



Full wwPDB EM Validation Report ⓘ

Sep 9, 2026 – 04:31 PM EDT

PDB ID : 9ZNC / pdb_00009znc
EMDB ID : EMD-74444
Title : CryoEM structure of the DNA-PK complex bound to N20 nucleosome
Authors : Lu, W.; He, Y.
Deposited on : 2025-12-12
Resolution : 3.93 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.dev133
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) : 2.50

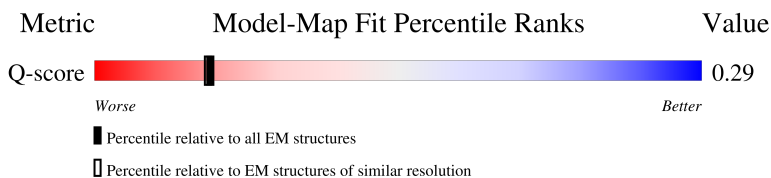
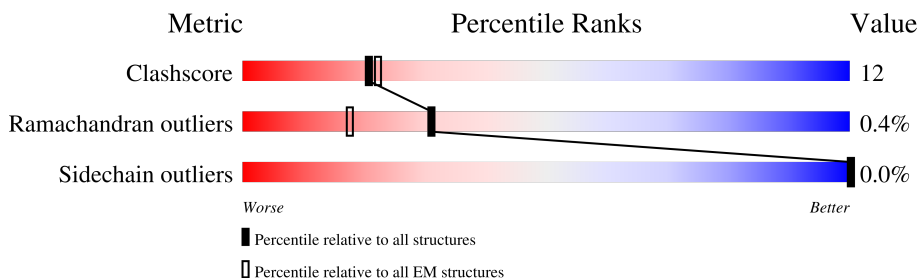
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.93 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7811 (3.43 - 4.43)

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	112	11% 66% 21% 12%
1	E	112	8% 60% 29% 10%
2	B	87	7% 71% 24% 5%
2	F	87	13% 64% 36%

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Mol	Chain	Length	Quality of chain
3	C	117	
3	G	117	
4	D	99	
4	H	99	
5	I	164	
6	M	4128	
7	N	20	
8	J	164	
9	K	609	
10	L	732	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 99079 atoms, of which 48461 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 Histone H3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	98	Total	C	H	N	O	S	0	0
			1654	509	846	156	140	3		
1	E	101	Total	C	H	N	O	S	0	0
			1714	526	881	161	143	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	83	Total	C	H	N	O	S	0	0
			1372	418	710	129	114	1		
2	F	87	Total	C	H	N	O	S	0	0
			1461	442	758	142	118	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	115	Total	C	H	N	O		0	0
			1828	552	948	175	153			
3	G	108	Total	C	H	N	O		0	0
			1728	525	896	163	144			

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	99	Total	C	H	N	O	S	0	0
			1613	493	828	146	144	2		
4	H	99	Total	C	H	N	O	S	0	0
			1613	493	828	146	144	2		

- Molecule 5 is a DNA chain called DNA (164-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
5	I	164	Total	C	H	N	O	P	0	0
			5223	1601	1842	634	983	163		

- Molecule 6 is a protein called DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	M	3662	Total	C	H	N	O	S	0	0
			58976	18776	29692	4946	5370	192		

- Molecule 7 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	20	Total	C	H	N	O	0	0
			141	60	40	20	21		

- Molecule 8 is a DNA chain called DNA (164-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	164	Total	C	H	N	O	P	0	0
			5178	1586	1841	607	981	163		

- Molecule 9 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	490	Total	C	H	N	O	S	0	0
			7998	2533	4044	671	733	17		

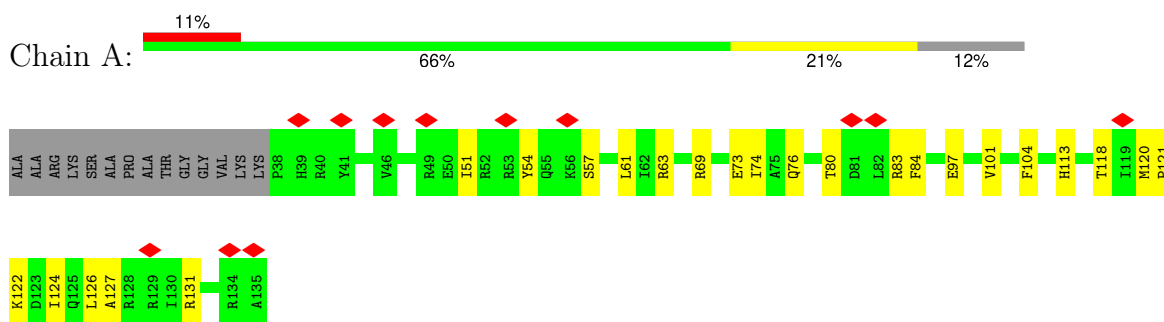
- Molecule 10 is a protein called DNA repair protein Ku80.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	535	Total	C	H	N	O	S	0	0
			8580	2736	4307	713	800	24		

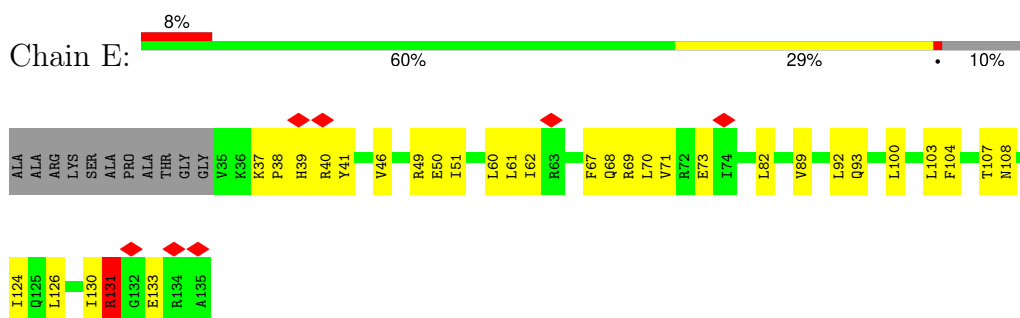
3 Residue-property plots [i](#)

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.

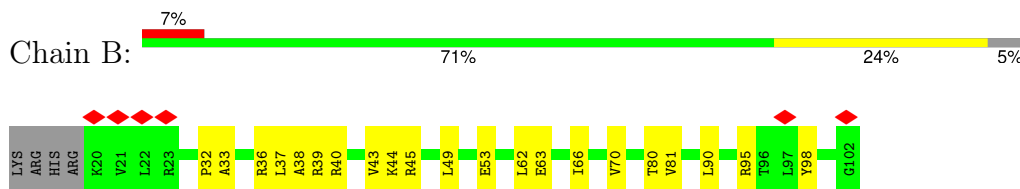
• Molecule 1: Histone H3



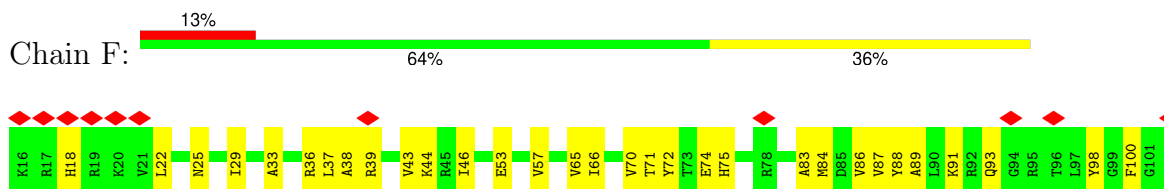
• Molecule 1: Histone H3



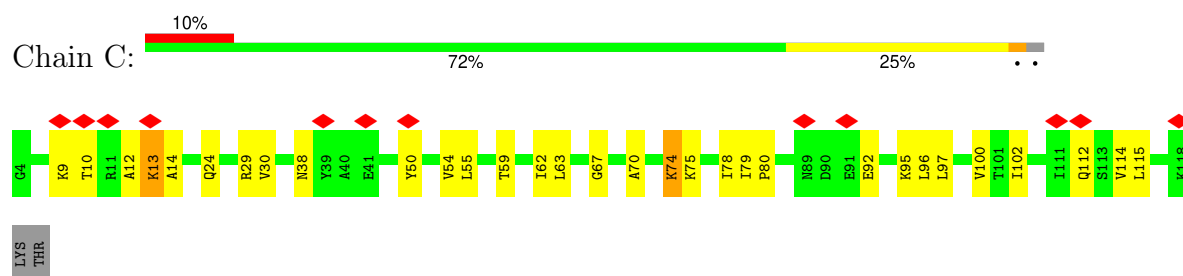
• Molecule 2: Histone H4



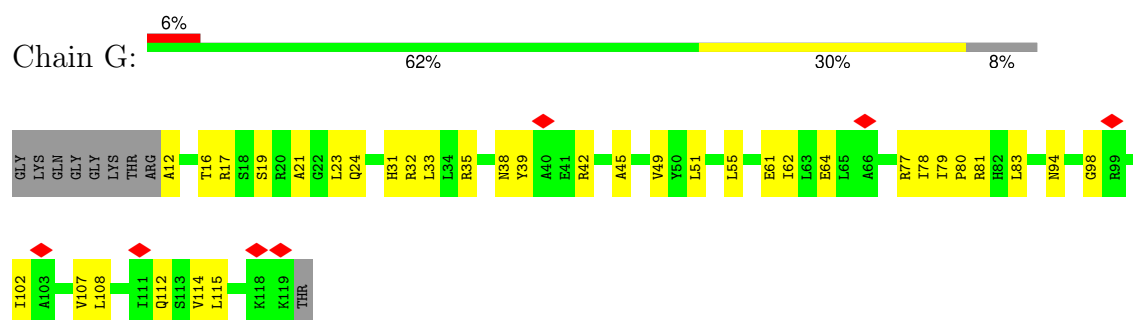
• Molecule 2: Histone H4



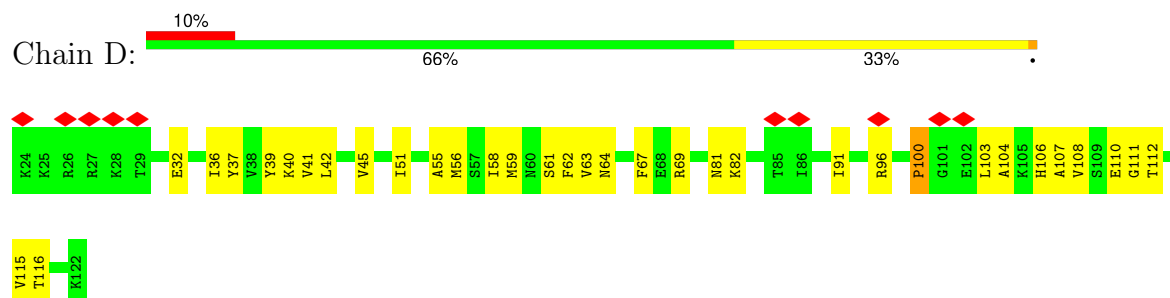
• Molecule 3: Histone H2A



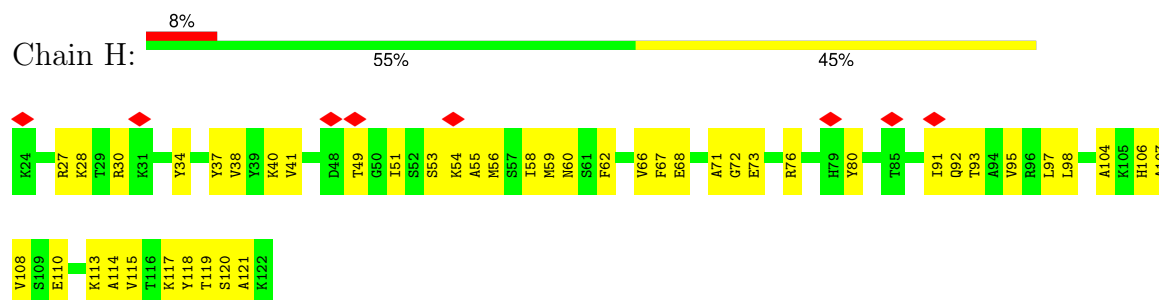
- Molecule 3: Histone H2A



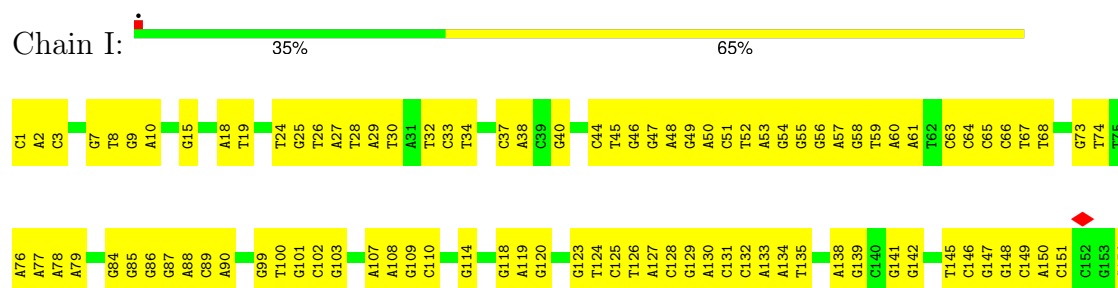
- Molecule 4: Histone H2B



- Molecule 4: Histone H2B

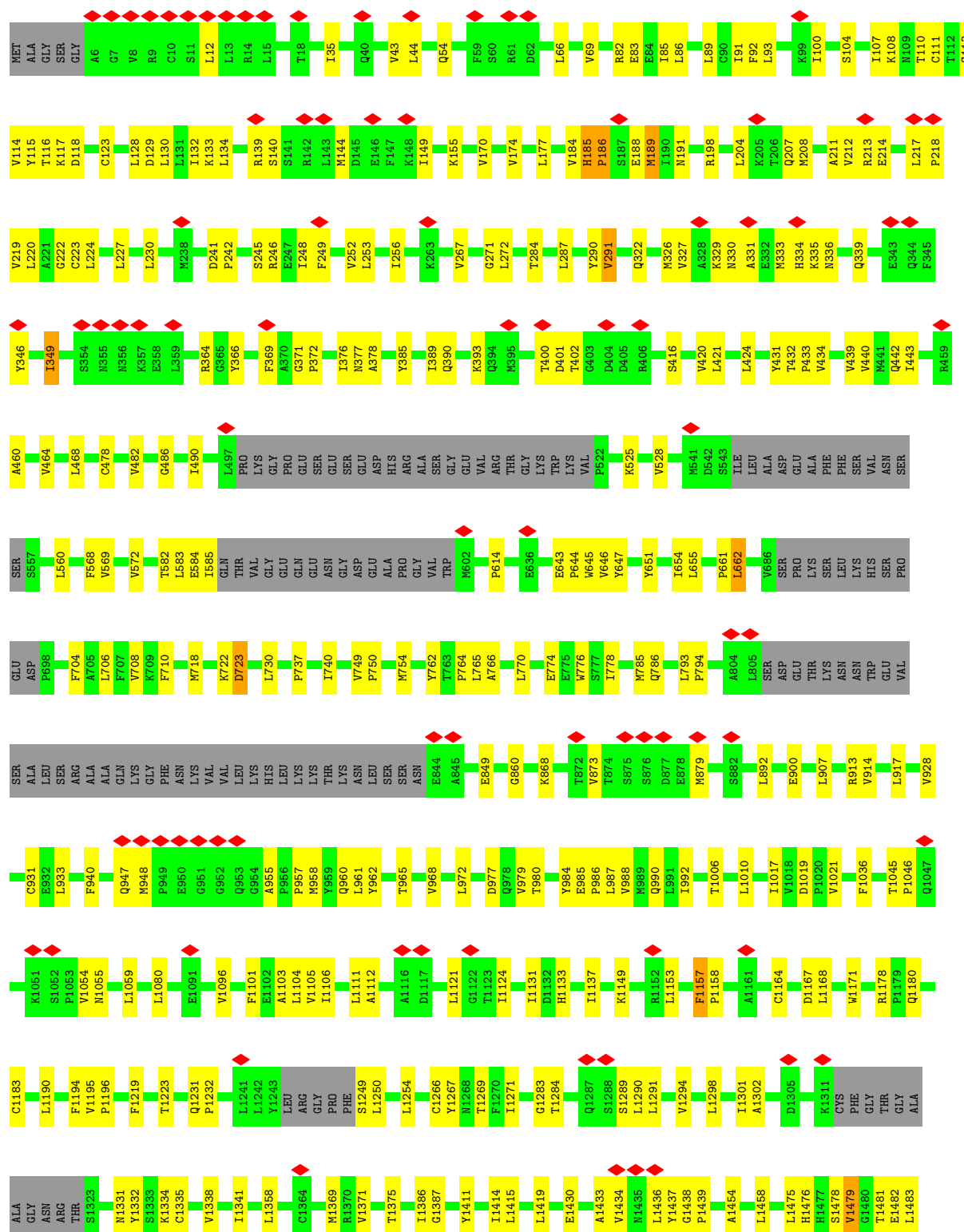


- Molecule 5: DNA (164-MER)

