG:HB2	1.99	0.44
4:D:417:ASN:HB3	4:D:453:PRO:C	2.37	0.44
4:D:227:LYS:NZ	4:D:243:ARG:HH12	2.15	0.44
1:A:327:GLU:H	1:A:327:GLU:HG3	1.52	0.44
4:D:58:GLN:HE21	4:D:58:GLN:HB3	1.70	0.44
4:D:239:MET:HE2	4:D:239:MET:HB3	1.65	0.44
1:A:596:ILE:HG12	1:A:611:PHE:HD2	1.82	0.44
4:D:119:ILE:CG2	4:D:120:TRP:N	2.80	0.44
4:D:130:THR:CA	4:D:133:LEU:HB2	2.48	0.44
4:D:229:LYS:HA	4:D:229:LYS:HD3	1.52	0.44
4:D:285:VAL:HG22	4:D:291:PHE:CE1	2.53	0.44
1:A:75:ARG:HH21	1:A:163:LEU:HD13	1.81	0.44
4:D:176:SER:HB3	4:D:179:ALA:HB3	2.00	0.44
4:D:343:LEU:O	4:D:346:PHE:HB3	2.18	0.44
4:D:346:PHE:CZ	4:D:385:TYR:CE2	3.05	0.43
4:D:347:ILE:HG23	4:D:463:VAL:HG11	2.00	0.43
1:A:549:LEU:HD11	1:A:556:GLN:HB2	2.00	0.43
2:B:521:ALA:O	2:B:525:ILE:HG12	2.18	0.43
2:B:727:ARG:HA	2:B:727:ARG:HD3	1.88	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:81:GLU:HG3	4:D:82:HIS:CE1	2.53	0.43
4:D:91:LYS:HD2	4:D:112:ASP:HA	1.90	0.43
4:D:119:ILE:HG23	4:D:120:TRP:N	2.32	0.43
1:A:74:HIS:HE2	1:A:77:GLU:HA	1.82	0.43
1:A:374:MET:HE3	1:A:374:MET:HB3	1.59	0.43
1:A:403:LEU:HD12	1:A:404:SER:H	1.83	0.43
2:B:683:LEU:O	2:B:686:GLU:HG2	2.18	0.43
4:D:342:ARG:HD3	4:D:416:ARG:HG3	2.00	0.43
1:A:413:LYS:HD3	1:A:454:ARG:HH12	1.82	0.43
1:A:589:LEU:HD22	2:B:546:MET:SD	2.59	0.43
4:D:49:LEU:HB3	4:D:53:GLU:HB2	2.00	0.43
4:D:91:LYS:HB2	4:D:110:LEU:HD13	2.00	0.43
4:D:113:LYS:CD	4:D:117:ARG:HH21	2.31	0.43
4:D:301:ILE:HG12	4:D:305:LYS:HG3	2.00	0.43
1:A:73:LYS:HG3	2:B:727:ARG:CZ	2.49	0.43
1:A:433:ALA:H	1:A:436:GLU:HG3	1.83	0.43
2:B:522:ASP:OD2	2:B:559:TYR:OH	2.29	0.43
4:D:34:ASN:CB	4:D:291:PHE:HB2	2.49	0.43
4:D:46:GLU:O	4:D:47:LEU:C	2.62	0.43
1:A:67:ASP:OD1	1:A:67:ASP:N	2.52	0.43
4:D:418:LEU:N	4:D:419:PRO:CD	2.72	0.43
5:E:234:C:O2	6:F:16:G:N1	2.49	0.43
2:B:163:LEU:O	2:B:167:LEU:HG	2.19	0.43
4:D:142:ASN:O	4:D:145:ASP:HB2	2.18	0.43
4:D:301:ILE:HG12	4:D:301:ILE:O	2.18	0.43
4:D:339:GLU:CD	4:D:340:ASP:H	2.26	0.43
4:D:379:LEU:HD12	4:D:379:LEU:HA	1.81	0.43
1:A:591:GLN:HG3	1:A:595:MET:HE3	2.00	0.43
4:D:50:SER:H	4:D:53:GLU:CD	2.27	0.43
4:D:196:MET:HE1	4:D:222:MET:SD	2.58	0.43
2:B:535:ILE:HD11	3:C:232:LEU:HD23	2.00	0.43
4:D:324:HIS:HB3	4:D:358:LEU:HG	1.99	0.43
6:F:4:A:N7	6:F:5:G:C6	2.87	0.43
6:F:21:U:O2'	6:F:22:U:O5'	2.36	0.43
1:A:543:LEU:HD12	1:A:563:LEU:HD23	2.00	0.43
1:A:686:LEU:O	1:A:690:ILE:HG13	2.18	0.43
2:B:545:GLN:O	2:B:549:GLN:HG3	2.19	0.43
1:A:78:ILE:HG23	1:A:80:GLU:HG3	2.01	0.42
1:A:178:ILE:CG2	1:A:182:MET:HE2	2.49	0.42
4:D:39:PHE:CD2	4:D:120:TRP:HA	2.53	0.42
4:D:68:LEU:O	4:D:69:SER:C	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:235:A:O2'	5:E:236:C:OP1	2.34	0.42
1:A:547:ASP:OD1	1:A:547:ASP:N	2.47	0.42
4:D:176:SER:C	4:D:178:ALA:N	2.75	0.42
1:A:28:LEU:H	1:A:28:LEU:HG	1.47	0.42
2:B:750:ILE:HD13	2:B:750:ILE:HA	1.77	0.42
4:D:130:THR:O	4:D:133:LEU:HB2	2.19	0.42
4:D:302:ASP:N	4:D:303:PRO:CD	2.82	0.42
2:B:131:TRP:HB2	2:B:220:ARG:HG2	2.01	0.42
3:C:118:TYR:O	3:C:122:VAL:HG23	2.18	0.42
3:C:208:GLU:O	3:C:212:VAL:HG12	2.19	0.42
4:D:159:MET:O	4:D:160:ASP:CB	2.67	0.42
1:A:75:ARG:HD2	1:A:113:LYS:HB2	2.02	0.42
4:D:39:PHE:CE2	4:D:120:TRP:HE3	2.38	0.42
4:D:88:ASP:OD1	4:D:91:LYS:HB2	2.19	0.42
4:D:135:HIS:O	4:D:138:ILE:HB	2.18	0.42
4:D:283:PRO:O	4:D:284:ALA:C	2.62	0.42
1:A:550:LEU:HD12	1:A:557:MET:HE2	2.01	0.42
3:C:60:ASP:OD1	3:C:61:LYS:N	2.52	0.42
4:D:139:TRP:HE3	4:D:275:CYS:HB2	1.85	0.42
4:D:205:ASN:O	4:D:207:TRP:N	2.52	0.42
1:A:51:PHE:CE1	1:A:62:VAL:HG12	2.55	0.42
1:A:64:GLU:HG2	1:A:67:ASP:CG	2.45	0.42
1:A:149:SER:OG	1:A:153:GLU:N	2.53	0.42
1:A:187:LEU:HD12	1:A:190:SER:HB2	2.02	0.42
4:D:232:THR:HG22	4:D:235:GLN:HG2	2.02	0.42
4:D:272:HIS:HD2	4:D:337:ALA:HB2	1.82	0.42
1:A:635:LYS:HD2	1:A:635:LYS:HA	1.80	0.42
1:A:688:GLU:O	1:A:692:GLU:HG3	2.20	0.42
4:D:269:SER:O	4:D:270:VAL:C	2.63	0.42
4:D:276:LEU:HD11	4:D:303:PRO:HB3	2.01	0.42
4:D:422:LYS:HZ3	4:D:422:LYS:HG3	1.66	0.42
1:A:365:GLN:HG2	1:A:366:LEU:N	2.35	0.42
2:B:722:ALA:HB1	3:C:4:ILE:HD11	2.01	0.42
3:C:225:SER:HB2	3:C:228:TYR:HD2	1.85	0.42
4:D:80:GLU:O	4:D:81:GLU:O	2.38	0.42
4:D:283:PRO:HA	4:D:286:ALA:HB3	2.02	0.42
4:D:289:TYR:HE2	4:D:291:PHE:HA	1.85	0.42
1:A:187:LEU:H	1:A:187:LEU:HG	1.66	0.41
2:B:344:PHE:HD1	2:B:344:PHE:HA	1.78	0.41
4:D:37:GLY:HA3	4:D:285:VAL:HG21	2.01	0.41
4:D:52:TYR:CE1	4:D:313:TYR:CG	3.08	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:163:MET:SD	4:D:163:MET:N	2.93	0.41
4:D:329:VAL:CG1	4:D:381:LEU:HD21	2.50	0.41
4:D:341:LEU:HA	4:D:344:LEU:HB2	2.01	0.41
1:A:207:ILE:HG23	1:A:211:MET:HB3	2.00	0.41
1:A:367:LYS:HE2	1:A:367:LYS:HB2	1.92	0.41
3:C:192:GLU:HG3	3:C:193:LEU:HD12	2.02	0.41
4:D:154:LEU:HD12	4:D:160:ASP:O	2.19	0.41
4:D:189:MET:HB3	4:D:226:LEU:HG	2.01	0.41
4:D:232:THR:OG1	4:D:266:LEU:CD1	2.67	0.41
6:F:18:U:H6	6:F:18:U:C3'	2.32	0.41
1:A:31:GLU:O	1:A:35:PHE:N	2.26	0.41
1:A:54:ILE:HG22	1:A:73:LYS:HD2	2.03	0.41
1:A:117:PHE:HB2	1:A:143:THR:CG2	2.50	0.41
1:A:361:LYS:HG3	1:A:363:THR:HG23	2.01	0.41
4:D:257:ILE:HG12	4:D:257:ILE:H	1.39	0.41
1:A:149:SER:CB	1:A:153:GLU:HG3	2.51	0.41
2:B:29:PRO:HD2	2:B:232:GLU:O	2.21	0.41
2:B:354:GLY:HA3	2:B:368:ILE:O	2.20	0.41
4:D:103:LYS:HE3	4:D:105:MET:SD	2.61	0.41
4:D:267:ARG:CZ	4:D:454:GLU:HB2	2.50	0.41
4:D:308:GLN:HE21	4:D:308:GLN:HB3	1.50	0.41
6:F:22:U:H6	6:F:22:U:P	2.43	0.41
1:A:676:LEU:HD13	2:B:486:ARG:HB3	2.02	0.41
2:B:579:LEU:HG	2:B:589:LEU:HD21	2.03	0.41
2:B:716:GLU:HG3	2:B:754:ARG:HH12	1.84	0.41
4:D:258:PHE:O	4:D:259:SER:C	2.62	0.41
4:D:331:MET:HE2	4:D:331:MET:HB2	1.71	0.41
4:D:384:ARG:HD2	4:D:384:ARG:HA	1.75	0.41
1:A:157:THR:O	1:A:158:LYS:HG2	2.20	0.41
1:A:219:LEU:HD21	1:A:226:LEU:HD13	2.01	0.41
1:A:327:GLU:CD	1:A:328:ARG:HG3	2.45	0.41
3:C:154:LEU:HB2	3:C:158:GLU:CG	2.49	0.41
4:D:119:ILE:O	4:D:120:TRP:C	2.62	0.41
1:A:256:LYS:HA	2:B:460:GLN:NE2	2.35	0.41
4:D:96:ILE:HG13	4:D:107:GLU:HG2	2.03	0.41
1:A:94:ILE:HD12	1:A:94:ILE:HA	1.70	0.41
1:A:619:TRP:CD1	2:B:11:LYS:HD3	2.56	0.41
2:B:554:ASP:OD2	2:B:555:TYR:N	2.54	0.41
4:D:157:THR:HG22	4:D:159:MET:N	2.29	0.41
1:A:165:GLU:CG	1:A:168:ARG:CG	2.63	0.41
1:A:437:TYR:HA	1:A:440:SER:OG	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:72:GLU:CD	3:C:101:ARG:HH22	2.28	0.41
4:D:100:VAL:CG1	4:D:101:ASP:H	2.29	0.41
4:D:168:GLN:HG2	4:D:337:ALA:HB2	2.03	0.41
4:D:238:MET:HA	4:D:241:GLN:NE2	2.35	0.41
6:F:23:A:H4'	6:F:24:U:OP1	2.17	0.41
1:A:53:PHE:CE2	1:A:72:LEU:HA	2.55	0.41
1:A:661:GLU:OE2	1:A:690:ILE:HA	2.20	0.41
2:B:689:TYR:HD1	3:C:31:ILE:HD12	1.86	0.41
3:C:108:THR:HG23	3:C:111:TYR:HD1	1.84	0.41
4:D:285:VAL:HG22	4:D:291:PHE:CZ	2.56	0.41
1:A:250:SER:O	1:A:253:VAL:HG22	2.21	0.40
2:B:287:ARG:HA	2:B:290:MET:CB	2.51	0.40
2:B:507:MET:HE2	2:B:507:MET:HB3	1.97	0.40
4:D:51:ASP:O	4:D:52:TYR:C	2.64	0.40
1:A:666:LEU:HD12	1:A:666:LEU:HA	1.96	0.40
2:B:155:LEU:HB3	2:B:169:ASP:OD1	2.22	0.40
4:D:163:MET:HB2	4:D:488:PHE:CE1	2.56	0.40
4:D:164:CYS:SG	4:D:166:LEU:HG	2.62	0.40
4:D:235:GLN:HE22	4:D:444:ILE:HB	1.87	0.40
4:D:277:PRO:HG2	4:D:280:VAL:HG23	2.03	0.40
1:A:443:ARG:HG2	2:B:546:MET:HE3	2.03	0.40
2:B:541:PRO:O	2:B:545:GLN:HG3	2.21	0.40
4:D:33:ILE:HD13	4:D:296:TYR:H	1.85	0.40
4:D:61:LEU:HB2	4:D:140:HIS:NE2	2.37	0.40
4:D:229:LYS:O	4:D:269:SER:N	2.39	0.40
4:D:238:MET:HA	4:D:241:GLN:CD	2.46	0.40
4:D:267:ARG:HH11	4:D:454:GLU:HB2	1.78	0.40
4:D:312:VAL:HG11	4:D:381:LEU:CD1	2.51	0.40
1:A:47:MET:HG2	1:A:170:ARG:NH1	2.37	0.40
1:A:213:ARG:NH2	2:B:60:GLU:OE2	2.55	0.40
1:A:425:LEU:HB3	2:B:549:GLN:OE1	2.21	0.40
2:B:333:PHE:O	2:B:336:ILE:HG22	2.21	0.40
4:D:87:LYS:HZ2	4:D:87:LYS:CA	2.33	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	701/716 (98%)	641 (91%)	59 (8%)	1 (0%)	48	78
2	B	732/757 (97%)	681 (93%)	51 (7%)	0	100	100
3	C	245/759 (32%)	226 (92%)	19 (8%)	0	100	100
4	D	428/498 (86%)	376 (88%)	48 (11%)	4 (1%)	14	45
All	All	2106/2730 (77%)	1924 (91%)	177 (8%)	5 (0%)	44	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	81	GLU
4	D	464	PHE
4	D	48	LYS
1	A	26	GLU
4	D	419	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	633/643 (98%)	604 (95%)	29 (5%)	24	57
2	B	649/670 (97%)	641 (99%)	8 (1%)	63	82
3	C	224/673 (33%)	222 (99%)	2 (1%)	70	85
4	D	368/418 (88%)	260 (71%)	108 (29%)	0	2
All	All	1874/2404 (78%)	1727 (92%)	147 (8%)	14	37