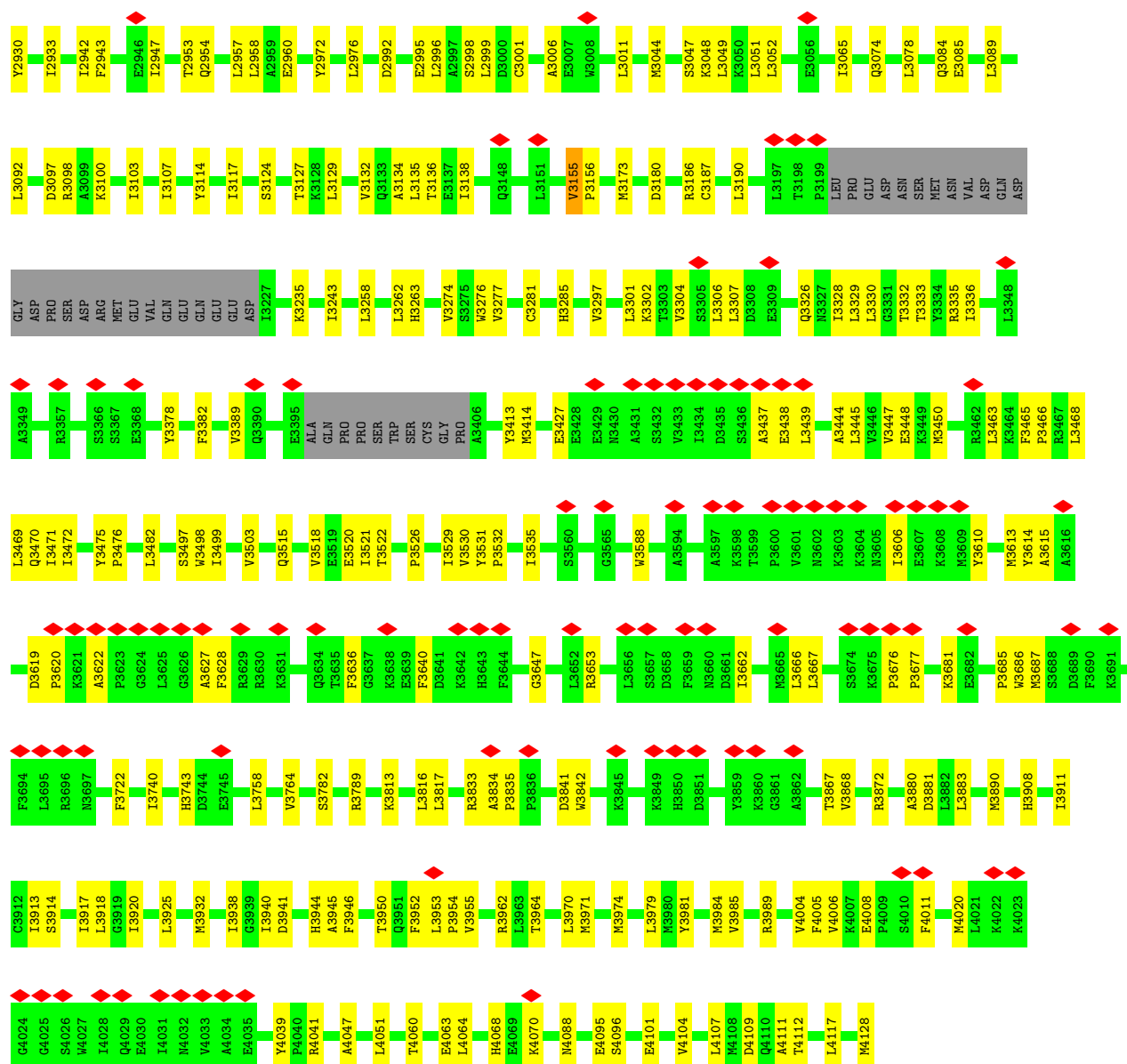


G155	A156
T157	T158
C159	T160
C161	G162
A163	T164

• Molecule 6: DNA-dependent protein kinase catalytic subunit







• Molecule 7: Unknown peptide



• Molecule 8: DNA (164-MER)



LYS	VAL	GLU	ILE	LYS	GLN	LEU	ASN	HIS	PHE	TRP	GLU	ILE	VAL	VAL	GLN	ASP	GLY	ILE	THR	LEU	ILE	THR	LYS	GLU	GLU	ALA	GLY	SER	SER	SER	VAL	THR	ALA	GLU	GLU	ALA	LYS	LYS	PHE	LEU	ALA	ALA	PRO	LYS	ASP	LYS	PRO	PRO	SER	GLY	ASP	THR	ALA	ALA	VAL	PHE	GLU	GLU	GLY	GLY	D724
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68925	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.809	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.12	Depositor
Map size ($\text{\AA}$)	474.5216, 474.5216, 474.5216	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0592, 1.0592, 1.0592	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	0.18	0/820	0.46	0/1099
1	E	0.21	0/845	0.55	1/1132 (0.1%)
2	B	0.21	0/669	0.43	0/894
2	F	0.22	0/711	0.51	0/948
3	C	0.19	0/890	0.51	0/1197
3	G	0.29	0/842	0.49	0/1135
4	D	0.17	0/796	0.39	0/1065
4	H	0.27	0/796	0.62	1/1065 (0.1%)
5	I	0.24	0/3797	0.54	0/5865
6	M	0.16	0/29884	0.46	2/40387 (0.0%)
8	J	0.23	0/3739	0.51	0/5763
9	K	0.18	0/4031	0.50	1/5429 (0.0%)
10	L	0.17	0/4359	0.50	0/5881
All	All	0.19	0/52179	0.48	5/71860 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
2	F	0	1
4	D	0	1
4	H	0	1
6	M	0	4
9	K	0	6
All	All	0	14

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	349	ILE	N-CA-CB	6.26	119.05	110.54
1	E	131	ARG	CG-CD-NE	5.54	124.19	112.00
9	K	304	ASN	N-CA-C	5.21	117.00	110.91
6	M	349	ILE	CB-CA-C	-5.19	105.13	112.14
4	H	54	LYS	CB-CG-CD	5.02	122.84	111.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	100	PRO	Peptide
1	E	131	ARG	Sidechain
2	F	18	HIS	Peptide
4	H	27	ARG	Peptide
9	K	206	LYS	Peptide
9	K	244	ARG	Peptide
9	K	277	VAL	Peptide
9	K	447	PRO	Peptide
9	K	474	ARG	Peptide
9	K	530	TYR	Peptide
6	M	1631	SER	Peptide
6	M	185	HIS	Peptide
6	M	222	GLY	Peptide
6	M	2778	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	808	846	846	41	0
1	E	833	881	880	43	0
2	B	662	710	709	32	0
2	F	703	758	755	41	0
3	C	880	948	945	43	0
3	G	832	896	895	54	0
4	D	785	828	825	38	0
4	H	785	828	825	55	0
5	I	3381	1842	1842	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	29284	29692	29680	604	0
7	N	101	40	24	0	0
8	J	3337	1841	1841	92	0
9	K	3954	4044	4042	84	0
10	L	4273	4307	4303	107	0
All	All	50618	48461	48412	1191	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1191) 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)
6:M:3052:LEU:HD22	6:M:3092:LEU:HD13	1.34	1.06
4:H:38:VAL:HG21	4:H:56:MET:HE1	1.42	1.00
6:M:256:ILE:HD11	6:M:272:LEU:HD23	1.53	0.90
6:M:3277:VAL:HG23	6:M:3307:LEU:HD23	1.55	0.88
3:C:114:VAL:HG12	1:E:112:ILE:HD12	1.59	0.85
3:C:115:LEU:HD22	2:F:44:LYS:NZ	1.91	0.85
10:L:519:PRO:O	10:L:522:VAL:HG22	1.82	0.80
6:M:2235:LEU:HG	6:M:2279:ILE:HD11	1.63	0.79
9:K:529:VAL:HG21	10:L:372:ALA:HB1	1.64	0.79
9:K:497:LEU:O	9:K:498:MET:HE2	1.81	0.79
9:K:493:LEU:HD22	10:L:323:PHE:CD2	2.20	0.76
6:M:1133:HIS:O	6:M:1137:ILE:HD12	1.86	0.76
6:M:1478:SER:O	6:M:1479:VAL:HG22	1.85	0.76
9:K:349:GLY:HA3	10:L:463:LEU:HD11	1.68	0.76
10:L:154:LEU:HD21	10:L:161:LEU:HD13	1.65	0.75
9:K:388:LYS:NZ	10:L:451:LEU:HD12	2.03	0.74
9:K:72:ILE:O	9:K:75:ILE:HG22	1.87	0.73
10:L:113:VAL:O	10:L:117:VAL:HG23	1.88	0.73
6:M:3107:ILE:HD13	6:M:3135:LEU:HD23	1.69	0.73
9:K:388:LYS:HZ2	10:L:451:LEU:HD12	1.54	0.73
3:C:50:TYR:HB3	4:D:91:ILE:HD11	1.71	0.72
3:G:24:GLN:HE22	4:H:40:LYS:HB2	1.55	0.72
6:M:421:LEU:HG	6:M:464:VAL:HG22	1.71	0.72
6:M:1291:LEU:HD21	6:M:1358:LEU:HD21	1.72	0.72
4:H:38:VAL:HG21	4:H:56:MET:CE	2.18	0.70
6:M:2245:TRP:O	6:M:2249:LEU:HD23	1.91	0.70
6:M:2563:LEU:HD12	6:M:2791:ILE:HG23	1.74	0.70
1:A:124:ILE:HD13	2:B:53:GLU:OE2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:3653:ARG:HH22	6:M:3662:ILE:HD13	1.54	0.70
6:M:1111:LEU:HD11	6:M:1131:ILE:HD13	1.74	0.69
6:M:3816:LEU:HD13	6:M:4128:MET:CE	2.22	0.69
6:M:718:MET:CE	6:M:730:LEU:HD21	2.23	0.69
6:M:1590:THR:O	6:M:1593:VAL:HG22	1.92	0.69
4:H:62:PHE:O	4:H:66:VAL:HG22	1.92	0.69
10:L:201:GLN:O	10:L:205:LEU:HD23	1.92	0.69
3:G:80:PRO:HB3	3:G:102:ILE:HG21	1.75	0.68
6:M:2854:PHE:O	6:M:2858:ILE:HD12	1.92	0.68
6:M:1878:ASP:OD2	6:M:1946:ASN:ND2	2.27	0.68
10:L:16:VAL:HG12	10:L:16:VAL:O	1.94	0.68
9:K:72:ILE:HG23	9:K:491:GLU:OE2	1.92	0.68
6:M:2185:MET:HA	6:M:2185:MET:HE2	1.74	0.68
6:M:100:ILE:HD11	6:M:134:LEU:HD13	1.76	0.68
3:G:33:LEU:HD22	4:H:67:PHE:CZ	2.29	0.68
6:M:2205:VAL:HG22	6:M:2206:PRO:HD2	1.74	0.67
6:M:3950:THR:HG23	6:M:4063:GLU:OE1	1.95	0.67
9:K:147:LEU:HD12	9:K:193:LEU:HD22	1.76	0.67
6:M:3047:SER:O	6:M:3051:LEU:HD23	1.95	0.67
9:K:493:LEU:HD13	10:L:323:PHE:CE2	2.30	0.67
6:M:1283:GLY:O	6:M:1284:THR:HG22	1.94	0.67
3:C:114:VAL:CG1	1:E:112:ILE:HD12	2.25	0.66
6:M:2954:GLN:O	6:M:2958:LEU:HD23	1.94	0.66
6:M:130:LEU:O	6:M:134:LEU:HD23	1.96	0.66
6:M:3302:LYS:HD3	6:M:3302:LYS:O	1.94	0.66
6:M:2953:THR:O	6:M:2957:LEU:HD23	1.96	0.66
1:A:61:LEU:HD13	2:B:37:LEU:HG	1.78	0.66
5:I:51:DC:H2'	5:I:52:DT:H71	1.78	0.66
6:M:139:ARG:HG2	6:M:140:SER:H	1.60	0.65
6:M:3468:LEU:O	6:M:3472:ILE:HD12	1.96	0.65
10:L:109:ASP:O	10:L:113:VAL:HG23	1.96	0.65
6:M:3883:LEU:HB2	6:M:3970:LEU:HD21	1.78	0.65
6:M:1415:LEU:HD12	6:M:1419:LEU:HD13	1.78	0.65
8:J:126:DG:H2'	8:J:127:DT:H72	1.78	0.65
3:G:83:LEU:HD13	4:H:59:MET:HE3	1.79	0.65
5:I:2:DA:N6	8:J:163:DT:N3	2.44	0.65
6:M:3297:VAL:HG12	6:M:3301:LEU:HD23	1.78	0.65
5:I:147:DG:H2''	5:I:148:DG:C8	2.32	0.64
6:M:1101:PHE:CE1	6:M:1153:LEU:HD11	2.32	0.64
10:L:423:GLN:O	10:L:424:LEU:HD22	1.98	0.64
6:M:256:ILE:HD11	6:M:272:LEU:CD2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:33:ALA:O	2:F:37:LEU:HD23	1.98	0.63
4:H:92:GLN:NE2	4:H:93:THR:HG23	2.13	0.63
9:K:466:VAL:HG21	10:L:389:MET:SD	2.39	0.63
1:E:61:LEU:CD2	2:F:37:LEU:HD22	2.28	0.63
6:M:460:ALA:O	6:M:464:VAL:HG23	1.99	0.63
6:M:1112:ALA:HB1	6:M:1180:GLN:HE21	1.63	0.63
6:M:3468:LEU:HD22	6:M:3469:LEU:HD22	1.80	0.63
6:M:2481:HIS:HA	6:M:2484:TYR:CE1	2.34	0.62
1:A:54:TYR:OH	1:A:61:LEU:HD12	1.99	0.62
6:M:2385:LEU:HD12	6:M:2385:LEU:O	1.99	0.62
6:M:2220:MET:N	6:M:2220:MET:HE2	2.13	0.62
6:M:3834:ALA:HB3	6:M:3835:PRO:HD3	1.82	0.62
2:F:88:TYR:O	2:F:91:LYS:HG2	1.99	0.62
6:M:1933:LEU:HD13	6:M:1936:ARG:HB2	1.82	0.62
6:M:3985:VAL:HG21	6:M:4101:GLU:HG3	1.82	0.61
4:H:114:ALA:HA	4:H:117:LYS:HE3	1.82	0.61
10:L:407:VAL:HG23	10:L:424:LEU:HD21	1.83	0.61
6:M:116:THR:HG22	6:M:117:LYS:H	1.64	0.61
6:M:992:ILE:HD11	6:M:1036:PHE:HB2	1.81	0.61
6:M:1582:LEU:HD21	6:M:1593:VAL:HB	1.82	0.61
9:K:94:LYS:O	9:K:104:VAL:HG22	2.01	0.61
6:M:1101:PHE:CZ	6:M:1153:LEU:HD11	2.35	0.61
6:M:2359:LYS:HD2	6:M:2359:LYS:O	2.00	0.61
6:M:3052:LEU:CD2	6:M:3092:LEU:HD13	2.21	0.61
6:M:1761:LEU:O	6:M:1765:VAL:HG23	2.00	0.60
6:M:3531:TYR:O	6:M:3535:ILE:HD12	2.01	0.60
9:K:505:ASP:OD1	9:K:507:THR:HG22	2.01	0.60
3:C:74:LYS:HE3	3:C:74:LYS:HA	1.84	0.60
5:I:73:DG:H2"	5:I:74:DT:H71	1.82	0.60
6:M:3186:ARG:O	6:M:3190:LEU:HD23	2.01	0.60
3:G:33:LEU:HD23	3:G:33:LEU:O	2.00	0.60
6:M:3627:ALA:O	6:M:3628:PHE:CD1	2.54	0.60
1:E:46:VAL:O	1:E:50:GLU:OE1	2.19	0.60
6:M:1301:ILE:O	6:M:1301:ILE:HG22	2.02	0.60
6:M:1430:GLU:OE2	6:M:1433:ALA:HB3	2.02	0.60
10:L:336:GLU:OE1	10:L:336:GLU:O	2.20	0.60
9:K:202:LEU:HD12	9:K:202:LEU:O	2.01	0.60
9:K:38:LEU:HD21	9:K:167:MET:HE3	1.83	0.59
10:L:11:VAL:HG11	10:L:114:SER:HB2	1.84	0.59
6:M:1693:VAL:O	6:M:1696:LEU:HD23	2.02	0.59
6:M:1839:PHE:HE1	6:M:1843:ILE:HD13	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:2155:GLU:HG3	6:M:2156:VAL:H	1.68	0.59
6:M:868:LYS:HE3	6:M:3173:MET:HB2	1.84	0.59
6:M:2272:VAL:HG12	6:M:2276:LEU:CD1	2.33	0.59
1:A:127:ALA:O	1:A:131:ARG:HG2	2.02	0.59
6:M:3468:LEU:CD2	6:M:3469:LEU:HD22	2.33	0.59
5:I:8:DT:H2'	5:I:9:DG:C8	2.37	0.59
6:M:349:ILE:HG23	6:M:366:TYR:CZ	2.38	0.59
3:G:17:ARG:HH12	8:J:31:DT:H3'	1.68	0.59
6:M:3497:SER:HG	6:M:3498:TRP:CD1	2.21	0.59
8:J:111:DC:C2'	8:J:112:DT:H71	2.31	0.59
3:G:45:ALA:O	3:G:49:VAL:HG23	2.03	0.59
10:L:343:LEU:O	10:L:343:LEU:HD23	2.02	0.59
6:M:1840:PHE:HB2	6:M:1880:MET:HE3	1.84	0.59
6:M:2146:LEU:HD23	6:M:2149:LEU:HD12	1.84	0.59
6:M:2563:LEU:HD12	6:M:2791:ILE:CG2	2.33	0.59
6:M:3089:LEU:CD1	6:M:3092:LEU:HD12	2.33	0.59
6:M:3816:LEU:HD13	6:M:4128:MET:HE2	1.84	0.59
10:L:339:CYS:HB3	10:L:340:PHE:HA	1.84	0.59
8:J:151:DG:H2'	8:J:152:DA:C8	2.37	0.58
3:G:39:TYR:CD2	4:H:71:ALA:HB1	2.38	0.58
4:D:39:TYR:CE1	4:D:51:ILE:HD11	2.39	0.58
6:M:3667:LEU:O	6:M:3667:LEU:HD23	2.04	0.58
6:M:1006:THR:O	6:M:1010:LEU:HD23	2.04	0.58
6:M:1294:VAL:O	6:M:1298:LEU:HD23	2.02	0.58
6:M:2510:LEU:HD13	6:M:2557:LEU:HG	1.84	0.58
3:C:74:LYS:HD2	9:K:533:ASP:OD1	2.04	0.58
6:M:1832:SER:C	6:M:1833:LEU:HD12	2.29	0.58
4:H:30:ARG:HH12	8:J:28:DC:H4'	1.68	0.57
6:M:873:VAL:HG12	6:M:879:MET:HG3	1.86	0.57
6:M:1105:VAL:HG23	6:M:1171:TRP:CZ2	2.38	0.57
6:M:2168:LEU:HA	6:M:2171:LEU:HB3	1.86	0.57
3:C:97:LEU:HD11	4:D:62:PHE:HE1	1.68	0.57
6:M:3470:GLN:HB3	6:M:4004:VAL:HG11	1.85	0.57
1:E:60:LEU:HD11	1:E:93:GLN:HG2	1.85	0.57
9:K:356:LEU:HD22	9:K:437:LEU:HD21	1.86	0.57
3:C:115:LEU:HD22	2:F:44:LYS:HZ2	1.69	0.57
6:M:4060:THR:O	6:M:4064:LEU:HD23	2.04	0.57
6:M:114:VAL:HG13	6:M:128:LEU:HD21	1.85	0.57
6:M:766:ALA:O	6:M:770:LEU:HD23	2.04	0.57
6:M:100:ILE:HD11	6:M:134:LEU:CD1	2.35	0.57
4:D:42:LEU:CD2	4:D:51:ILE:HG23	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:24:GLN:NE2	4:H:37:TYR:O	2.38	0.56
6:M:1855:PHE:HB2	6:M:1858:LEU:HD21	1.87	0.56
6:M:3518:VAL:HG23	6:M:3529:ILE:CD1	2.35	0.56
8:J:99:DG:H2''	8:J:100:DG:C8	2.41	0.56
10:L:351:VAL:HG13	10:L:351:VAL:O	2.05	0.56
5:I:123:DG:H2'	5:I:124:DT:C6	2.40	0.56
6:M:93:LEU:HG	6:M:100:ILE:HD12	1.88	0.56
6:M:402:THR:HG22	6:M:402:THR:O	2.06	0.56
6:M:1575:LEU:O	6:M:1579:VAL:HG22	2.06	0.56
6:M:4107:LEU:HD23	6:M:4107:LEU:O	2.04	0.56
8:J:10:DC:H2''	8:J:11:DC:C6	2.40	0.56
10:L:261:ILE:HG22	10:L:377:LEU:HD22	1.86	0.56
10:L:279:VAL:HG12	10:L:280:ASP:N	2.20	0.56
6:M:1586:SER:HB2	6:M:1593:VAL:HG21	1.88	0.56
6:M:1711:ARG:HG3	6:M:1761:LEU:HD21	1.87	0.56
9:K:361:TYR:C	9:K:362:LEU:HD22	2.31	0.56
6:M:1371:VAL:O	6:M:1375:THR:HG23	2.06	0.56
6:M:2779:ASP:OD1	6:M:2782:ASP:HB3	2.06	0.56
4:H:38:VAL:CG2	4:H:56:MET:HE1	2.27	0.56
9:K:105:LEU:HD23	9:K:106:GLN:HG2	1.88	0.56
10:L:356:PHE:CD1	10:L:422:VAL:HG11	2.40	0.56
8:J:74:DC:C2'	8:J:75:DT:H71	2.36	0.56
1:A:54:TYR:C	2:B:39:ARG:NH2	2.64	0.55
1:E:61:LEU:HD21	2:F:37:LEU:HD22	1.88	0.55
6:M:4112:THR:HG22	6:M:4112:THR:O	2.05	0.55
6:M:1839:PHE:CE1	6:M:1843:ILE:HG21	2.42	0.55
6:M:3306:LEU:C	6:M:3307:LEU:HD12	2.32	0.55
1:E:71:VAL:HG23	2:F:66:ILE:HD11	1.88	0.55
6:M:2272:VAL:HG12	6:M:2276:LEU:HD13	1.86	0.55
6:M:2361:ILE:HG23	6:M:2400:VAL:CG2	2.36	0.55
9:K:388:LYS:NZ	10:L:451:LEU:O	2.39	0.55
10:L:495:LEU:HD12	10:L:499:LEU:HD23	1.88	0.55
2:F:70:VAL:O	2:F:74:GLU:OE1	2.24	0.55
6:M:322:GLN:O	6:M:326:MET:HE1	2.07	0.55
6:M:1888:ASP:O	6:M:1896:ILE:HG21	2.06	0.55
6:M:3518:VAL:O	6:M:3522:THR:HG23	2.06	0.55
6:M:3920:ILE:HD13	6:M:3945:ALA:HA	1.89	0.55
9:K:40:PHE:CD1	9:K:67:ILE:HG23	2.41	0.55
10:L:339:CYS:CB	10:L:340:PHE:HA	2.36	0.55
6:M:1949:ILE:HD11	6:M:2100:LEU:HB2	1.89	0.55
6:M:2539:LEU:HD21	6:M:2813:PHE:CD2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:3925:LEU:HD21	6:M:3962:ARG:HE	1.70	0.55
6:M:4047:ALA:O	6:M:4051:LEU:HD23	2.07	0.55
10:L:164:PHE:C	10:L:165:LEU:HD22	2.31	0.55
4:D:104:ALA:O	4:D:108:VAL:HG23	2.07	0.55
6:M:1054:VAL:O	6:M:1054:VAL:HG13	2.07	0.55
8:J:126:DG:C2'	8:J:127:DT:H72	2.36	0.55
5:I:148:DG:H1'	5:I:149:DC:C4	2.41	0.55
6:M:188:GLU:O	6:M:189:MET:O	2.24	0.55
6:M:900:GLU:OE2	6:M:2535:THR:HG23	2.07	0.55
5:I:2:DA:N6	8:J:163:DT:C4	2.75	0.54
5:I:138:DA:H1'	5:I:139:DG:C5	2.42	0.54
6:M:1715:GLU:O	6:M:1718:ILE:HG22	2.06	0.54
6:M:2183:HIS:CE1	6:M:2186:VAL:HG23	2.42	0.54
6:M:2238:ILE:HG23	6:M:2279:ILE:HD13	1.90	0.54
6:M:2930:TYR:HA	6:M:2933:ILE:HG22	1.89	0.54
6:M:1946:ASN:HA	6:M:1949:ILE:HG22	1.88	0.54
6:M:416:SER:O	6:M:420:VAL:HG22	2.08	0.54
9:K:97:VAL:HG12	9:K:97:VAL:O	2.08	0.54
1:A:61:LEU:HD11	2:B:36:ARG:CB	2.37	0.54
8:J:92:DC:H2''	8:J:93:DC:H5'	1.89	0.54
10:L:231:LEU:HD21	10:L:511:HIS:CD2	2.43	0.54
5:I:2:DA:C6	8:J:163:DT:N3	2.75	0.54
6:M:1678:LEU:HD12	6:M:1679:LEU:HD12	1.90	0.54
6:M:2445:LYS:O	6:M:2445:LYS:HG3	2.08	0.54
3:G:21:ALA:C	4:H:117:LYS:NZ	2.65	0.54
5:I:156:DA:H2''	5:I:157:DT:C7	2.38	0.54
5:I:156:DA:H2''	5:I:157:DT:H73	1.90	0.54
6:M:214:GLU:OE2	6:M:219:VAL:HG21	2.09	0.54
6:M:1845:VAL:HG13	6:M:1846:ASP:H	1.73	0.54
4:H:34:TYR:HB2	4:H:60:ASN:OD1	2.08	0.53
5:I:77:DA:H2''	5:I:78:DA:C8	2.43	0.53
6:M:2958:LEU:CD1	6:M:4101:GLU:HG2	2.37	0.53
8:J:111:DC:H2''	8:J:112:DT:H71	1.89	0.53
10:L:91:LEU:O	10:L:94:ILE:HG22	2.09	0.53
1:E:103:LEU:HG	1:E:124:ILE:HD11	1.90	0.53
6:M:2144:LEU:O	6:M:2144:LEU:HD23	2.08	0.53
6:M:2536:LEU:O	6:M:2540:LEU:HD13	2.09	0.53
6:M:3297:VAL:HG12	6:M:3301:LEU:CD2	2.38	0.53
8:J:121:DG:C2	8:J:122:DG:C6	2.96	0.53
4:H:104:ALA:O	4:H:108:VAL:HG12	2.09	0.53
6:M:708:VAL:HG22	6:M:740:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:914:VAL:HG21	6:M:933:LEU:HD22	1.90	0.53
6:M:3463:LEU:O	6:M:3463:LEU:HD23	2.09	0.53
3:G:112:GLN:HE22	3:G:114:VAL:HG23	1.73	0.53
6:M:214:GLU:O	6:M:214:GLU:HG2	2.08	0.53
6:M:3470:GLN:CB	6:M:4004:VAL:HG11	2.38	0.53
9:K:146:VAL:HG13	9:K:147:LEU:HD22	1.91	0.53
6:M:129:ASP:O	6:M:132:ILE:HG22	2.08	0.53
6:M:1437:TYR:CE2	6:M:1510:LEU:HD21	2.43	0.53
6:M:2281:MET:HB3	6:M:2329:TYR:OH	2.08	0.53
5:I:130:DA:H2'	5:I:131:DC:C5	2.44	0.53
6:M:654:ILE:HG21	6:M:706:LEU:HD21	1.90	0.53
9:K:362:LEU:HD21	10:L:267:ILE:HG21	1.91	0.53
1:A:126:LEU:O	1:A:127:ALA:C	2.50	0.53
5:I:66:DC:H2''	5:I:67:DT:C6	2.43	0.53
6:M:246:ARG:HA	6:M:249:PHE:CZ	2.44	0.53
10:L:154:LEU:HD23	10:L:215:LEU:HD13	1.89	0.53
6:M:1843:ILE:CD1	6:M:1876:ILE:HD12	2.39	0.53
6:M:3940:ILE:HG23	6:M:3940:ILE:O	2.09	0.53
6:M:230:LEU:HD23	6:M:230:LEU:H	1.74	0.53
6:M:1743:MET:HE3	6:M:1774:MET:HE2	1.90	0.53
6:M:2428:ASP:O	6:M:2429:ASP:CG	2.52	0.53
6:M:2442:MET:HE1	6:M:2446:LEU:HD21	1.90	0.53
3:C:112:GLN:N	3:C:115:LEU:HD12	2.24	0.52
8:J:12:DC:C2	8:J:13:DG:C8	2.97	0.52
1:E:68:GLN:O	1:E:71:VAL:HG12	2.10	0.52
1:E:82:LEU:CD1	2:F:70:VAL:HG22	2.40	0.52
5:I:119:DA:H2''	5:I:120:DG:C8	2.44	0.52
6:M:1019:ASP:OD1	6:M:1021:VAL:HG12	2.09	0.52
4:H:106:HIS:O	4:H:110:GLU:OE1	2.27	0.52
6:M:43:VAL:HG13	6:M:44:LEU:HD22	1.92	0.52
6:M:962:TYR:HA	6:M:965:THR:HG22	1.91	0.52
6:M:1479:VAL:O	6:M:1482:GLU:HG3	2.09	0.52
6:M:3084:GLN:HE21	6:M:3135:LEU:HD12	1.74	0.52
6:M:990:GLN:HB2	6:M:2780:LEU:O	2.08	0.52
9:K:280:ALA:HB3	10:L:428:GLU:OE1	2.09	0.52
10:L:32:GLU:HA	10:L:35:LYS:HG2	1.91	0.52
10:L:467:ASP:O	10:L:468:GLU:HG2	2.09	0.52
2:B:98:TYR:HB2	3:G:102:ILE:HD13	1.90	0.52
6:M:2462:VAL:N	6:M:2473:MET:HE1	2.24	0.52
6:M:3842:TRP:CZ2	6:M:3867:THR:HG23	2.45	0.52
8:J:86:DT:H2''	8:J:87:DT:C7	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:3301:LEU:HA	6:M:3304:VAL:HG12	1.91	0.52