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	28	LEU
1	A	30	ILE
1	A	48	TYR
1	A	66	ASP
1	A	73	LYS
1	A	77	GLU
1	A	84	ARG
1	A	94	ILE
1	A	102	LYS
1	A	125	ARG
1	A	131	TYR
1	A	133	GLU
1	A	138	ILE
1	A	140	SER
1	A	141	GLU
1	A	143	THR
1	A	148	PHE
1	A	179	ARG
1	A	182	MET
1	A	187	LEU
1	A	211	MET
1	A	212	ARG
1	A	327	GLU
1	A	361	LYS
1	A	374	MET
1	A	440	SER
1	A	499	ASN
1	A	548	MET
2	B	289	MET
2	B	442	GLN
2	B	444	SER
2	B	445	ASP
2	B	570	THR
2	B	571	ARG
2	B	727	ARG
2	B	750	ILE
3	C	38	ARG
3	C	135	PHE
4	D	33	ILE
4	D	38	ARG
4	D	41	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	51	ASP
4	D	55	ARG
4	D	58	GLN
4	D	60	SER
4	D	61	LEU
4	D	62	THR
4	D	66	MET
4	D	69	SER
4	D	73	GLU
4	D	74	ARG
4	D	75	ARG
4	D	78	TYR
4	D	79	LEU
4	D	81	GLU
4	D	82	HIS
4	D	87	LYS
4	D	88	ASP
4	D	98	LYS
4	D	99	ARG
4	D	101	ASP
4	D	103	LYS
4	D	107	GLU
4	D	112	ASP
4	D	113	LYS
4	D	115	GLU
4	D	117	ARG
4	D	119	ILE
4	D	125	ASN
4	D	127	ASP
4	D	136	MET
4	D	138	ILE
4	D	150	ARG
4	D	154	LEU
4	D	156	ARG
4	D	157	THR
4	D	162	ARG
4	D	163	MET
4	D	166	LEU
4	D	168	GLN
4	D	172	LEU
4	D	174	ARG
4	D	175	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	183	VAL
4	D	184	LYS
4	D	189	MET
4	D	191	MET
4	D	193	LEU
4	D	198	LYS
4	D	199	ARG
4	D	213	ARG
4	D	214	LYS
4	D	220	GLU
4	D	221	ARG
4	D	225	ILE
4	D	226	LEU
4	D	227	LYS
4	D	229	LYS
4	D	232	THR
4	D	235	GLN
4	D	238	MET
4	D	239	MET
4	D	242	VAL
4	D	244	GLU
4	D	246	ARG
4	D	252	GLU
4	D	257	ILE
4	D	259	SER
4	D	264	LEU
4	D	265	ILE
4	D	267	ARG
4	D	270	VAL
4	D	273	LYS
4	D	276	LEU
4	D	290	ASP
4	D	292	GLU
4	D	294	GLU
4	D	302	ASP
4	D	304	PHE
4	D	306	LEU
4	D	308	GLN
4	D	309	ASN
4	D	312	VAL
4	D	317	ARG
4	D	319	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	327	GLN
4	D	331	MET
4	D	338	PHE
4	D	339	GLU
4	D	340	ASP
4	D	344	LEU
4	D	353	SER
4	D	355	ARG
4	D	358	LEU
4	D	360	THR
4	D	412	PHE
4	D	414	VAL
4	D	415	GLN
4	D	416	ARG
4	D	418	LEU
4	D	421	ASP
4	D	422	LYS
4	D	454	GLU
4	D	455	GLU
4	D	456	VAL
4	D	479	PHE