6:M:3883:LEU:CB	6:M:3970:LEU:HD21	2.39	0.52
9:K:301:ARG:NH2	10:L:294:VAL:HG22	2.24	0.52
9:K:361:TYR:CE1	10:L:422:VAL:HG22	2.45	0.52
9:K:478:PHE:O	10:L:427:MET:HB2	2.09	0.52
1:A:74:ILE:HD12	2:B:66:ILE:HD13	1.91	0.52
6:M:478:CYS:O	6:M:482:VAL:HG23	2.10	0.52
8:J:52:DA:H2'	8:J:53:DC:C6	2.45	0.52
4:H:56:MET:HE3	4:H:56:MET:O	2.10	0.52
6:M:184:VAL:HG12	6:M:184:VAL:O	2.10	0.52
1:A:61:LEU:HD11	2:B:36:ARG:HB3	1.92	0.52
3:C:95:LYS:HE2	4:D:100:PRO:HB3	1.90	0.52
5:I:61:DA:C2	8:J:105:DT:O2	2.63	0.52
3:G:16:THR:HG23	3:G:19:SER:H	1.74	0.52
6:M:2089:ASN:CG	6:M:2094:MET:HE3	2.35	0.52
2:F:88:TYR:CZ	4:H:80:TYR:CE1	2.98	0.51
1:E:61:LEU:CD1	2:F:36:ARG:HE	2.24	0.51
6:M:2166:SER:N	6:M:2167:PRO:HD2	2.24	0.51
6:M:2461:PHE:HB2	6:M:2473:MET:CE	2.40	0.51
6:M:3636:PHE:O	6:M:3640:PHE:HB2	2.11	0.51
6:M:873:VAL:HG13	6:M:873:VAL:O	2.11	0.51
6:M:1482:GLU:O	6:M:1486:LEU:HD23	2.09	0.51
9:K:490:LEU:HD23	9:K:490:LEU:O	2.10	0.51
10:L:339:CYS:HB3	10:L:340:PHE:CA	2.40	0.51
3:C:38:ASN:HB3	3:G:38:ASN:OD1	2.10	0.51
3:G:24:GLN:NE2	4:H:40:LYS:HE2	2.25	0.51
4:H:28:LYS:HZ3	5:I:141:DG:H5''	1.76	0.51
5:I:154:DG:H2''	5:I:155:DG:C8	2.46	0.51
6:M:569:VAL:O	6:M:572:VAL:HG22	2.11	0.51
6:M:1195:VAL:HG23	6:M:1196:PRO:HD3	1.92	0.51
6:M:1626:TRP:HA	6:M:1629:CYS:HB3	1.91	0.51
6:M:1757:MET:O	6:M:1761:LEU:HD23	2.11	0.51
6:M:2205:VAL:HG22	6:M:2206:PRO:CD	2.39	0.51
6:M:2361:ILE:O	6:M:2364:LEU:HD23	2.11	0.51
6:M:1369:MET:HE2	6:M:1414:ILE:HG23	1.93	0.51
9:K:84:ALA:O	9:K:85:VAL:HG12	2.10	0.51
9:K:246:VAL:HG23	9:K:246:VAL:O	2.09	0.51
4:D:58:ILE:HG13	2:F:98:TYR:HB3	1.92	0.51
1:E:108:ASN:O	1:E:112:ILE:HG22	2.11	0.51
6:M:913:ARG:O	6:M:917:LEU:HD23	2.10	0.51
6:M:1845:VAL:HG13	6:M:1846:ASP:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:38:ALA:HB1	2:F:43:VAL:HB	1.92	0.51
4:H:91:ILE:O	4:H:95:VAL:HG23	2.10	0.51
6:M:3173:MET:HE1	6:M:3782:SER:C	2.36	0.51
6:M:3526:PRO:O	6:M:3530:VAL:HG23	2.11	0.51
6:M:3883:LEU:HB3	6:M:3970:LEU:HD11	1.92	0.51
6:M:85:ILE:O	6:M:89:LEU:HD23	2.10	0.51
6:M:3427:GLU:OE2	6:M:3437:ALA:HB2	2.11	0.51
8:J:123:DC:C2	8:J:124:DA:N7	2.79	0.51
10:L:205:LEU:HA	10:L:208:VAL:HG12	1.93	0.51
6:M:93:LEU:HD21	6:M:107:ILE:HD13	1.92	0.51
6:M:1916:ILE:HA	6:M:1919:CYS:SG	2.50	0.51
6:M:2274:ILE:HG23	6:M:2322:VAL:HG11	1.93	0.51
6:M:2359:LYS:C	6:M:2361:ILE:H	2.18	0.51
8:J:2:DT:H2'	8:J:3:DC:C1'	2.41	0.51
10:L:246:HIS:CD2	10:L:246:HIS:O	2.64	0.51
6:M:1718:ILE:HD11	6:M:1765:VAL:HG22	1.92	0.51
1:A:61:LEU:C	1:A:61:LEU:HD23	2.37	0.50
1:A:104:PHE:CG	2:B:38:ALA:HA	2.45	0.50
6:M:189:MET:HE1	6:M:191:ASN:O	2.11	0.50
6:M:3414:MET:HA	6:M:3414:MET:HE2	1.93	0.50
2:F:83:ALA:O	2:F:87:VAL:HG23	2.11	0.50
6:M:346:TYR:HA	6:M:349:ILE:CG1	2.41	0.50
6:M:2340:SER:O	6:M:2344:LEU:HD13	2.11	0.50
6:M:116:THR:HG22	6:M:117:LYS:N	2.26	0.50
6:M:3052:LEU:C	6:M:3052:LEU:HD23	2.36	0.50
6:M:3515:GLN:O	6:M:3518:VAL:HG12	2.11	0.50
6:M:1267:TYR:CD2	6:M:1290:LEU:HD13	2.47	0.50
6:M:1933:LEU:HD12	6:M:1933:LEU:O	2.11	0.50
10:L:163:PHE:H	10:L:224:ILE:HG22	1.77	0.50
6:M:1626:TRP:HE1	6:M:1671:VAL:HG22	1.77	0.50
6:M:3124:SER:O	6:M:3127:THR:HG22	2.10	0.50
5:I:10:DA:H61	8:J:155:DT:H3	1.60	0.50
6:M:139:ARG:HG2	6:M:140:SER:N	2.25	0.50
6:M:431:TYR:O	6:M:434:VAL:HG12	2.10	0.50
6:M:2100:LEU:C	6:M:2100:LEU:HD23	2.37	0.50
6:M:2459:VAL:HG13	6:M:2505:VAL:HG11	1.92	0.50
6:M:464:VAL:O	6:M:468:LEU:HD23	2.12	0.50
4:D:111:GLY:O	4:D:115:VAL:HG23	2.11	0.49
2:F:89:ALA:O	2:F:93:GLN:HG3	2.12	0.49
6:M:223:CYS:O	6:M:227:LEU:HD13	2.12	0.49
3:C:50:TYR:O	3:C:54:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:69:ARG:NE	4:D:69:ARG:HA	2.27	0.49
3:G:24:GLN:NE2	4:H:40:LYS:HB2	2.24	0.49
6:M:3438:GLU:HG2	6:M:3439:LEU:N	2.27	0.49
6:M:3614:TYR:O	6:M:3615:ALA:HB3	2.12	0.49
6:M:3640:PHE:CE1	6:M:3666:LEU:HD13	2.47	0.49
10:L:28:GLU:OE2	10:L:32:GLU:HB3	2.12	0.49
6:M:400:THR:HG22	6:M:401:ASP:OD1	2.12	0.49
6:M:1776:GLU:HG3	6:M:1777:LEU:HD12	1.94	0.49
8:J:112:DT:H6	8:J:112:DT:H5'	1.76	0.49
3:G:80:PRO:HG3	4:H:55:ALA:HA	1.93	0.49
6:M:1946:ASN:O	6:M:1949:ILE:HG22	2.11	0.49
6:M:3764:VAL:HG21	6:M:3941:ASP:OD2	2.12	0.49
9:K:207:LYS:HB3	9:K:208:PRO:HD2	1.93	0.49
1:A:118:THR:HA	2:B:45:ARG:HG2	1.94	0.49
6:M:2220:MET:HE2	6:M:2220:MET:CA	2.42	0.49
6:M:3326:GLN:O	6:M:3330:LEU:HD23	2.12	0.49
1:A:126:LEU:HD21	1:E:113:HIS:ND1	2.27	0.49
6:M:220:LEU:HD21	6:M:267:VAL:HG21	1.94	0.49
6:M:762:TYR:CD2	6:M:765:LEU:HD13	2.48	0.49
6:M:1430:GLU:HG3	6:M:1434:VAL:HG13	1.95	0.49
9:K:143:LEU:HD23	9:K:182:LYS:HA	1.94	0.49
6:M:3389:VAL:HG22	6:M:3389:VAL:O	2.11	0.49
10:L:166:PRO:O	10:L:167:PHE:C	2.55	0.49
3:C:50:TYR:CE1	4:D:111:GLY:HA3	2.48	0.49
4:D:42:LEU:HD22	4:D:51:ILE:HG23	1.94	0.49
6:M:1675:TYR:O	6:M:1679:LEU:HD13	2.13	0.49
6:M:2474:TYR:O	6:M:2478:MET:HG3	2.13	0.49
6:M:3606:ILE:O	6:M:3606:ILE:HG22	2.12	0.49
10:L:266:SER:O	10:L:267:ILE:C	2.56	0.49
1:A:61:LEU:HD11	2:B:36:ARG:C	2.38	0.49
8:J:42:DC:H2''	8:J:43:DA:O5'	2.12	0.49
9:K:258:ARG:C	9:K:259:LEU:HD12	2.38	0.49
9:K:477:SER:O	9:K:478:PHE:CG	2.66	0.49
3:G:17:ARG:O	3:G:21:ALA:HB2	2.12	0.49
6:M:1112:ALA:HB1	6:M:1180:GLN:NE2	2.28	0.49
9:K:289:TYR:CD1	10:L:297:LEU:HD12	2.47	0.49
10:L:262:ALA:HB3	10:L:366:ALA:O	2.13	0.49
5:I:27:DA:H2'	5:I:28:DT:H72	1.95	0.48
5:I:27:DA:N6	8:J:137:DA:N6	2.60	0.48
5:I:32:DT:H2'	5:I:33:DC:C5	2.48	0.48
6:M:3281:CYS:HB3	6:M:3329:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:114:DG:C2	8:J:52:DA:C2	3.01	0.48
6:M:718:MET:HE3	6:M:730:LEU:HD21	1.93	0.48
6:M:933:LEU:C	6:M:933:LEU:HD23	2.37	0.48
6:M:1718:ILE:CD1	6:M:1765:VAL:HG22	2.43	0.48
6:M:3627:ALA:O	6:M:3628:PHE:HD1	1.95	0.48
6:M:3636:PHE:O	6:M:3640:PHE:CB	2.61	0.48
9:K:201:ASP:O	9:K:202:LEU:C	2.56	0.48
2:F:39:ARG:NH1	2:F:44:LYS:HA	2.28	0.48
6:M:198:ARG:NH2	9:K:312:LEU:HB3	2.28	0.48
6:M:207:GLN:HA	6:M:211:ALA:HA	1.95	0.48
6:M:1386:ILE:HG22	6:M:1387:GLY:N	2.28	0.48
6:M:2540:LEU:HD21	6:M:2832:ILE:HB	1.95	0.48
2:B:39:ARG:HA	2:B:43:VAL:HG12	1.95	0.48
2:B:62:LEU:O	2:B:63:GLU:C	2.56	0.48
3:C:102:ILE:HG13	4:D:58:ILE:CD1	2.44	0.48
3:G:33:LEU:HD23	3:G:33:LEU:C	2.38	0.48
5:I:65:DC:H2''	5:I:66:DC:C5	2.49	0.48
1:E:112:ILE:HG23	1:E:113:HIS:CD2	2.48	0.48
6:M:568:PHE:O	6:M:572:VAL:HG13	2.13	0.48
6:M:1438:GLY:N	6:M:1439:PRO:HD2	2.28	0.48
6:M:2461:PHE:C	6:M:2473:MET:HE1	2.38	0.48
6:M:3129:LEU:O	6:M:3132:VAL:HG12	2.14	0.48
8:J:42:DC:H4'	8:J:43:DA:OP1	2.12	0.48
3:G:32:ARG:HH12	8:J:29:DA:H2'	1.79	0.48
6:M:1411:TYR:CZ	6:M:1414:ILE:HG21	2.49	0.48
6:M:1670:GLU:HA	6:M:1673:THR:HG22	1.96	0.48
6:M:3089:LEU:HD13	6:M:3092:LEU:HD12	1.94	0.48
8:J:63:DG:C4	8:J:64:DC:C5	3.02	0.48
10:L:376:ALA:O	10:L:377:LEU:HB3	2.12	0.48
3:C:55:LEU:HD21	4:D:63:VAL:HG13	1.96	0.48
5:I:130:DA:H2''	5:I:131:DC:C6	2.49	0.48
6:M:2359:LYS:C	6:M:2361:ILE:N	2.72	0.48
9:K:130:ARG:O	9:K:134:MET:HG2	2.14	0.48
6:M:860:GLY:HA3	6:M:3136:THR:HG21	1.94	0.48
6:M:2201:THR:N	6:M:2202:PRO:HD2	2.29	0.48
6:M:2311:ARG:HB3	6:M:2315:VAL:O	2.14	0.48
10:L:149:ILE:HG23	10:L:150:ILE:HD12	1.94	0.48
10:L:220:GLY:HA2	10:L:223:GLU:OE1	2.13	0.48
6:M:253:LEU:HA	6:M:256:ILE:HG22	1.95	0.48
6:M:708:VAL:HA	6:M:740:ILE:HD11	1.95	0.48
6:M:907:LEU:HD23	6:M:907:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:2307:MET:SD	6:M:2307:MET:C	2.97	0.48
8:J:44:DG:H2'	8:J:45:DC:C6	2.49	0.48
1:E:69:ARG:HB2	2:F:25:ASN:ND2	2.29	0.48
3:G:78:ILE:HD11	4:H:49:THR:HG21	1.95	0.48
6:M:987:LEU:O	6:M:990:GLN:HG3	2.13	0.48
6:M:1870:LYS:O	6:M:1874:TYR:CD2	2.67	0.48
6:M:2443:MET:N	6:M:2444:PRO:CD	2.76	0.48
4:D:39:TYR:HE1	4:D:51:ILE:HD11	1.78	0.47
2:F:71:THR:OG1	4:H:97:LEU:HD21	2.13	0.47
3:G:32:ARG:O	3:G:35:ARG:HG2	2.13	0.47
5:I:54:DG:H2''	5:I:55:DG:C8	2.48	0.47
5:I:141:DG:C2'	5:I:142:DG:C8	2.97	0.47
6:M:737:PRO:O	6:M:740:ILE:HG22	2.13	0.47
6:M:776:TRP:HB3	6:M:785:MET:HE1	1.96	0.47
6:M:985:GLU:HG3	6:M:986:PRO:HD3	1.96	0.47
6:M:2361:ILE:HG23	6:M:2400:VAL:HG21	1.95	0.47
3:C:29:ARG:CZ	4:D:32:GLU:OE2	2.62	0.47
5:I:73:DG:H4'	5:I:74:DT:OP1	2.13	0.47
5:I:146:DC:H2''	5:I:147:DG:C8	2.49	0.47
6:M:2405:VAL:HG22	6:M:2406:GLU:N	2.30	0.47
6:M:3089:LEU:HD12	6:M:3092:LEU:HD12	1.93	0.47
1:A:127:ALA:O	1:A:131:ARG:N	2.47	0.47
6:M:82:ARG:O	6:M:86:LEU:HD23	2.15	0.47
6:M:1301:ILE:HG22	6:M:1334:LYS:HD2	1.96	0.47
6:M:1920:TYR:HE1	6:M:1952:ILE:HD11	1.79	0.47
9:K:90:THR:HG21	9:K:103:TYR:HB2	1.96	0.47
10:L:528:ILE:HB	10:L:529:PRO:HD3	1.96	0.47
6:M:110:THR:O	6:M:110:THR:HG22	2.13	0.47
6:M:2215:LEU:O	6:M:2219:LEU:HD13	2.15	0.47
6:M:3962:ARG:O	6:M:3962:ARG:HG3	2.14	0.47
1:E:61:LEU:HD11	2:F:36:ARG:CB	2.45	0.47
2:F:84:MET:HB3	2:F:88:TYR:CE2	2.49	0.47
3:G:55:LEU:CD2	4:H:66:VAL:HG23	2.45	0.47
6:M:1149:LYS:HA	6:M:1149:LYS:HE2	1.96	0.47
6:M:1483:LEU:HD11	6:M:1514:LEU:HD13	1.96	0.47
8:J:92:DC:C2'	8:J:93:DC:H5'	2.45	0.47
9:K:207:LYS:O	9:K:208:PRO:C	2.58	0.47
9:K:424:LYS:O	9:K:424:LYS:HD3	2.15	0.47
10:L:407:VAL:HG23	10:L:424:LEU:CD2	2.45	0.47
1:A:54:TYR:CD2	1:A:54:TYR:O	2.68	0.47
2:B:44:LYS:HD2	3:G:115:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:LEU:CD2	2:F:65:VAL:HG11	2.45	0.47
5:I:107:DA:H1'	5:I:108:DA:C8	2.49	0.47
6:M:224:LEU:HD23	6:M:271:GLY:HA2	1.96	0.47
6:M:1190:LEU:HG	6:M:1194:PHE:CE2	2.49	0.47
6:M:2364:LEU:HB3	6:M:2378:PHE:CD2	2.49	0.47
8:J:1:DA:HO5'	8:J:1:DA:H8	1.61	0.47
1:A:54:TYR:HB3	2:B:39:ARG:NE	2.29	0.47
3:C:114:VAL:HG12	1:E:112:ILE:CD1	2.40	0.47
1:E:100:LEU:O	1:E:104:PHE:CD2	2.68	0.47
4:H:117:LYS:C	4:H:117:LYS:HD2	2.40	0.47
5:I:67:DT:H2''	5:I:68:DT:H72	1.96	0.47
6:M:290:TYR:O	6:M:290:TYR:CD1	2.67	0.47
6:M:291:VAL:HG12	6:M:291:VAL:O	2.14	0.47
6:M:1882:SER:O	6:M:1883:ARG:HG2	2.15	0.47
6:M:1920:TYR:CE1	6:M:1952:ILE:HD11	2.50	0.47
6:M:1952:ILE:HG22	6:M:1961:PHE:CD1	2.50	0.47
6:M:2943:PHE:HA	6:M:2947:ILE:HG23	1.97	0.47
6:M:3302:LYS:O	6:M:3302:LYS:CD	2.61	0.47
6:M:3475:TYR:N	6:M:3476:PRO:HD2	2.30	0.47
6:M:3953:LEU:O	6:M:3954:PRO:C	2.57	0.47
10:L:294:VAL:HG23	10:L:294:VAL:O	2.14	0.47
10:L:364:VAL:O	10:L:364:VAL:HG23	2.14	0.47
5:I:109:DG:H2''	5:I:110:DC:C6	2.50	0.47
6:M:960:GLN:HG2	6:M:961:LEU:N	2.29	0.47
6:M:2326:ILE:HA	6:M:2329:TYR:CD2	2.50	0.47
6:M:3124:SER:HA	6:M:3127:THR:HG22	1.96	0.47
3:C:78:ILE:HB	4:D:51:ILE:HG22	1.97	0.47
3:G:21:ALA:C	4:H:117:LYS:HZ1	2.23	0.47
5:I:89:DC:H2''	5:I:90:DA:C8	2.50	0.47
6:M:1157:PHE:H	6:M:1158:PRO:CD	2.27	0.47
6:M:2197:THR:O	6:M:2198:GLY:C	2.58	0.47
8:J:64:DC:H2'	8:J:65:DA:H8	1.80	0.47
5:I:148:DG:H1'	5:I:149:DC:C5	2.50	0.47
6:M:333:MET:HE3	6:M:333:MET:HA	1.97	0.47
6:M:582:THR:HB	6:M:584:GLU:OE1	2.15	0.47
6:M:3932:MET:HE3	6:M:3932:MET:O	2.15	0.47
1:A:83:ARG:O	2:B:80:THR:HA	2.15	0.46
4:H:62:PHE:CE1	4:H:66:VAL:HG13	2.50	0.46
6:M:1802:TYR:CE2	6:M:1843:ILE:HG22	2.50	0.46
6:M:2568:MET:HG2	6:M:2568:MET:O	2.15	0.46
3:G:107:VAL:HG22	3:G:108:LEU:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:1195:VAL:N	6:M:1196:PRO:HD2	2.30	0.46
5:I:161:DC:H2''	5:I:162:DG:C8	2.50	0.46
6:M:2555:LEU:O	6:M:2559:THR:HG23	2.15	0.46
6:M:2992:ASP:O	6:M:2996:LEU:HD23	2.16	0.46
6:M:3297:VAL:O	6:M:3301:LEU:HD23	2.15	0.46
6:M:3613:MET:HE1	6:M:3647:GLY:O	2.16	0.46
8:J:64:DC:H2'	8:J:65:DA:C8	2.50	0.46
9:K:84:ALA:O	9:K:85:VAL:O	2.33	0.46
1:A:127:ALA:C	1:A:131:ARG:HG2	2.40	0.46
3:C:97:LEU:N	3:C:97:LEU:HD12	2.30	0.46
1:E:70:LEU:O	1:E:73:GLU:HB2	2.15	0.46
3:G:62:ILE:CD1	4:H:62:PHE:HE2	2.29	0.46
6:M:116:THR:HG22	6:M:117:LYS:HG3	1.97	0.46
6:M:2480:ILE:O	6:M:2484:TYR:CD1	2.68	0.46
10:L:24:ILE:HG13	10:L:24:ILE:O	2.15	0.46
3:C:13:LYS:HD2	3:C:14:ALA:N	2.30	0.46
1:E:49:ARG:HD3	1:E:49:ARG:N	2.30	0.46
2:F:44:LYS:O	2:F:46:ILE:HD12	2.16	0.46
6:M:115:TYR:CG	6:M:155:LYS:HE2	2.51	0.46
6:M:335:LYS:O	6:M:339:GLN:HG2	2.15	0.46
6:M:1249:SER:C	6:M:1250:LEU:HD12	2.40	0.46
6:M:2485:ARG:O	6:M:2486:ASP:C	2.57	0.46
6:M:2589:TYR:HD1	6:M:2775:TYR:HH	1.62	0.46
10:L:34:ALA:O	10:L:37:VAL:HG12	2.16	0.46
1:E:73:GLU:HA	2:F:22:LEU:HD11	1.97	0.46
5:I:24:DT:H2''	5:I:25:DG:O5'	2.14	0.46
6:M:1478:SER:O	6:M:1479:VAL:CG2	2.58	0.46
6:M:3100:LYS:HA	6:M:3103:ILE:HG22	1.96	0.46
3:C:24:GLN:OE1	4:D:40:LYS:NZ	2.48	0.46
1:E:67:PHE:CG	1:E:93:GLN:OE1	2.68	0.46
2:F:83:ALA:HB1	2:F:100:PHE:CD2	2.51	0.46
5:I:123:DG:C2	8:J:43:DA:C2	3.03	0.46
5:I:128:DC:C2'	5:I:129:DG:C8	2.98	0.46
6:M:643:GLU:N	6:M:644:PRO:HD2	2.31	0.46
6:M:3789:ARG:HB2	6:M:3938:ILE:HG22	1.98	0.46
6:M:3913:ILE:HB	6:M:3984:MET:HG2	1.98	0.46
5:I:7:DG:H2'	5:I:8:DT:H72	1.97	0.46
6:M:3134:ALA:O	6:M:3138:ILE:HG12	2.16	0.46
6:M:3285:HIS:CE1	6:M:3333:THR:HG23	2.51	0.46
6:M:3619:ASP:HB2	6:M:3620:PRO:HD2	1.96	0.46
8:J:20:DA:H2''	8:J:21:DG:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:311:LEU:C	9:K:312:LEU:HD22	2.41	0.46
10:L:157:CYS:O	10:L:158:ASP:OD1	2.33	0.46
1:A:122:LYS:O	1:A:126:LEU:HD23	2.16	0.46
2:B:62:LEU:O	2:B:66:ILE:HD12	2.15	0.46
2:F:53:GLU:O	2:F:57:VAL:HG22	2.16	0.46
6:M:1101:PHE:HE1	6:M:1153:LEU:HD11	1.79	0.46
6:M:2198:GLY:O	6:M:2199:LEU:HD12	2.16	0.46
6:M:3816:LEU:HD21	6:M:3883:LEU:CD2	2.46	0.46
10:L:13:CYS:HG	10:L:59:PHE:HE2	1.62	0.46
10:L:216:GLU:HB2	10:L:220:GLY:HA3	1.98	0.46
2:F:88:TYR:HB3	2:F:91:LYS:HE3	1.97	0.46
3:G:39:TYR:CE2	4:H:71:ALA:HB1	2.51	0.46
5:I:99:DG:H2'	5:I:100:DT:H71	1.98	0.46
6:M:948:MET:O	6:M:948:MET:SD	2.74	0.46
6:M:1131:ILE:HD12	6:M:1131:ILE:H	1.81	0.46
6:M:2372:PRO:N	6:M:2373:PRO:CD	2.79	0.46
6:M:3274:VAL:HA	6:M:3277:VAL:HG12	1.98	0.46
6:M:3465:PHE:N	6:M:3466:PRO:CD	2.79	0.46
8:J:11:DC:C4	8:J:12:DC:N4	2.84	0.46
8:J:92:DC:H2'	8:J:93:DC:C6	2.51	0.46
9:K:146:VAL:O	9:K:149:VAL:HG12	2.16	0.46
9:K:360:HIS:HB3	9:K:438:PRO:HD3	1.98	0.46
10:L:251:LEU:O	10:L:259:ILE:HA	2.16	0.46
3:C:12:ALA:O	3:C:13:LYS:O	2.34	0.45
3:C:115:LEU:HD13	2:F:44:LYS:HZ1	1.80	0.45
6:M:1017:ILE:HD11	6:M:1080:LEU:HD22	1.97	0.45
6:M:1080:LEU:C	6:M:1080:LEU:HD23	2.41	0.45
6:M:1960:LYS:O	10:L:728:LEU:HD11	2.16	0.45
6:M:2135:ASN:OD1	6:M:2137:ILE:HG22	2.17	0.45
6:M:2220:MET:HE2	6:M:2220:MET:HA	1.97	0.45
6:M:2995:GLU:O	6:M:2999:LEU:HD23	2.16	0.45
8:J:1:DA:H2''	8:J:2:DT:H71	1.97	0.45
3:G:79:ILE:HD12	3:G:81:ARG:CG	2.46	0.45
6:M:2496:GLN:O	6:M:2499:PHE:HB3	2.16	0.45
6:M:2584:CYS:SG	6:M:2781:PRO:HD2	2.56	0.45
6:M:3628:PHE:CE2	6:M:3686:TRP:HA	2.52	0.45
8:J:45:DC:H4'	8:J:46:DT:OP1	2.16	0.45
8:J:116:DC:H2'	8:J:117:DT:H71	1.96	0.45
10:L:97:LYS:HG3	10:L:97:LYS:O	2.17	0.45
2:B:90:LEU:HB3	2:B:95:ARG:O	2.16	0.45
4:H:53:SER:O	4:H:56:MET:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:67:PHE:CD2	4:H:68:GLU:N	2.85	0.45
5:I:158:DT:C2	5:I:159:DC:C5	3.04	0.45
6:M:66:LEU:HA	6:M:69:VAL:HG22	1.98	0.45
6:M:91:ILE:HG13	6:M:92:PHE:N	2.30	0.45
6:M:241:ASP:HB3	6:M:242:PRO:HD3	1.97	0.45
6:M:2916:LEU:HD21	6:M:2920:VAL:HB	1.98	0.45
6:M:3114:TYR:O	6:M:3117:ILE:HG22	2.16	0.45
5:I:67:DT:H2''	5:I:68:DT:C7	2.46	0.45
6:M:2361:ILE:HA	6:M:2364:LEU:CD2	2.46	0.45
8:J:84:DC:C2	8:J:85:DG:C5	3.04	0.45
9:K:361:TYR:O	9:K:362:LEU:HD22	2.16	0.45
3:G:78:ILE:HB	4:H:51:ILE:HD12	1.98	0.45
5:I:33:DC:H2''	5:I:34:DT:H71	1.99	0.45
6:M:892:LEU:HD21	6:M:940:PHE:CE1	2.51	0.45
6:M:3065:ILE:HD13	6:M:3089:LEU:HD23	1.97	0.45
10:L:284:LEU:O	10:L:284:LEU:HD12	2.17	0.45
3:G:21:ALA:O	3:G:23:LEU:N	2.49	0.45
5:I:1:DC:C6	5:I:2:DA:C2	3.05	0.45
5:I:134:DA:C8	5:I:135:DT:H72	2.51	0.45
8:J:3:DC:H2''	8:J:4:DG:C8	2.52	0.45
1:A:54:TYR:O	1:A:54:TYR:CG	2.70	0.45
1:A:61:LEU:HD21	2:B:36:ARG:HB2	1.99	0.45
2:B:39:ARG:C	2:B:39:ARG:HH11	2.24	0.45
3:C:102:ILE:HG13	4:D:58:ILE:HD11	1.99	0.45
5:I:101:DG:H2''	5:I:102:DC:C6	2.52	0.45
5:I:126:DT:H4'	5:I:127:DA:H5'	1.99	0.45
6:M:704:PHE:O	6:M:708:VAL:HG23	2.16	0.45
6:M:3097:ASP:OD2	6:M:3098:ARG:N	2.49	0.45
8:J:71:DG:C4	8:J:72:DC:C5	3.04	0.45
10:L:378:SER:HA	10:L:381:ILE:HG22	1.99	0.45
3:G:42:ARG:HD2	5:I:129:DG:O3'	2.17	0.45
4:H:113:LYS:O	4:H:117:LYS:HG3	2.17	0.45
5:I:160:DT:H2''	5:I:161:DC:C6	2.50	0.45
6:M:1946:ASN:C	6:M:1946:ASN:HD22	2.24	0.45
6:M:2235:LEU:O	6:M:2238:ILE:HG22	2.17	0.45
6:M:3447:VAL:HG23	6:M:3448:GLU:N	2.32	0.45
3:G:79:ILE:CD1	3:G:81:ARG:HG3	2.46	0.45
6:M:184:VAL:C	6:M:186:PRO:HD2	2.42	0.45
6:M:525:LYS:O	6:M:528:VAL:HG12	2.16	0.45
6:M:1231:GLN:N	6:M:1232:PRO:CD	2.80	0.45
6:M:1877:LEU:HA	6:M:1880:MET:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:2543:ASN:OD1	6:M:2839:ASP:HB3	2.16	0.45
9:K:146:VAL:HG13	9:K:147:LEU:N	2.32	0.45
10:L:342:VAL:HG22	10:L:344:GLY:H	1.82	0.45
1:E:73:GLU:HG2	2:F:22:LEU:HD13	1.99	0.45
6:M:129:ASP:O	6:M:133:LYS:HG2	2.17	0.45
6:M:371:GLY:N	6:M:372:PRO:CD	2.80	0.45
6:M:1103:ALA:HA	6:M:1106:ILE:HG22	1.99	0.45
6:M:1684:LEU:HD12	6:M:1684:LEU:N	2.32	0.45
6:M:2274:ILE:HD12	6:M:2274:ILE:H	1.82	0.45
6:M:3074:GLN:O	6:M:3078:LEU:HD23	2.17	0.45
6:M:3619:ASP:OD1	6:M:3622:ALA:HB3	2.17	0.45
6:M:3971:MET:O	6:M:3974:MET:O	2.35	0.45
8:J:86:DT:H2''	8:J:87:DT:H72	1.99	0.45
9:K:493:LEU:HD13	10:L:323:PHE:CZ	2.52	0.45
10:L:279:VAL:HG13	10:L:285:LYS:O	2.17	0.45
6:M:1475:LEU:O	6:M:1476:HIS:C	2.60	0.44
6:M:1718:ILE:HG13	6:M:1722:PHE:CD2	2.52	0.44
6:M:3531:TYR:HB2	6:M:3532:PRO:HD3	1.99	0.44
6:M:4111:ALA:O	6:M:4117:LEU:HD21	2.18	0.44
9:K:525:PHE:O	9:K:528:LEU:HB3	2.17	0.44
3:G:24:GLN:HE21	4:H:40:LYS:HE2	1.82	0.44
5:I:40:DG:C2	8:J:126:DG:C2	3.05	0.44
5:I:128:DC:H2'	5:I:129:DG:C8	2.52	0.44
5:I:132:DC:C2	5:I:133:DA:N7	2.85	0.44
6:M:330:ASN:O	6:M:331:ALA:HB3	2.16	0.44
6:M:400:THR:HG22	6:M:401:ASP:N	2.33	0.44
6:M:1104:LEU:HD23	6:M:1168:LEU:HD11	1.99	0.44
6:M:1646:LEU:HD11	6:M:1692:ALA:HB2	1.97	0.44
6:M:3499:ILE:O	6:M:3503:VAL:HG22	2.17	0.44
10:L:66:ASN:OD1	10:L:67:PRO:HD2	2.18	0.44
3:C:30:VAL:HG13	4:D:67:PHE:HE2	1.83	0.44
4:H:72:GLY:O	4:H:76:ARG:HG3	2.18	0.44
6:M:213:ARG:HE	9:K:405:ASN:HB2	1.83	0.44
6:M:1369:MET:CE	6:M:1414:ILE:HG23	2.48	0.44
6:M:2145:PHE:O	6:M:2149:LEU:HG	2.17	0.44
6:M:2219:LEU:C	6:M:2220:MET:HE2	2.42	0.44
6:M:2325:LEU:O	6:M:2329:TYR:CD1	2.70	0.44
6:M:2947:ILE:HG23	6:M:2947:ILE:O	2.17	0.44
6:M:2972:TYR:O	6:M:2976:LEU:HD23	2.17	0.44
6:M:3389:VAL:HG23	6:M:3413:TYR:CE1	2.52	0.44
6:M:3833:ARG:HG2	6:M:3841:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:88:DT:H2''	8:J:89:DT:C6	2.53	0.44
10:L:279:VAL:CG1	10:L:280:ASP:N	2.80	0.44
3:G:33:LEU:CD2	4:H:67:PHE:CZ	2.98	0.44
4:H:115:VAL:O	4:H:119:THR:HG23	2.16	0.44
5:I:158:DT:H1'	5:I:159:DC:C6	2.52	0.44
6:M:327:VAL:HA	6:M:330:ASN:OD1	2.17	0.44
6:M:336:ASN:HA	6:M:339:GLN:HG2	2.00	0.44
6:M:1593:VAL:HA	6:M:1596:VAL:HG12	1.99	0.44
6:M:2088:LEU:CD1	6:M:2144:LEU:HD22	2.47	0.44
6:M:2170:GLN:OE1	6:M:2170:GLN:O	2.36	0.44
6:M:2175:GLU:O	6:M:2175:GLU:HG2	2.17	0.44
8:J:79:DC:H2''	8:J:80:DC:C5	2.52	0.44
8:J:86:DT:H2''	8:J:87:DT:C6	2.52	0.44
8:J:120:DA:H2''	8:J:121:DG:C8	2.53	0.44
9:K:85:VAL:CG1	9:K:106:GLN:HG3	2.48	0.44
3:G:24:GLN:HE21	4:H:37:TYR:HA	1.82	0.44
3:G:102:ILE:HD12	4:H:58:ILE:HG21	1.99	0.44
6:M:1933:LEU:HD12	6:M:1933:LEU:C	2.42	0.44
6:M:3243:ILE:HD11	6:M:3258:LEU:HB3	1.99	0.44
6:M:3816:LEU:HD21	6:M:3883:LEU:HD22	1.98	0.44
9:K:193:LEU:HD11	9:K:198:ILE:HG21	2.00	0.44
9:K:375:VAL:HG13	10:L:541:GLU:H	1.82	0.44
9:K:466:VAL:HG23	10:L:345:PHE:CG	2.53	0.44
10:L:43:GLN:OE1	10:L:491:PHE:HB3	2.18	0.44
6:M:3011:LEU:HD23	6:M:3047:SER:HB3	2.00	0.44
6:M:3880:ALA:O	6:M:3881:ASP:OD1	2.35	0.44
1:E:112:ILE:HG23	1:E:113:HIS:N	2.32	0.44
5:I:84:DG:H4'	5:I:85:DG:OP1	2.18	0.44
6:M:170:VAL:O	6:M:174:VAL:HG23	2.18	0.44
6:M:346:TYR:HA	6:M:349:ILE:HG12	1.98	0.44
6:M:3470:GLN:HG2	6:M:4004:VAL:HG21	1.99	0.44
8:J:104:DT:H2''	8:J:105:DT:C6	2.53	0.44
9:K:71:TYR:OH	9:K:115:ARG:HB2	2.18	0.44
10:L:39:THR:O	10:L:43:GLN:HG3	2.17	0.44
4:H:28:LYS:HZ3	5:I:141:DG:C5'	2.31	0.44
5:I:119:DA:N6	8:J:45:DC:N4	2.65	0.44
5:I:158:DT:C2	5:I:159:DC:C4	3.06	0.44
6:M:1715:GLU:OE2	6:M:1715:GLU:C	2.61	0.44
6:M:1855:PHE:O	6:M:1856:THR:HG23	2.17	0.44
10:L:451:LEU:O	10:L:454:VAL:HG22	2.17	0.44
5:I:37:DC:H2'	5:I:38:DA:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:177:LEU:C	6:M:177:LEU:HD23	2.42	0.44
6:M:208:MET:SD	6:M:208:MET:C	3.01	0.44
6:M:486:GLY:O	6:M:490:ILE:HG12	2.17	0.44
6:M:646:VAL:HG13	6:M:647:TYR:N	2.33	0.44
6:M:1519:PHE:CE1	6:M:1570:GLU:HG2	2.52	0.44
6:M:1668:PHE:N	6:M:1669:PRO:HD2	2.33	0.44
6:M:1782:PHE:HA	6:M:1785:ILE:HG22	2.00	0.44
6:M:3155:VAL:HB	6:M:3156:PRO:HD3	2.00	0.44
1:A:51:ILE:O	2:B:39:ARG:NH2	2.51	0.43
4:H:106:HIS:O	4:H:107:ALA:C	2.61	0.43
5:I:129:DG:C4	5:I:130:DA:N7	2.86	0.43
6:M:1266:CYS:O	6:M:1269:THR:HG22	2.17	0.43
6:M:1550:VAL:O	6:M:1551:ILE:O	2.35	0.43
6:M:1696:LEU:N	6:M:1697:PRO:CD	2.80	0.43
6:M:2998:SER:HA	6:M:3001:CYS:SG	2.58	0.43
8:J:10:DC:H2''	8:J:11:DC:C5	2.53	0.43
8:J:38:DT:O3'	8:J:39:DA:C8	2.71	0.43
10:L:415:ASN:CG	10:L:416:TYR:H	2.26	0.43
3:G:80:PRO:HD3	4:H:55:ALA:HB2	2.00	0.43
5:I:26:DT:H2''	5:I:27:DA:H8	1.83	0.43
5:I:86:DG:H2''	5:I:87:DG:C8	2.53	0.43
6:M:185:HIS:HA	6:M:189:MET:HB3	2.00	0.43
6:M:1298:LEU:O	6:M:1302:ALA:HB2	2.19	0.43
6:M:1839:PHE:O	6:M:1843:ILE:HG12	2.17	0.43
6:M:2219:LEU:O	6:M:2223:VAL:HG23	2.19	0.43
8:J:43:DA:H2''	8:J:44:DG:C8	2.53	0.43
8:J:44:DG:C2'	8:J:45:DC:C6	3.01	0.43
9:K:173:ASP:OD2	9:K:213:ILE:HG22	2.18	0.43
2:B:44:LYS:HB2	3:G:115:LEU:HD11	2.00	0.43
3:C:95:LYS:CE	4:D:100:PRO:HB3	2.47	0.43
3:G:21:ALA:C	3:G:23:LEU:N	2.76	0.43
4:H:73:GLU:OE1	4:H:98:LEU:HG	2.19	0.43
6:M:762:TYR:CD1	6:M:764:PRO:HD2	2.53	0.43
6:M:1574:ASN:O	6:M:1575:LEU:C	2.62	0.43
6:M:1839:PHE:CE1	6:M:1843:ILE:HD13	2.51	0.43
6:M:2307:MET:HE3	6:M:2352:HIS:HB3	2.00	0.43
6:M:3450:MET:HE1	6:M:3471:ILE:HD13	2.01	0.43
6:M:3743:HIS:CG	6:M:3743:HIS:O	2.72	0.43
6:M:3908:HIS:HA	6:M:3911:ILE:HG22	2.00	0.43
6:M:4039:TYR:CE2	6:M:4041:ARG:HB2	2.53	0.43
8:J:17:DC:H2''	8:J:18:DC:C5	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:113:ALA:O	9:K:116:ILE:HG22	2.18	0.43
10:L:253:ILE:HD12	10:L:342:VAL:CG1	2.48	0.43
3:C:67:GLY:O	3:C:70:ALA:HB3	2.18	0.43
4:D:81:ASN:O	4:D:82:LYS:HG2	2.18	0.43
1:E:62:ILE:HD11	2:F:37:LEU:HD21	2.00	0.43
6:M:584:GLU:O	6:M:585:ILE:C	2.60	0.43
6:M:1358:LEU:HD23	6:M:1358:LEU:C	2.43	0.43
6:M:1514:LEU:HD12	6:M:1514:LEU:C	2.44	0.43
6:M:2854:PHE:CE1	6:M:2858:ILE:HD11	2.53	0.43
6:M:3173:MET:HE1	6:M:3782:SER:OG	2.18	0.43
6:M:3722:PHE:CD2	6:M:3740:ILE:HG22	2.53	0.43
6:M:3890:MET:HE3	6:M:3932:MET:HE3	2.00	0.43
8:J:47:DC:H1'	8:J:48:DT:C6	2.53	0.43
9:K:439:PHE:O	9:K:442:ASP:OD1	2.36	0.43
1:A:51:ILE:HA	2:B:39:ARG:NH2	2.34	0.43
3:G:38:ASN:OD1	3:G:38:ASN:O	2.37	0.43
6:M:1080:LEU:HD23	6:M:1080:LEU:O	2.19	0.43
6:M:1563:PHE:O	6:M:1567:ILE:HG12	2.19	0.43
6:M:1782:PHE:O	6:M:1785:ILE:HG22	2.19	0.43
6:M:2428:ASP:O	6:M:2429:ASP:CB	2.65	0.43
6:M:2533:SER:HA	6:M:2565:MET:HE2	2.01	0.43
6:M:3444:ALA:C	6:M:3445:LEU:HD22	2.44	0.43
8:J:91:DA:C4	8:J:92:DC:C5	3.07	0.43
8:J:150:DC:H2'	8:J:151:DG:C8	2.54	0.43
10:L:198:THR:HG23	10:L:201:GLN:H	1.83	0.43
6:M:947:GLN:O	6:M:948:MET:HB3	2.18	0.43
6:M:2345:VAL:O	6:M:2349:LEU:HD23	2.18	0.43
6:M:3084:GLN:NE2	6:M:3135:LEU:HD12	2.33	0.43
6:M:3981:TYR:CE1	6:M:4104:VAL:HG23	2.53	0.43
10:L:242:ARG:HG2	10:L:243:HIS:N	2.33	0.43
10:L:246:HIS:O	10:L:246:HIS:HD2	2.00	0.43
3:C:92:GLU:OE1	4:D:103:LEU:HG	2.19	0.43
4:D:36:ILE:HG13	4:D:37:TYR:N	2.34	0.43
3:G:51:LEU:HD21	4:H:67:PHE:HD1	1.83	0.43
5:I:26:DT:H5''	5:I:26:DT:H6	1.83	0.43
5:I:58:DG:H2''	5:I:59:DT:C7	2.49	0.43
6:M:204:LEU:HD12	6:M:223:CYS:SG	2.58	0.43
6:M:212:VAL:HG23	6:M:213:ARG:N	2.33	0.43
6:M:651:TYR:CE1	6:M:655:LEU:HD11	2.54	0.43
6:M:722:LYS:O	6:M:723:ASP:OD1	2.36	0.43
6:M:1338:VAL:O	6:M:1341:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:1484:LEU:HD12	6:M:1485:SER:N	2.33	0.43
6:M:1820:VAL:HG23	6:M:1821:ASP:N	2.32	0.43
6:M:2499:PHE:HD2	6:M:2500:LYS:HG3	1.84	0.43
6:M:3262:LEU:O	6:M:3263:HIS:C	2.61	0.43
6:M:4006:VAL:C	6:M:4011:PHE:HZ	2.26	0.43
8:J:28:DC:H1'	8:J:29:DA:N7	2.33	0.43
6:M:424:LEU:C	6:M:424:LEU:HD23	2.43	0.43
6:M:2957:LEU:HD13	6:M:2960:GLU:OE2	2.19	0.43
8:J:65:DA:H2'	8:J:66:DC:C6	2.53	0.43
9:K:207:LYS:HB3	9:K:208:PRO:CD	2.47	0.43
1:A:63:ARG:HG3	8:J:92:DC:OP1	2.19	0.43
2:B:45:ARG:HH12	5:I:87:DG:H5''	1.84	0.43
3:G:31:HIS:CD2	3:G:35:ARG:NH2	2.86	0.43
3:G:94:ASN:O	3:G:98:GLY:N	2.51	0.43
5:I:44:DC:H4'	5:I:45:DT:OP1	2.18	0.43
5:I:45:DT:H1'	5:I:46:DG:C5	2.54	0.43
5:I:118:DG:H1'	5:I:119:DA:C8	2.54	0.43
5:I:150:DA:H2''	5:I:151:DC:C5	2.54	0.43
6:M:390:GLN:HA	6:M:393:LYS:HZ3	1.83	0.43
6:M:928:VAL:HA	6:M:931:CYS:SG	2.59	0.43
6:M:977:ASP:OD1	6:M:979:VAL:HG12	2.19	0.43
6:M:1124:ILE:H	6:M:1124:ILE:HD12	1.83	0.43
6:M:2249:LEU:C	6:M:2249:LEU:HD12	2.43	0.43
6:M:3914:SER:O	6:M:3917:ILE:HG22	2.19	0.43
8:J:3:DC:C2'	8:J:4:DG:N7	2.81	0.43
9:K:350:PHE:HB3	9:K:394:VAL:HG12	2.01	0.43
10:L:402:ASN:OD1	10:L:402:ASN:O	2.35	0.43
1:E:39:HIS:O	9:K:516:LYS:HE3	2.19	0.43
3:G:94:ASN:O	3:G:98:GLY:CA	2.67	0.43
5:I:26:DT:C2'	5:I:27:DA:H8	2.32	0.43
5:I:108:DA:C6	5:I:109:DG:C6	3.07	0.43
6:M:1675:TYR:CE1	6:M:1679:LEU:HD11	2.54	0.43
6:M:2320:ALA:HB1	6:M:2362:VAL:CG1	2.49	0.43
6:M:3438:GLU:HG2	6:M:3439:LEU:H	1.83	0.43
6:M:3468:LEU:O	6:M:3472:ILE:CD1	2.64	0.43
6:M:3520:GLU:OE2	6:M:3521:ILE:HG13	2.18	0.43
6:M:4095:GLU:CD	6:M:4096:SER:HG	2.27	0.43
8:J:76:DG:H4'	8:J:77:DT:OP1	2.18	0.43
10:L:14:MET:HE3	10:L:34:ALA:HB3	2.01	0.43
1:A:76:GLN:NE2	1:A:80:THR:HG22	2.34	0.42
1:A:120:MET:HB2	1:A:122:LYS:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:VAL:HG11	2:F:98:TYR:CZ	2.54	0.42
1:E:70:LEU:HD11	2:F:29:ILE:HG12	2.00	0.42
3:G:17:ARG:O	3:G:21:ALA:CB	2.66	0.42
6:M:560:LEU:C	6:M:560:LEU:HD23	2.44	0.42
6:M:849:GLU:OE2	6:M:849:GLU:N	2.50	0.42
6:M:1335:CYS:HA	6:M:1338:VAL:HG22	2.01	0.42
6:M:1918:LEU:O	6:M:1922:ALA:HB2	2.18	0.42
6:M:2837:LEU:C	6:M:2837:LEU:HD23	2.44	0.42
6:M:3044:MET:O	6:M:3048:LYS:HG2	2.19	0.42
6:M:3813:LYS:O	6:M:3817:LEU:HD13	2.19	0.42
8:J:102:DG:C2	8:J:103:DA:C6	3.07	0.42
1:A:61:LEU:HD21	2:B:33:ALA:HA	2.00	0.42
5:I:9:DG:C2	5:I:10:DA:C5	3.08	0.42
5:I:48:DA:C4	5:I:49:DG:N7	2.87	0.42
5:I:134:DA:H5'	5:I:134:DA:H8	1.84	0.42
6:M:12:LEU:HD12	6:M:54:GLN:NE2	2.34	0.42
6:M:108:LYS:HE2	6:M:149:ILE:HG13	2.01	0.42
6:M:708:VAL:HG22	6:M:740:ILE:CD1	2.48	0.42
6:M:774:GLU:O	6:M:778:ILE:HG12	2.19	0.42
6:M:1646:LEU:HD21	6:M:1691:GLN:HG3	2.01	0.42
6:M:2958:LEU:HD12	6:M:4101:GLU:HG2	2.01	0.42
6:M:4068:HIS:C	6:M:4070:LYS:H	2.28	0.42
9:K:277:VAL:O	9:K:277:VAL:HG23	2.19	0.42
9:K:462:MET:HG3	9:K:465:ILE:HB	2.02	0.42
10:L:367:ALA:HB3	10:L:371:GLU:CD	2.44	0.42
3:C:9:LYS:O	3:C:10:THR:C	2.61	0.42
4:D:112:THR:O	4:D:116:THR:HG23	2.18	0.42
2:F:72:TYR:HE1	4:H:97:LEU:HD13	1.84	0.42
6:M:3868:VAL:O	6:M:3872:ARG:HG2	2.18	0.42
6:M:3946:PHE:CZ	6:M:4006:VAL:HG21	2.53	0.42
8:J:25:DG:H2''	8:J:26:DC:C6	2.54	0.42
8:J:75:DT:H2''	8:J:76:DG:C8	2.54	0.42
8:J:110:DC:H2''	8:J:111:DC:C5	2.55	0.42
1:E:46:VAL:C	1:E:50:GLU:OE1	2.62	0.42
6:M:83:GLU:HB3	6:M:123:CYS:SG	2.59	0.42
6:M:940:PHE:HD2	6:M:2576:MET:HE1	1.84	0.42
6:M:1526:GLU:O	6:M:1529:VAL:HG12	2.18	0.42
6:M:2825:THR:OG1	6:M:2828:GLU:OE2	2.37	0.42
6:M:4088:ASN:OD1	6:M:4109:ASP:OD2	2.37	0.42
9:K:40:PHE:CE1	9:K:67:ILE:HG23	2.54	0.42
9:K:388:LYS:NZ	10:L:455:ASP:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:403:ARG:HG3	9:K:404:ARG:H	1.84	0.42
10:L:339:CYS:HB3	10:L:340:PHE:C	2.45	0.42
1:E:61:LEU:HD11	2:F:36:ARG:HB3	2.01	0.42
5:I:60:DA:C2	8:J:106:DA:C2	3.07	0.42
6:M:252:VAL:O	6:M:256:ILE:HG22	2.19	0.42
6:M:287:LEU:HD21	6:M:329:LYS:HG2	2.01	0.42
6:M:1055:ASN:O	6:M:1059:LEU:CD2	2.68	0.42