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

Mol	Chain	Res	Type
1	A	52	HIS
1	A	92	ASN
1	A	128	HIS
1	A	136	ASN
1	A	146	HIS
1	A	359	ASN
1	A	471	ASN
1	A	591	GLN
1	A	703	ASN
1	A	708	ASN
2	B	16	ASN
2	B	58	ASN
2	B	137	GLN
2	B	145	ASN
2	B	247	GLN
2	B	276	ASN
2	B	310	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	328	ASN
2	B	367	GLN
2	B	442	GLN
2	B	536	ASN
2	B	603	ASN
2	B	687	GLN
3	C	110	HIS
3	C	160	GLN
3	C	236	GLN
3	C	242	GLN
4	D	34	ASN
4	D	76	ASN
4	D	122	GLN
4	D	140	HIS
4	D	168	GLN
4	D	235	GLN
4	D	241	GLN
4	D	272	HIS
4	D	309	ASN
4	D	364	GLN
4	D	415	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	E	13/14 (92%)	9 (69%)	2 (15%)
6	F	23/24 (95%)	13 (56%)	1 (4%)
All	All	36/38 (94%)	22 (61%)	3 (8%)

All (22) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	E	230	U
5	E	232	G
5	E	233	U
5	E	234	C
5	E	235	A
5	E	236	C
5	E	237	C
5	E	238	C
5	E	241	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	5	G
6	F	7	A
6	F	8	A
6	F	11	A
6	F	13	G
6	F	16	G
6	F	17	U
6	F	19	U
6	F	20	U
6	F	21	U
6	F	22	U
6	F	23	A
6	F	24	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	E	231	U
5	E	235	A
6	F	23	A

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64766. These allow visual inspection of the internal detail of the map and identification of artifacts.