6:M:1335:CYS:O	6:M:1338:VAL:HG22	2.20	0.42
6:M:1735:ARG:O	6:M:1738:ASN:OD1	2.37	0.42
6:M:1776:GLU:O	6:M:1779:GLN:HG2	2.19	0.42
6:M:2091:HIS:CG	6:M:2092:GLU:N	2.87	0.42
6:M:2484:TYR:CE2	6:M:2499:PHE:CD1	3.07	0.42
6:M:2820:MET:HE3	6:M:2820:MET:HA	2.00	0.42
6:M:3681:LYS:HE3	6:M:3687:MET:HB2	2.01	0.42
8:J:111:DC:H2'	8:J:112:DT:H71	2.01	0.42
10:L:138:LEU:HD11	10:L:165:LEU:HD11	2.01	0.42
3:C:63:LEU:HD21	4:D:59:MET:HE3	2.01	0.42
4:D:106:HIS:O	4:D:110:GLU:OE1	2.37	0.42
6:M:785:MET:O	6:M:786:GLN:C	2.62	0.42
8:J:45:DC:H2''	8:J:46:DT:H71	2.01	0.42
8:J:74:DC:H2''	8:J:75:DT:H71	2.01	0.42
8:J:87:DT:H2''	8:J:88:DT:C6	2.53	0.42
1:A:131:ARG:NH2	1:E:131:ARG:HE	2.18	0.42
3:C:95:LYS:HD2	3:C:95:LYS:C	2.44	0.42
1:E:82:LEU:HD13	2:F:70:VAL:HG22	2.01	0.42
3:G:24:GLN:NE2	4:H:37:TYR:HA	2.35	0.42
3:G:61:GLU:O	3:G:64:GLU:HG3	2.19	0.42
5:I:49:DG:H2''	5:I:50:DA:C8	2.54	0.42
6:M:793:LEU:N	6:M:794:PRO:HD2	2.33	0.42
6:M:931:CYS:HB2	6:M:984:TYR:HE2	1.84	0.42
6:M:985:GLU:HA	6:M:988:VAL:HG12	2.02	0.42
6:M:1481:THR:O	6:M:1484:LEU:HG	2.20	0.42
6:M:2089:ASN:O	6:M:2089:ASN:OD1	2.37	0.42
6:M:2165:LEU:C	6:M:2165:LEU:HD23	2.44	0.42
6:M:2389:PHE:O	6:M:2390:HIS:ND1	2.53	0.42
6:M:2405:VAL:HG22	6:M:2406:GLU:H	1.85	0.42
6:M:2775:TYR:CG	6:M:2776:ARG:N	2.87	0.42
6:M:3276:TRP:HZ3	6:M:3307:LEU:HD21	1.85	0.42
8:J:21:DG:C6	8:J:22:DG:C6	3.08	0.42
10:L:164:PHE:HA	10:L:225:TYR:O	2.19	0.42
1:A:121:PRO:CG	2:B:49:LEU:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:LEU:HB3	2:F:44:LYS:NZ	2.35	0.42
4:D:96:ARG:CZ	4:D:108:VAL:HG21	2.50	0.42
5:I:63:DC:H1'	5:I:64:DC:C5	2.55	0.42
5:I:134:DA:H2'	5:I:135:DT:H72	2.01	0.42
6:M:211:ALA:CB	6:M:214:GLU:O	2.67	0.42
6:M:245:SER:HA	6:M:248:ILE:HG12	2.01	0.42
6:M:654:ILE:HD12	6:M:710:PHE:CG	2.55	0.42
6:M:1289:SER:O	6:M:1290:LEU:C	2.62	0.42
6:M:2368:THR:O	6:M:2369:LYS:HG2	2.20	0.42
6:M:2780:LEU:CB	6:M:2781:PRO:HD3	2.49	0.42
8:J:3:DC:H2''	8:J:4:DG:N7	2.34	0.42
9:K:141:TYR:OH	9:K:175:PRO:CB	2.67	0.42
9:K:193:LEU:CD1	9:K:198:ILE:HB	2.49	0.42
10:L:356:PHE:O	10:L:423:GLN:O	2.38	0.42
3:C:79:ILE:HB	3:C:80:PRO:HD2	2.01	0.42
6:M:979:VAL:HG13	6:M:980:THR:N	2.34	0.42
6:M:1509:GLN:C	6:M:1509:GLN:CD	2.88	0.42
6:M:2540:LEU:HD21	6:M:2832:ILE:CG2	2.49	0.42
6:M:3606:ILE:O	6:M:3606:ILE:CG2	2.67	0.42
9:K:130:ARG:O	9:K:133:ASP:OD1	2.37	0.42
9:K:435:VAL:O	9:K:435:VAL:HG13	2.19	0.42
4:D:106:HIS:O	4:D:107:ALA:C	2.61	0.42
6:M:1178:ARG:HD2	6:M:1183:CYS:SG	2.59	0.42
6:M:2484:TYR:CD2	6:M:2499:PHE:HD1	2.38	0.42
8:J:77:DT:O3'	8:J:78:DC:C6	2.73	0.42
8:J:85:DG:H2''	8:J:86:DT:H5''	2.01	0.42
9:K:275:ASN:OD1	9:K:275:ASN:O	2.38	0.42
9:K:301:ARG:HB2	9:K:303:PHE:CE2	2.55	0.42
10:L:367:ALA:HB3	10:L:371:GLU:OE1	2.19	0.42
10:L:373:ALA:O	10:L:376:ALA:O	2.37	0.42
1:E:41:TYR:CD2	5:I:101:DG:OP1	2.73	0.41
5:I:87:DG:H2''	5:I:88:DA:N7	2.34	0.41
5:I:147:DG:H4'	5:I:148:DG:OP1	2.20	0.41
6:M:241:ASP:HB3	6:M:242:PRO:CD	2.50	0.41
6:M:931:CYS:HB2	6:M:984:TYR:CE2	2.55	0.41
6:M:1876:ILE:HG13	6:M:1877:LEU:N	2.35	0.41
6:M:2309:PHE:HB2	6:M:2316:TYR:O	2.20	0.41
6:M:2528:GLU:O	6:M:2528:GLU:HG3	2.20	0.41
8:J:74:DC:H2'	8:J:75:DT:H71	2.01	0.41
8:J:100:DG:H2''	8:J:101:DG:N7	2.35	0.41
8:J:158:DC:H2''	8:J:159:DC:C5	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:348:MET:HE2	10:L:477:PHE:CZ	2.55	0.41
3:C:59:THR:HA	3:C:62:ILE:HG12	2.03	0.41
4:D:55:ALA:O	4:D:58:ILE:HG22	2.20	0.41
1:E:40:ARG:HA	5:I:101:DG:C5'	2.50	0.41
3:G:24:GLN:OE1	4:H:41:VAL:HG23	2.19	0.41
5:I:49:DG:C6	5:I:50:DA:N6	2.88	0.41
6:M:364:ARG:O	6:M:369:PHE:CD2	2.73	0.41
6:M:643:GLU:O	6:M:646:VAL:HG12	2.20	0.41
6:M:1331:ASN:OD1	6:M:1332:TYR:N	2.53	0.41
6:M:1633:TRP:CZ2	6:M:1674:THR:HG22	2.55	0.41
6:M:2320:ALA:HB1	6:M:2362:VAL:HG11	2.00	0.41
6:M:3476:PRO:HD3	6:M:3482:LEU:HD13	2.02	0.41
8:J:20:DA:C2'	8:J:21:DG:C8	3.03	0.41
9:K:465:ILE:HG13	9:K:521:LEU:HD23	2.02	0.41
10:L:36:LYS:O	10:L:39:THR:HG22	2.20	0.41
10:L:115:MET:HE1	10:L:154:LEU:HB2	2.02	0.41
10:L:253:ILE:HD12	10:L:342:VAL:HG11	2.01	0.41
10:L:261:ILE:CG2	10:L:377:LEU:HD22	2.50	0.41
10:L:339:CYS:CB	10:L:340:PHE:CA	2.98	0.41
4:D:37:TYR:O	4:D:41:VAL:HG22	2.20	0.41
1:E:51:ILE:HD11	2:F:44:LYS:HG3	2.01	0.41
4:H:120:SER:O	4:H:121:ALA:HB3	2.19	0.41
5:I:157:DT:C5	5:I:158:DT:C4	3.09	0.41
6:M:1219:PHE:O	6:M:1223:THR:HG23	2.20	0.41
6:M:1952:ILE:HA	6:M:1955:VAL:HG22	2.03	0.41
6:M:1963:GLN:HG2	6:M:1965:PHE:CZ	2.55	0.41
6:M:2402:LEU:HB2	6:M:2438:ILE:HD11	2.02	0.41
6:M:4006:VAL:O	6:M:4006:VAL:HG12	2.21	0.41
8:J:118:DC:H1'	8:J:119:DC:C6	2.55	0.41
9:K:146:VAL:HG13	9:K:147:LEU:CD2	2.49	0.41
9:K:411:VAL:HG21	9:K:434:LEU:HD23	2.01	0.41
1:A:57:SER:O	2:B:40:ARG:NH1	2.54	0.41
1:A:69:ARG:O	1:A:73:GLU:HG2	2.20	0.41
1:A:131:ARG:HA	1:A:131:ARG:NE	2.34	0.41
1:E:73:GLU:CD	2:F:22:LEU:HD13	2.44	0.41
5:I:47:DG:H5'	5:I:47:DG:C8	2.56	0.41
6:M:432:THR:N	6:M:433:PRO:HD2	2.35	0.41
6:M:892:LEU:HD23	6:M:892:LEU:C	2.46	0.41
6:M:1563:PHE:O	6:M:1564:SER:C	2.63	0.41
6:M:2104:MET:SD	6:M:2104:MET:C	3.03	0.41
6:M:3065:ILE:HD13	6:M:3089:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:3628:PHE:CD2	6:M:3685:PRO:HB2	2.55	0.41
10:L:56:LEU:HD21	10:L:58:LEU:HD21	2.02	0.41
3:C:50:TYR:CD2	4:D:91:ILE:HG13	2.56	0.41
1:E:131:ARG:HB3	1:E:133:GLU:HG3	2.02	0.41
5:I:15:DG:C2	8:J:151:DG:C2	3.09	0.41
5:I:24:DT:C2'	5:I:25:DG:C8	3.03	0.41
5:I:55:DG:H2''	5:I:56:DG:C8	2.56	0.41
6:M:661:PRO:O	6:M:662:LEU:HB2	2.20	0.41
6:M:754:MET:HA	6:M:754:MET:HE2	2.01	0.41
6:M:1267:TYR:O	6:M:1271:ILE:HD12	2.20	0.41
6:M:1619:ALA:HA	6:M:1622:ILE:HG22	2.02	0.41
6:M:1897:ASN:HD22	6:M:1902:GLY:HA2	1.86	0.41
6:M:2311:ARG:HG3	6:M:2313:LYS:H	1.86	0.41
6:M:2353:GLN:HG2	6:M:2382:VAL:HG12	2.03	0.41
6:M:2860:ASP:HA	6:M:2863:CYS:SG	2.60	0.41
6:M:3676:PRO:N	6:M:3677:PRO:HD2	2.35	0.41
6:M:3758:LEU:O	6:M:3758:LEU:HD12	2.20	0.41
8:J:67:DG:H2''	8:J:68:DT:C7	2.50	0.41
8:J:78:DC:H2''	8:J:79:DC:C6	2.56	0.41
9:K:192:ASP:C	9:K:192:ASP:OD1	2.63	0.41
2:B:32:PRO:CD	5:I:79:DA:OP2	2.69	0.41
3:C:97:LEU:HD11	4:D:62:PHE:CE1	2.51	0.41
4:D:59:MET:O	4:D:63:VAL:HG23	2.20	0.41
5:I:29:DA:H2'	5:I:30:DT:H71	2.02	0.41
5:I:124:DT:H2''	5:I:125:DC:C6	2.56	0.41
5:I:129:DG:C2	5:I:130:DA:C5	3.08	0.41
6:M:440:VAL:O	6:M:443:ILE:HG22	2.20	0.41
6:M:968:VAL:O	6:M:972:LEU:HG	2.20	0.41
6:M:1164:CYS:HB3	6:M:1167:ASP:OD2	2.21	0.41
6:M:1743:MET:HE2	6:M:1743:MET:HB3	1.96	0.41
6:M:1790:SER:O	6:M:1794:GLN:OE1	2.38	0.41
6:M:1818:SER:O	6:M:1819:PHE:C	2.64	0.41
6:M:1878:ASP:OD1	6:M:1878:ASP:C	2.63	0.41
6:M:2529:THR:HG23	6:M:2530:ARG:H	1.84	0.41
6:M:2792:THR:N	6:M:2793:PRO:HD2	2.36	0.41
6:M:3881:ASP:OD1	6:M:3881:ASP:C	2.63	0.41
6:M:4008:GLU:O	6:M:4011:PHE:CE1	2.74	0.41
10:L:56:LEU:HD23	10:L:57:VAL:N	2.36	0.41
1:A:124:ILE:HD12	1:A:124:ILE:H	1.84	0.41
3:C:96:LEU:C	3:C:97:LEU:HD12	2.46	0.41
3:G:79:ILE:CD1	3:G:81:ARG:CG	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:102:DC:H2''	5:I:103:DG:C8	2.56	0.41
5:I:138:DA:O3'	5:I:139:DG:C8	2.74	0.41
6:M:955:ALA:O	6:M:957:PRO:HD3	2.20	0.41
6:M:1927:MET:HE3	6:M:1969:GLU:OE1	2.21	0.41
6:M:2304:VAL:O	6:M:2307:MET:CG	2.69	0.41
6:M:2363:CYS:O	6:M:2367:VAL:HG23	2.21	0.41
6:M:3914:SER:O	6:M:3918:LEU:HD23	2.20	0.41
10:L:335:SER:O	10:L:336:GLU:HB3	2.20	0.41
1:A:54:TYR:H	2:B:39:ARG:HH21	1.69	0.41
1:A:97:GLU:O	1:A:101:VAL:HG22	2.21	0.41
1:A:113:HIS:HD2	1:E:126:LEU:HB2	1.85	0.41
5:I:53:DA:H2''	5:I:54:DG:C8	2.55	0.41
5:I:56:DG:O3'	5:I:57:DA:C8	2.74	0.41
5:I:76:DA:H2''	5:I:77:DA:C8	2.56	0.41
6:M:2196:TRP:C	6:M:2198:GLY:H	2.29	0.41
6:M:2780:LEU:HB2	6:M:2781:PRO:HD3	2.01	0.41
6:M:3332:THR:HA	6:M:3335:ARG:HG2	2.03	0.41
6:M:4005:PHE:O	6:M:4011:PHE:CE1	2.73	0.41
10:L:11:VAL:HG23	10:L:118:ILE:HD11	2.02	0.41
10:L:28:GLU:OE1	10:L:29:SER:O	2.39	0.41
10:L:526:SER:O	10:L:527:GLN:C	2.62	0.41
1:A:84:PHE:CD1	2:B:81:VAL:HG12	2.56	0.41
3:G:77:ARG:NE	8:J:20:DA:OP1	2.53	0.41
5:I:18:DA:C8	5:I:19:DT:H72	2.55	0.41
5:I:58:DG:C8	5:I:59:DT:H72	2.56	0.41
6:M:35:ILE:H	6:M:35:ILE:HD12	1.86	0.41
6:M:217:LEU:N	6:M:218:PRO:CD	2.84	0.41
6:M:334:HIS:NE2	6:M:376:ILE:HD11	2.36	0.41
6:M:377:ASN:O	6:M:378:ALA:HB3	2.20	0.41
6:M:958:MET:O	6:M:962:TYR:HB2	2.21	0.41
6:M:1019:ASP:OD1	6:M:1019:ASP:C	2.64	0.41
6:M:1254:LEU:HD23	6:M:1254:LEU:H	1.86	0.41
6:M:1454:ALA:O	6:M:1458:LEU:HG	2.20	0.41
6:M:1537:VAL:HG22	6:M:1554:SER:HA	2.03	0.41
6:M:1861:SER:O	6:M:1864:ASP:OD1	2.39	0.41
6:M:2108:LEU:HD23	6:M:2108:LEU:H	1.85	0.41
6:M:2147:ALA:O	6:M:2151:ILE:HG12	2.20	0.41
6:M:2157:PHE:HA	6:M:2164:TRP:CZ3	2.56	0.41
6:M:2200:ALA:HB1	6:M:2245:TRP:CZ3	2.55	0.41
6:M:2278:GLY:O	6:M:2281:MET:HG3	2.21	0.41
6:M:2319:ALA:HB1	6:M:2323:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:2534:ASN:O	6:M:2538:ARG:HB2	2.20	0.41
6:M:2942:ILE:HD13	6:M:3974:MET:HG2	2.03	0.41
6:M:3006:ALA:HB1	6:M:3180:ASP:OD2	2.21	0.41
6:M:3277:VAL:HG23	6:M:3307:LEU:HB3	2.03	0.41
6:M:3952:PHE:CD2	6:M:3954:PRO:HD2	2.56	0.41
8:J:23:DC:H2''	8:J:24:DC:C6	2.56	0.41
8:J:114:DG:H2'	8:J:115:DT:C6	2.55	0.41
9:K:75:ILE:HG12	10:L:316:TYR:CZ	2.56	0.41
9:K:349:GLY:HA2	10:L:461:MET:HE3	2.02	0.41
10:L:20:MET:HE2	10:L:137:ASP:HB3	2.02	0.41
10:L:357:MET:O	10:L:423:GLN:OE1	2.39	0.41
1:A:131:ARG:CZ	1:E:130:ILE:HG12	2.52	0.41
2:B:66:ILE:O	2:B:70:VAL:HG23	2.21	0.41
4:D:67:PHE:CD1	4:D:67:PHE:C	2.99	0.41
5:I:7:DG:C2	5:I:8:DT:C2	3.08	0.41
5:I:48:DA:H2''	5:I:49:DG:H8	1.86	0.41
6:M:104:SER:HB3	6:M:144:MET:HE1	2.02	0.41
6:M:204:LEU:HD23	6:M:204:LEU:C	2.46	0.41
6:M:749:VAL:N	6:M:750:PRO:HD2	2.35	0.41
6:M:2529:THR:HG23	6:M:2530:ARG:N	2.36	0.41
6:M:2901:LEU:HD23	6:M:2901:LEU:O	2.21	0.41
6:M:3636:PHE:O	6:M:3640:PHE:N	2.54	0.41
9:K:77:SER:O	9:K:251:THR:HG23	2.20	0.41
10:L:489:ARG:HG3	10:L:508:ILE:HG22	2.02	0.41
3:C:12:ALA:O	3:C:13:LYS:C	2.64	0.40
3:C:115:LEU:CD2	2:F:44:LYS:NZ	2.74	0.40
1:E:37:LYS:N	1:E:38:PRO:HD2	2.37	0.40
4:H:38:VAL:HG21	4:H:56:MET:SD	2.62	0.40
6:M:385:TYR:CE1	6:M:389:ILE:CG2	3.04	0.40
6:M:439:VAL:O	6:M:442:GLN:HG3	2.20	0.40
6:M:706:LEU:HD23	6:M:706:LEU:O	2.21	0.40
6:M:1045:THR:HG23	6:M:1046:PRO:HD2	2.03	0.40
6:M:1951:VAL:O	6:M:1955:VAL:HG13	2.21	0.40
6:M:2212:ALA:O	6:M:2216:LEU:HD23	2.20	0.40
6:M:2559:THR:O	6:M:2563:LEU:HD23	2.21	0.40
6:M:3328:ILE:O	6:M:3332:THR:HG23	2.20	0.40
6:M:3333:THR:O	6:M:3336:ILE:HG22	2.21	0.40
6:M:3954:PRO:O	6:M:3955:VAL:HG13	2.20	0.40
6:M:3962:ARG:NH1	6:M:3964:THR:HG21	2.36	0.40
6:M:3989:ARG:NH2	6:M:4101:GLU:OE2	2.54	0.40
8:J:54:DC:H2''	8:J:55:DG:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:10:THR:O	3:C:10:THR:HG23	2.21	0.40
3:C:96:LEU:HD11	4:D:100:PRO:CD	2.52	0.40
4:D:56:MET:C	4:D:56:MET:SD	3.04	0.40
1:E:60:LEU:CD1	1:E:93:GLN:HG2	2.51	0.40
1:E:107:THR:OG1	1:E:124:ILE:HD12	2.21	0.40
4:H:51:ILE:HD11	4:H:55:ALA:CB	2.52	0.40
4:H:51:ILE:HD11	4:H:55:ALA:HB1	2.02	0.40
5:I:25:DG:H2'	5:I:26:DT:C5	2.57	0.40
5:I:77:DA:C2'	5:I:78:DA:C8	3.04	0.40
5:I:145:DT:H2''	5:I:146:DC:C6	2.57	0.40
6:M:111:CYS:C	6:M:113:SER:H	2.30	0.40
6:M:118:ASP:OD1	6:M:123:CYS:HB2	2.21	0.40
6:M:1813:SER:OG	6:M:1868:THR:HG21	2.21	0.40
6:M:3588:TRP:NE1	6:M:3610:TYR:CE2	2.89	0.40
9:K:66:CYS:O	9:K:70:VAL:HG12	2.20	0.40
3:C:75:LYS:HE3	3:C:75:LYS:HB3	1.98	0.40
3:G:78:ILE:HD12	3:G:78:ILE:H	1.86	0.40
5:I:2:DA:H2'	5:I:3:DC:C6	2.56	0.40
5:I:26:DT:C2	5:I:27:DA:C8	3.08	0.40
5:I:130:DA:C2'	5:I:131:DC:C5	3.05	0.40
5:I:150:DA:H1'	5:I:151:DC:C5	2.56	0.40
6:M:1436:LEU:HG	6:M:1436:LEU:O	2.21	0.40
6:M:1515:LEU:O	6:M:1518:ALA:HB3	2.21	0.40
6:M:1590:THR:HB	6:M:1632:TRP:HE1	1.86	0.40
6:M:1747:LEU:HD23	6:M:1762:MET:HE3	2.03	0.40
6:M:1948:ALA:O	6:M:1952:ILE:HG13	2.22	0.40
6:M:2869:LEU:N	6:M:2869:LEU:HD23	2.36	0.40
6:M:3049:LEU:CD1	6:M:3085:GLU:HG3	2.52	0.40
6:M:3378:TYR:O	6:M:3382:PHE:CD1	2.74	0.40
6:M:3944:HIS:HD2	6:M:4020:MET:HE2	1.86	0.40
8:J:143:DC:H2''	8:J:144:DC:C6	2.57	0.40
9:K:69:SER:HB3	9:K:243:LEU:O	2.20	0.40
1:A:61:LEU:HD13	2:B:37:LEU:CG	2.48	0.40
1:A:74:ILE:CD1	2:B:66:ILE:HD13	2.51	0.40
4:D:61:SER:O	4:D:64:ASN:OD1	2.40	0.40
1:E:71:VAL:HG11	1:E:89:VAL:HG13	2.02	0.40
2:F:75:HIS:HD2	4:H:93:THR:HG21	1.87	0.40
2:F:84:MET:O	2:F:88:TYR:CG	2.75	0.40
5:I:87:DG:C4	5:I:88:DA:C6	3.09	0.40
6:M:184:VAL:HG11	6:M:191:ASN:HD21	1.86	0.40
6:M:583:LEU:HD13	6:M:614:PRO:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:645:TRP:O	6:M:646:VAL:C	2.65	0.40
6:M:1010:LEU:HD21	6:M:1036:PHE:CE1	2.56	0.40
6:M:1096:VAL:O	6:M:1096:VAL:HG22	2.22	0.40
6:M:1121:LEU:HD22	6:M:1124:ILE:HD11	2.04	0.40
4:D:41:VAL:O	4:D:45:VAL:HG22	2.21	0.40
2:F:83:ALA:O	2:F:86:VAL:HG12	2.21	0.40
3:G:12:ALA:HB3	8:J:32:DT:H4'	2.03	0.40
3:G:17:ARG:CD	4:H:118:TYR:OH	2.70	0.40
6:M:330:ASN:OD1	6:M:330:ASN:C	2.63	0.40
6:M:1055:ASN:O	6:M:1059:LEU:HD22	2.21	0.40
6:M:1900:PHE:CD2	6:M:1901:HIS:HB2	2.56	0.40
6:M:2232:ARG:O	6:M:2236:GLU:OE1	2.39	0.40
6:M:3187:CYS:SG	6:M:3235:LYS:HE3	2.61	0.40
9:K:361:TYR:HE2	10:L:358:GLY:C	2.29	0.40
10:L:91:LEU:HD13	10:L:495:LEU:CD1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	96/112 (86%)	91 (95%)	5 (5%)	0	100	100
1	E	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	B	81/87 (93%)	76 (94%)	5 (6%)	0	100	100
2	F	85/87 (98%)	79 (93%)	6 (7%)	0	100	100
3	C	113/117 (97%)	98 (87%)	13 (12%)	2 (2%)	6	34
3	G	106/117 (91%)	104 (98%)	2 (2%)	0	100	100
4	D	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
4	H	97/99 (98%)	88 (91%)	9 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	M	3632/4128 (88%)	3265 (90%)	354 (10%)	13 (0%)	30	65
9	K	486/609 (80%)	429 (88%)	54 (11%)	3 (1%)	21	56
10	L	529/732 (72%)	461 (87%)	65 (12%)	3 (1%)	21	56
All	All	5421/6299 (86%)	4876 (90%)	524 (10%)	21 (0%)	31	65