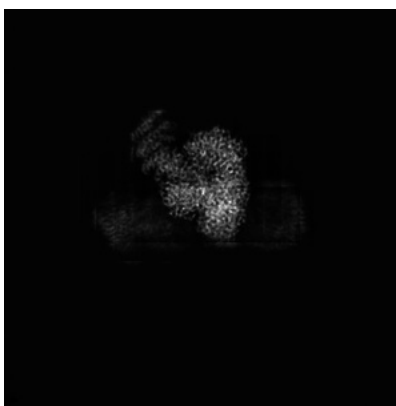
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

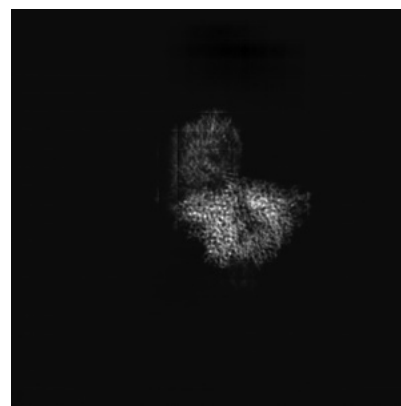
6.1.1 Primary map



X

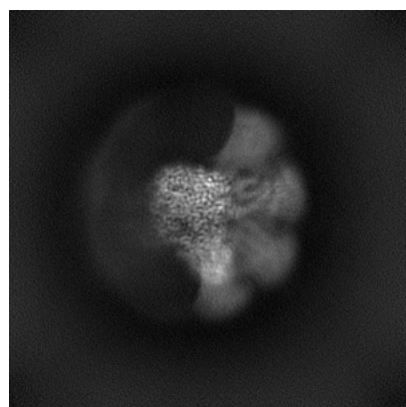


Y

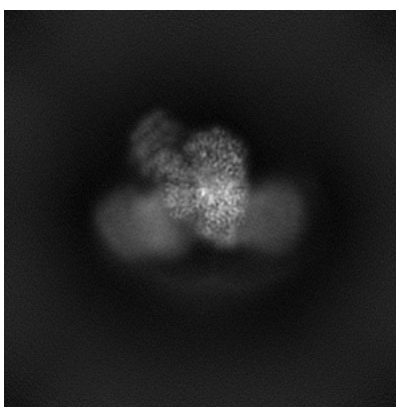


Z

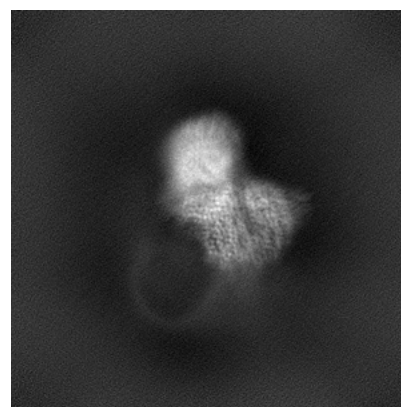
6.1.2 Raw map



X



Y

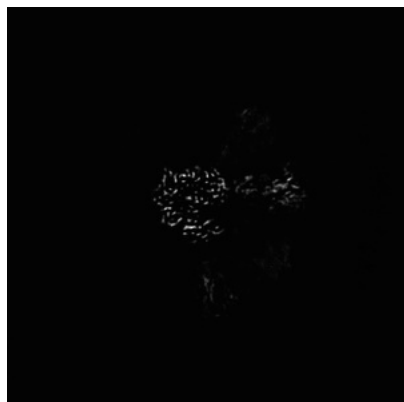


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 180

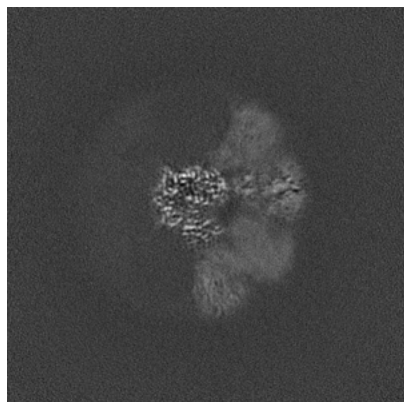


Y Index: 180

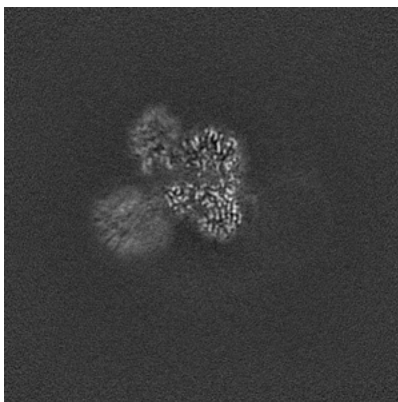


Z Index: 180

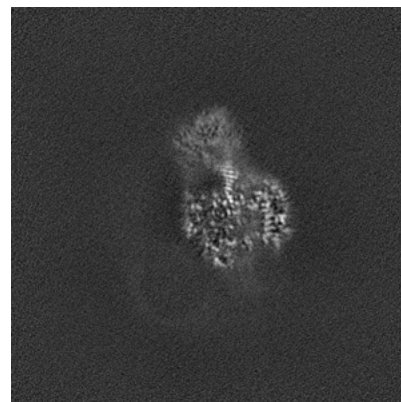
6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

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

6.3 Largest variance slices [i](#)

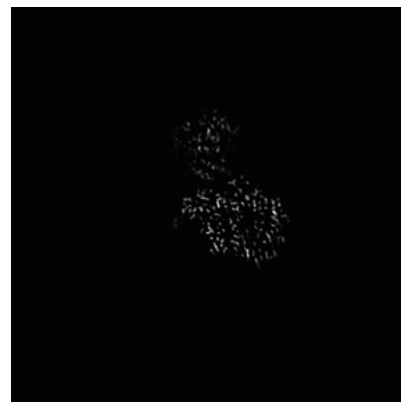
6.3.1 Primary map



X Index: 197

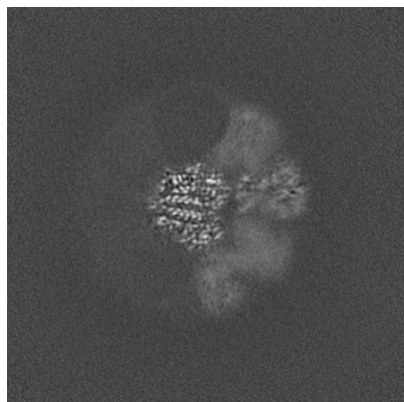


Y Index: 180

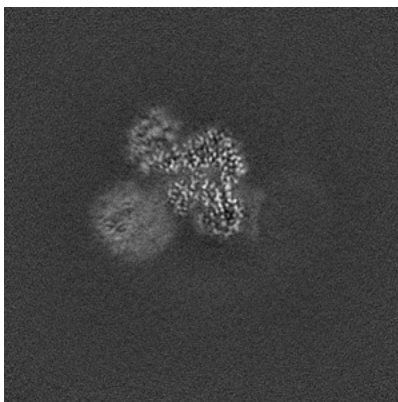


Z Index: 203

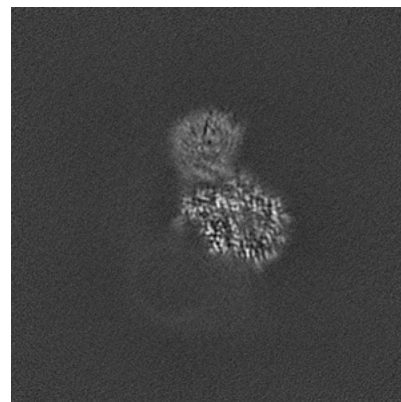
6.3.2 Raw map



X Index: 186



Y Index: 185

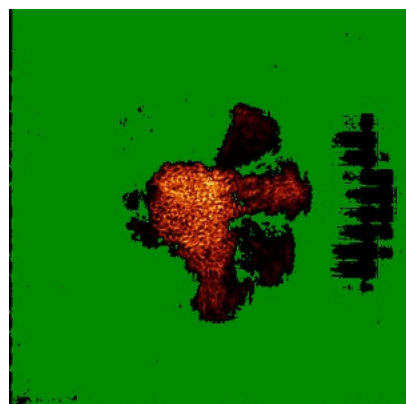


Z Index: 203

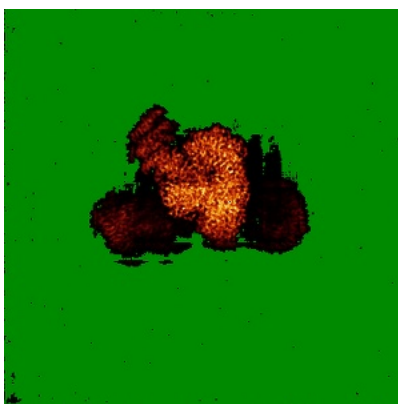
The images above show the largest variance slices of the map in three orthogonal directions.

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

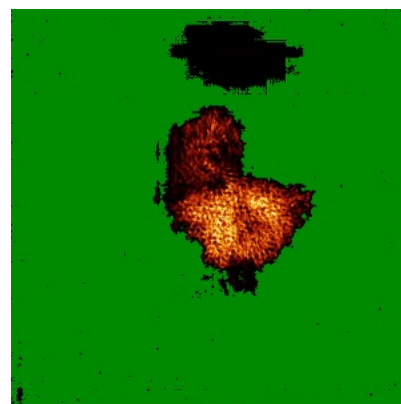
6.4.1 Primary map



X

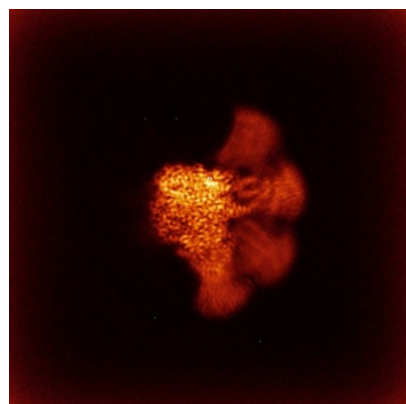


Y

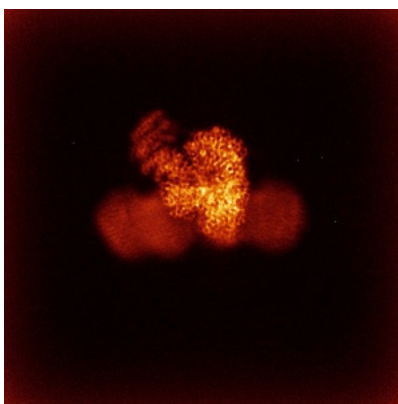


Z

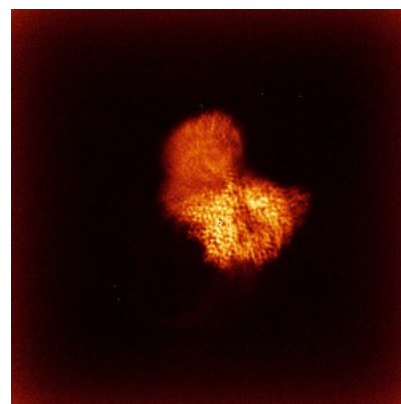
6.4.2 Raw map



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.

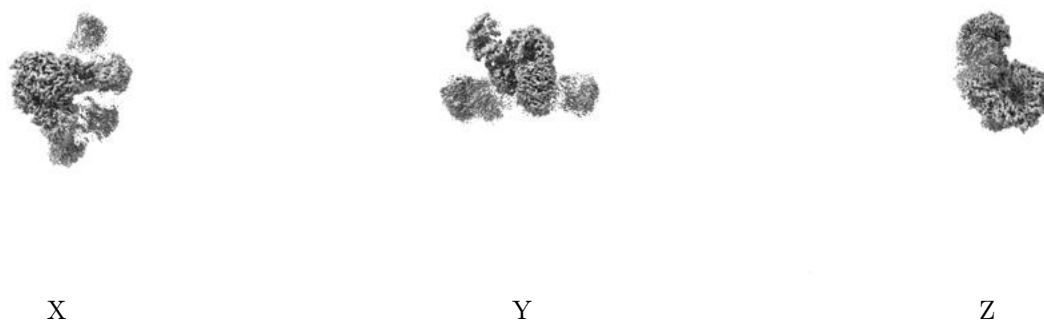
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. 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.

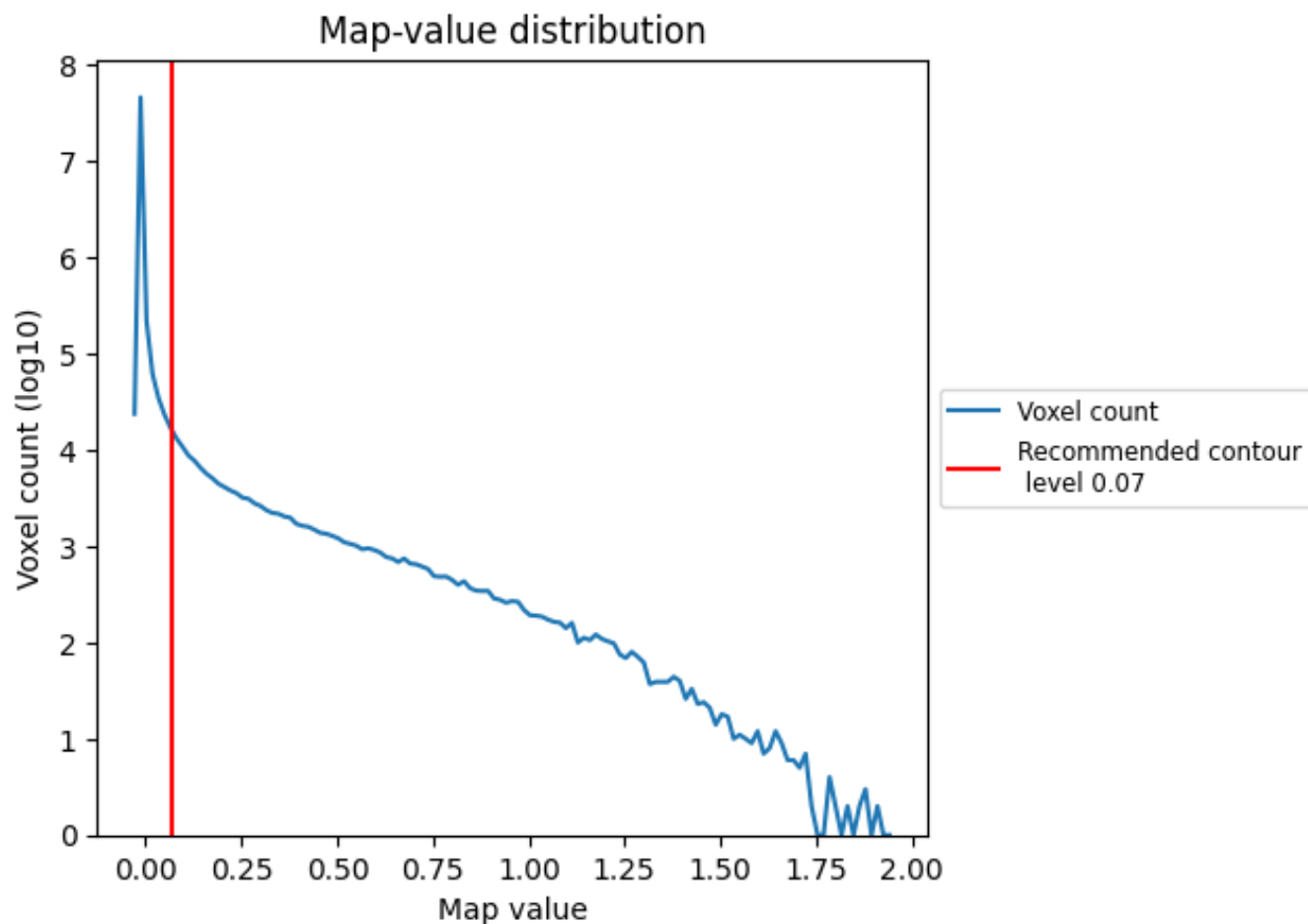
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