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	13	LYS
6	M	186	PRO
6	M	189	MET
6	M	2429	ASP
9	K	85	VAL
6	M	291	VAL
6	M	723	ASP
6	M	1157	PHE
6	M	1551	ILE
9	K	216	PHE
10	L	27	ILE
10	L	320	ILE
3	C	74	LYS
6	M	3155	VAL
6	M	2390	HIS
6	M	3979	LEU
9	K	473	TYR
6	M	284	THR
6	M	662	LEU
6	M	1479	VAL
10	L	166	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	85/93 (91%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	88/93 (95%)	88 (100%)	0	100	100
2	B	68/72 (94%)	68 (100%)	0	100	100
2	F	72/72 (100%)	72 (100%)	0	100	100
3	C	89/91 (98%)	89 (100%)	0	100	100
3	G	85/91 (93%)	85 (100%)	0	100	100
4	D	85/85 (100%)	85 (100%)	0	100	100
4	H	85/85 (100%)	85 (100%)	0	100	100
6	M	3266/3671 (89%)	3265 (100%)	1 (0%)	100	100
9	K	444/548 (81%)	444 (100%)	0	100	100
10	L	481/649 (74%)	481 (100%)	0	100	100
All	All	4848/5550 (87%)	4847 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	M	1946	ASN