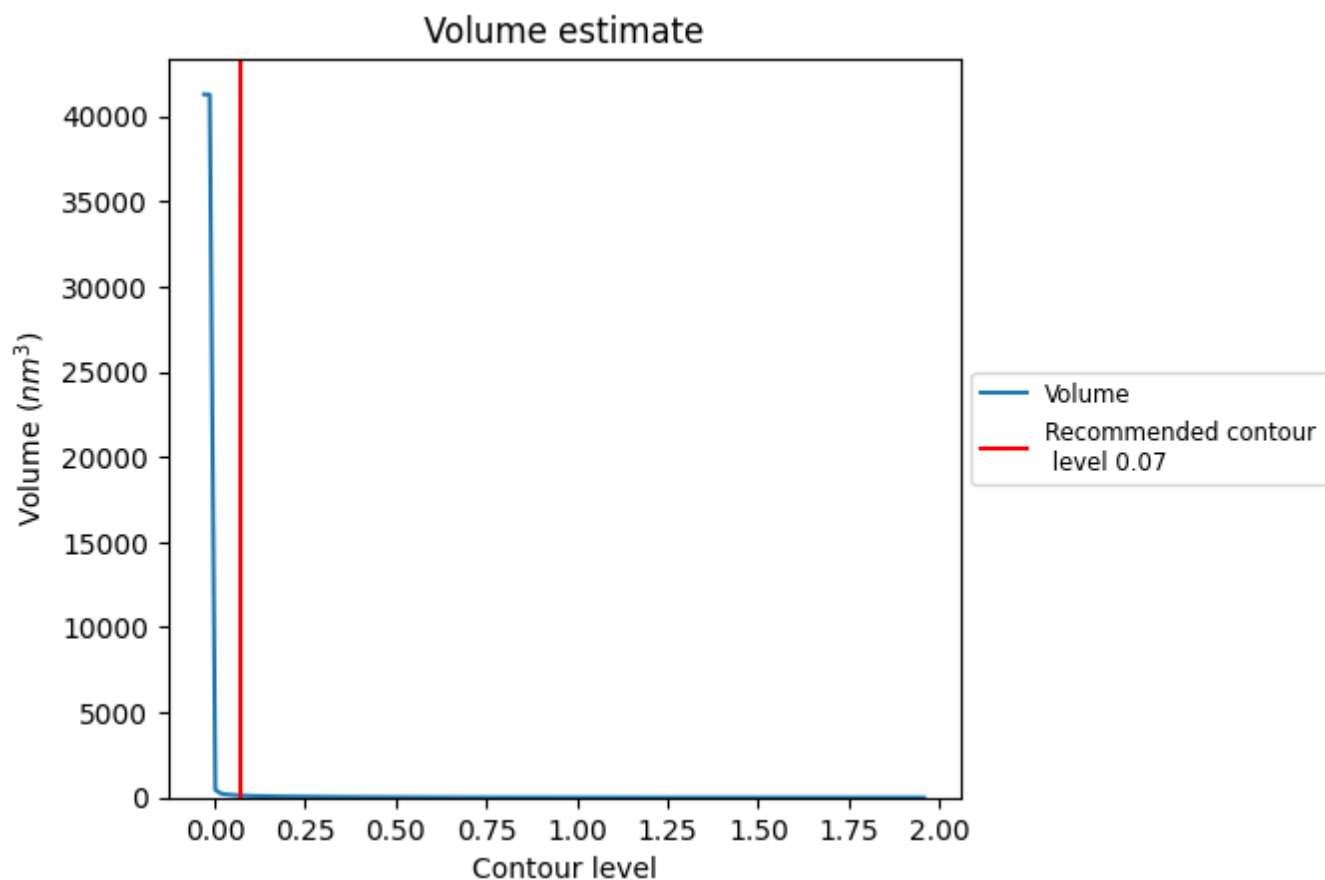
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

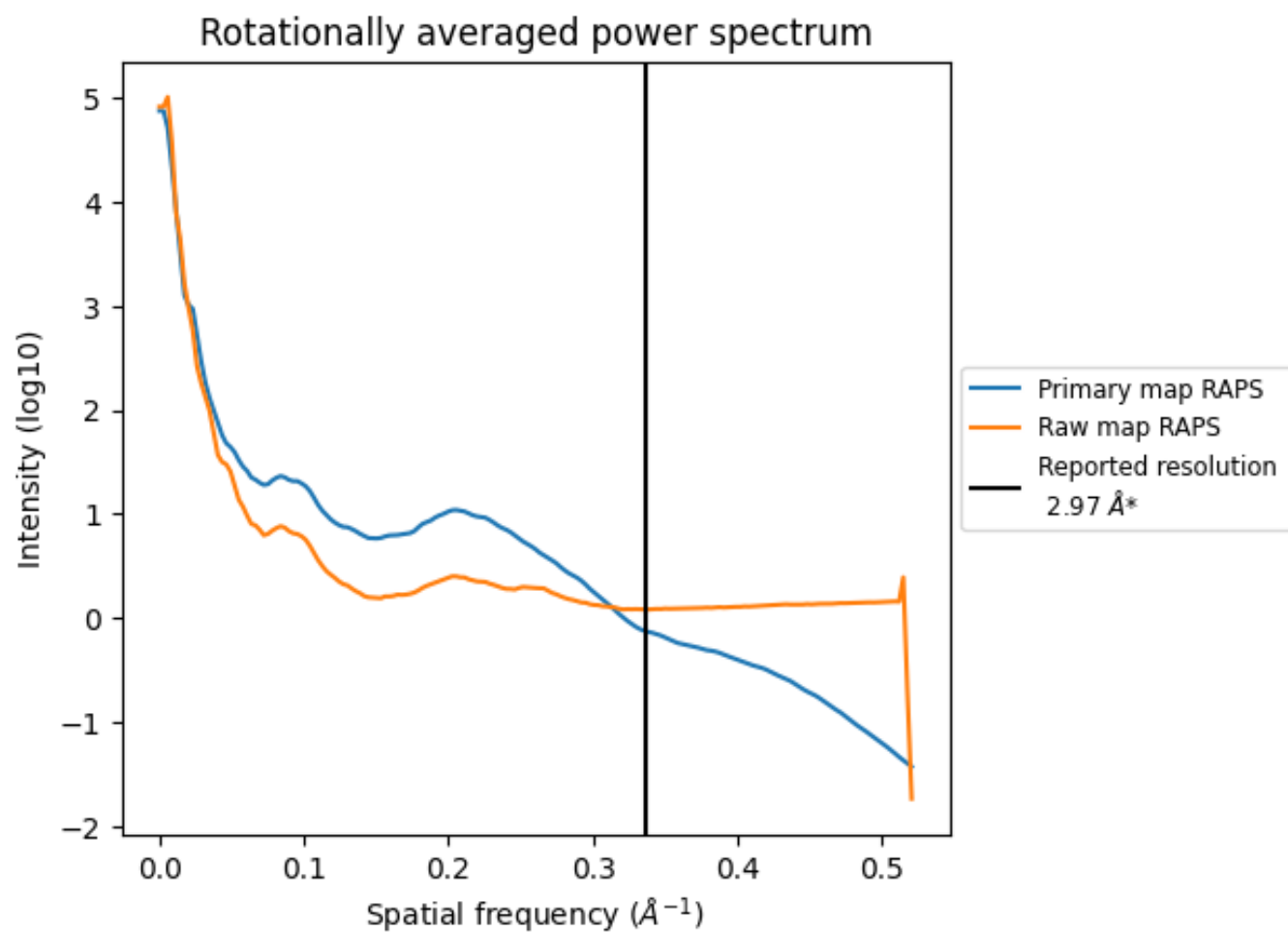
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 125 nm³; this corresponds to an approximate mass of 113 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 [i](#)

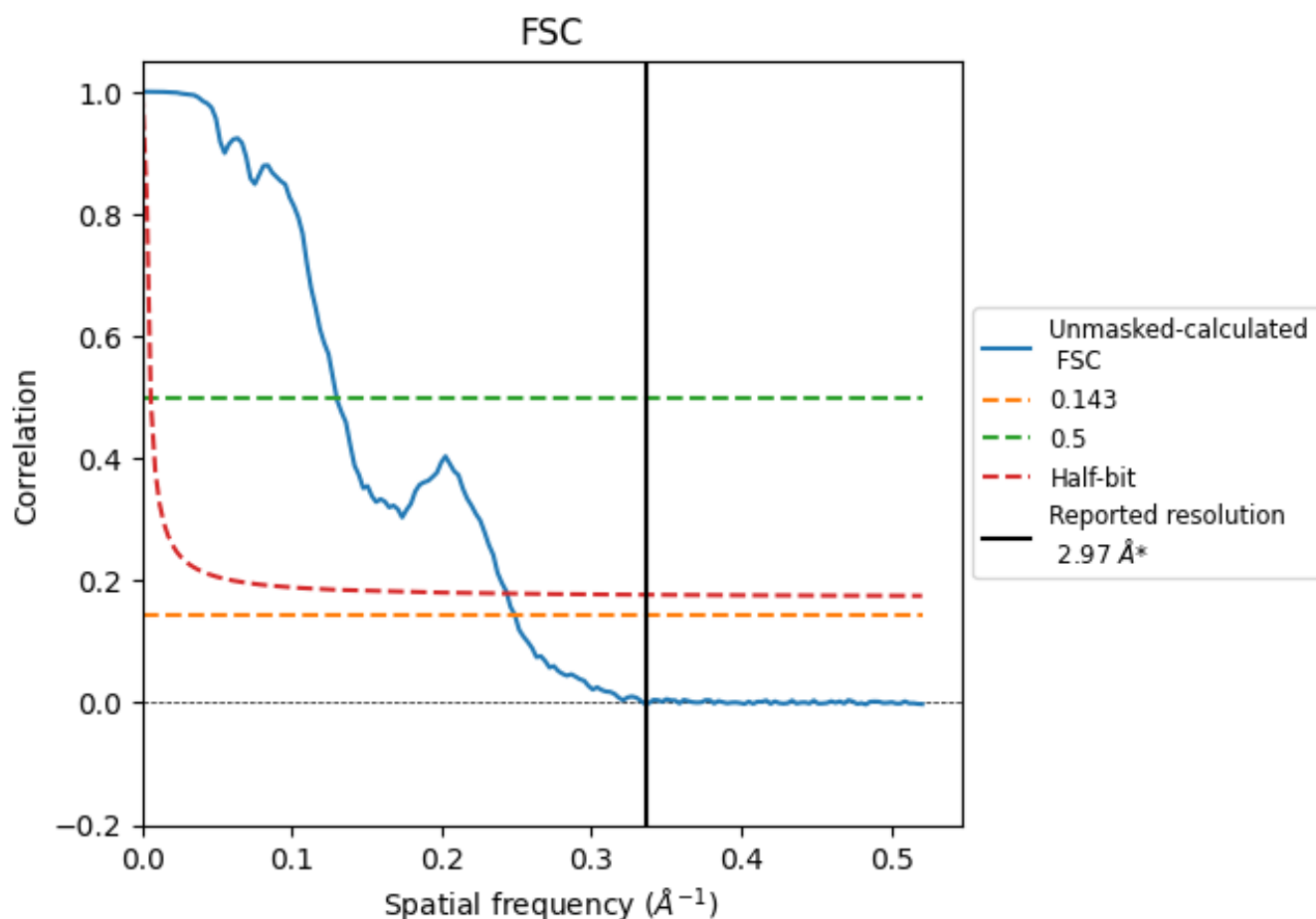


*Reported resolution corresponds to spatial frequency of 0.337 $\text{\AA}^{-1}$

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 0.337 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

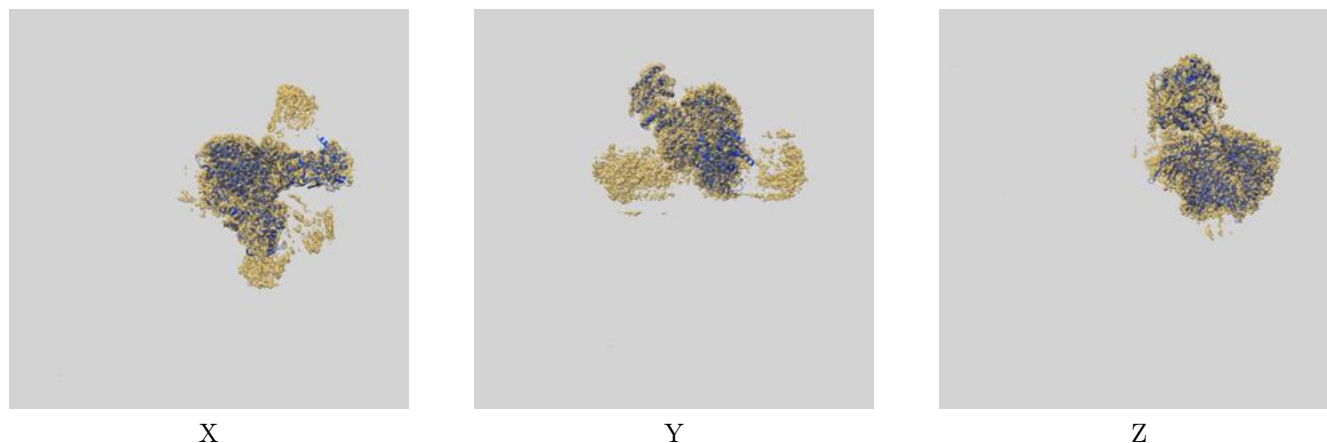
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.02	7.70	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.02 differs from the reported value 2.97 by more than 10 %

9 Map-model fit [i](#)

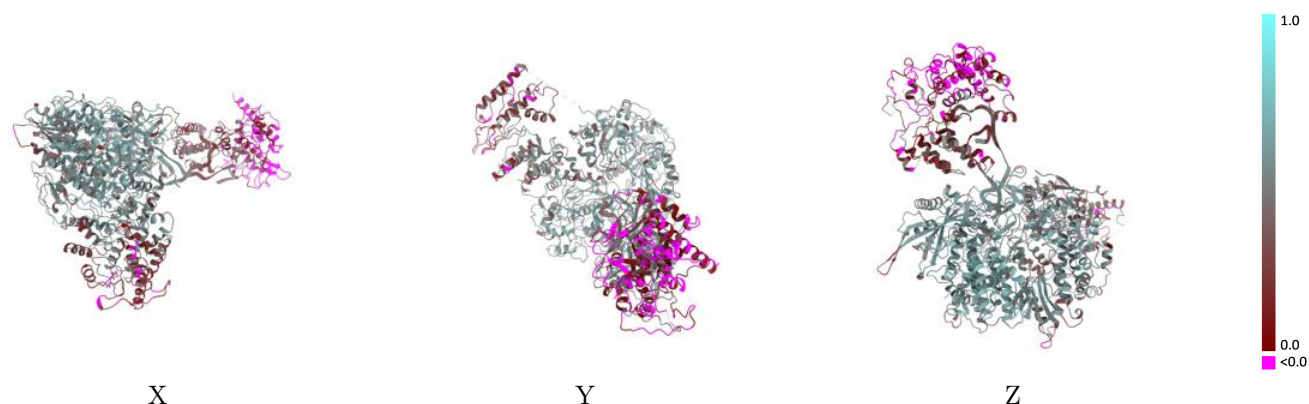
This section contains information regarding the fit between EMDB map EMD-64766 and PDB model 9V44. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



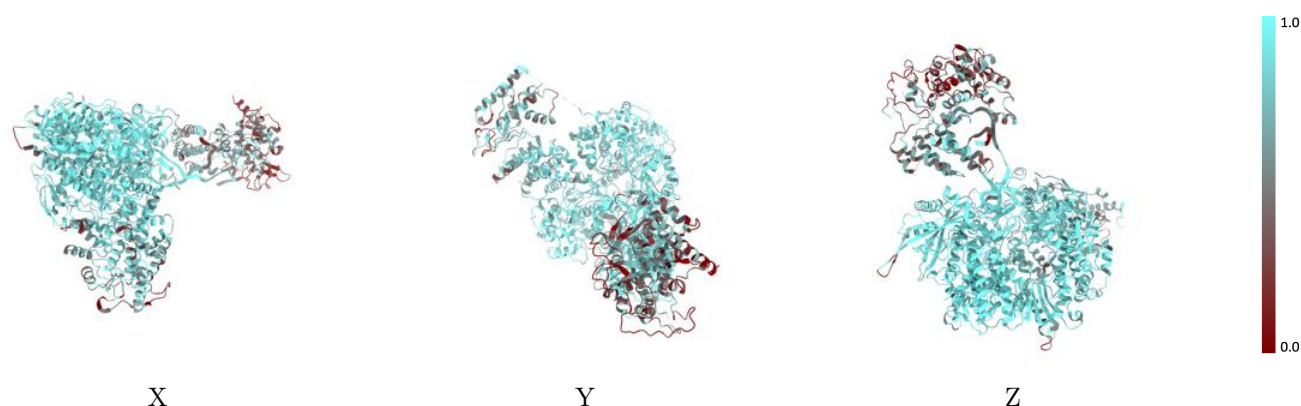
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



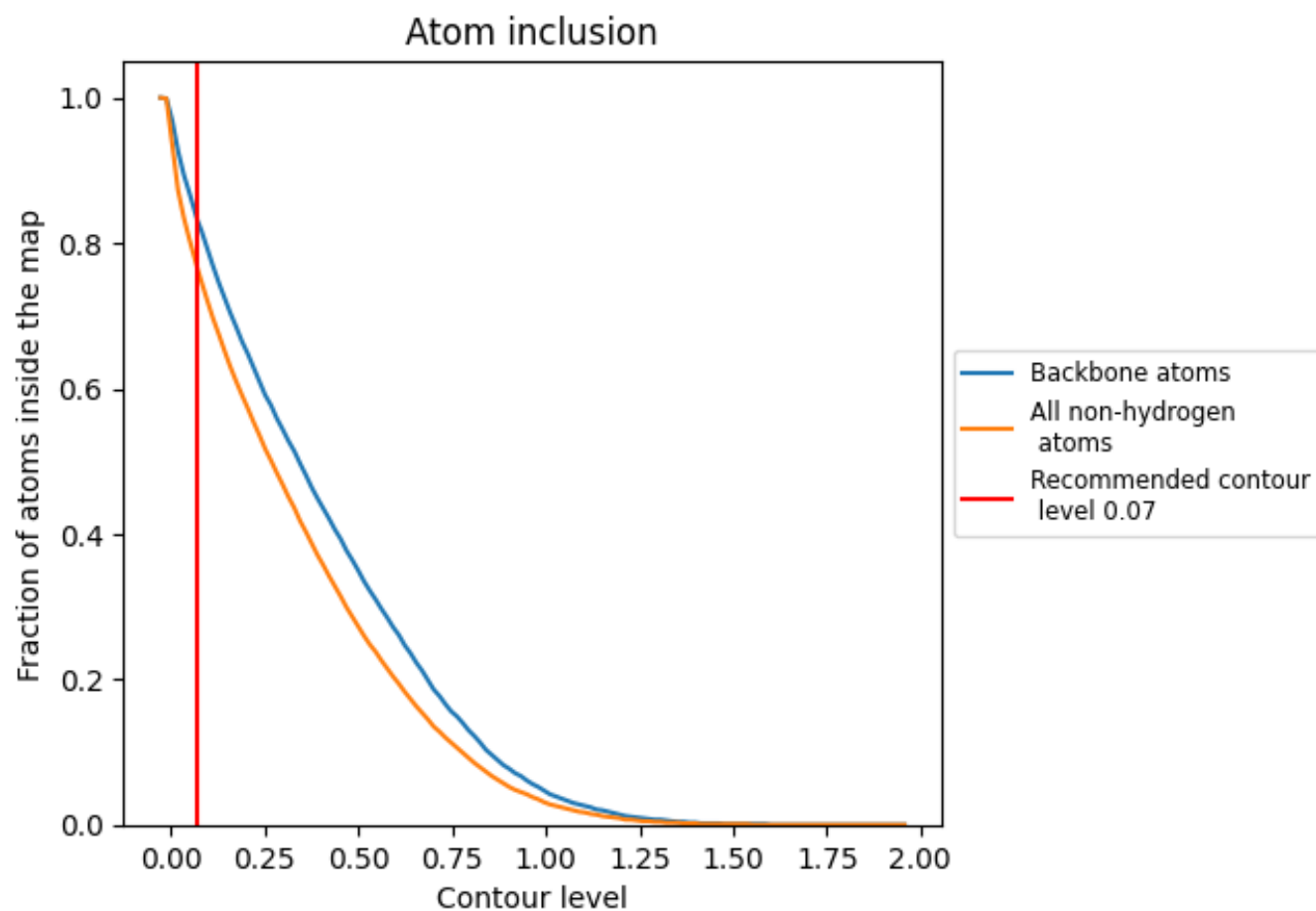
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 76% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7650	0.4290
A	0.8050	0.4700
B	0.8750	0.5370
C	0.8360	0.5040
D	0.4600	0.1260
E	0.7010	0.4330
F	0.8270	0.4780