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

Mol	Chain	Res	Type
1	E	85	GLN
1	E	93	GLN
2	F	25	ASN
3	G	24	GLN
3	G	31	HIS
3	G	89	ASN
6	M	485	GLN
6	M	1126	GLN
6	M	1175	HIS
6	M	1418	HIS
6	M	1476	HIS
6	M	1926	ASN
6	M	1946	ASN
6	M	1974	ASN
6	M	2170	GLN
6	M	2183	HIS
6	M	2222	HIS

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Mol	Chain	Res	Type
6	M	2971	GLN
6	M	3084	GLN
6	M	3093	GLN
6	M	3105	ASN
6	M	3327	ASN
6	M	3339	ASN
6	M	3569	GLN
6	M	3716	HIS
6	M	3777	GLN
6	M	3903	HIS
6	M	3908	HIS
6	M	3944	HIS
6	M	3966	GLN
9	K	101	ASN
9	K	163	HIS
9	K	304	ASN
9	K	484	GLN
9	K	489	ASN
10	L	246	HIS
10	L	492	GLN
10	L	496	HIS
10	L	500	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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 [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74444. These allow visual inspection of the internal detail of the map and identification of artifacts.

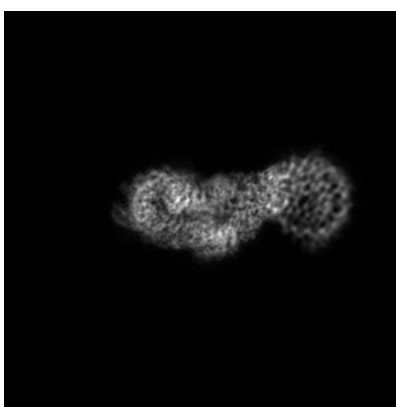
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

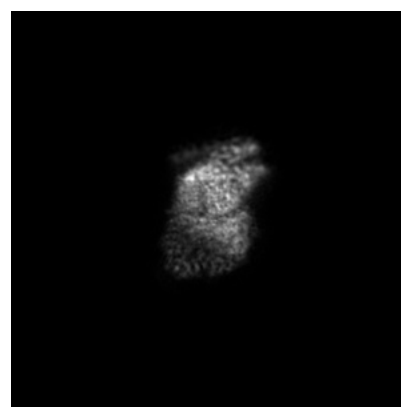
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 224



Y Index: 224



Z Index: 224

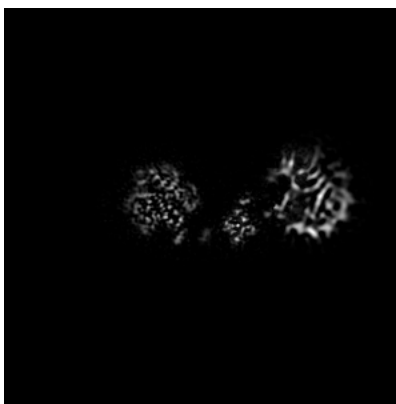
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

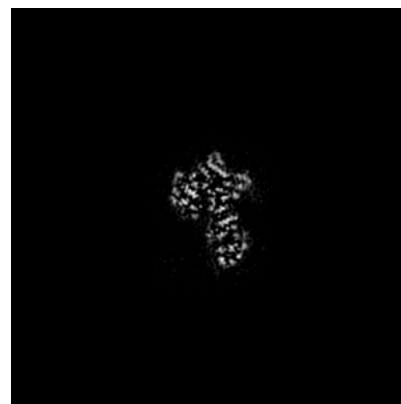
6.3.1 Primary map



X Index: 243



Y Index: 261

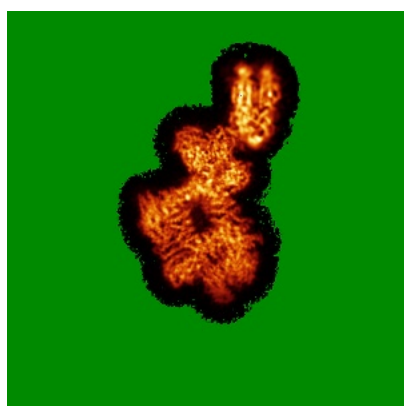


Z Index: 194

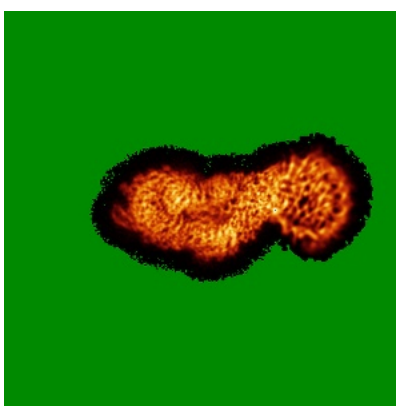
The images above show the largest variance slices of the map in three orthogonal directions.

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

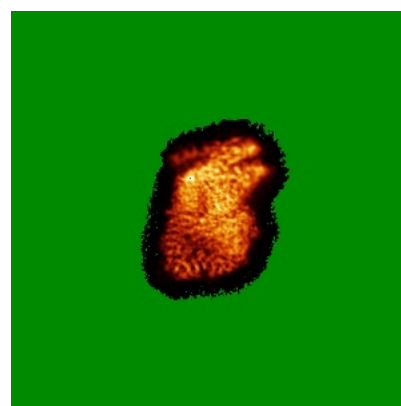
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

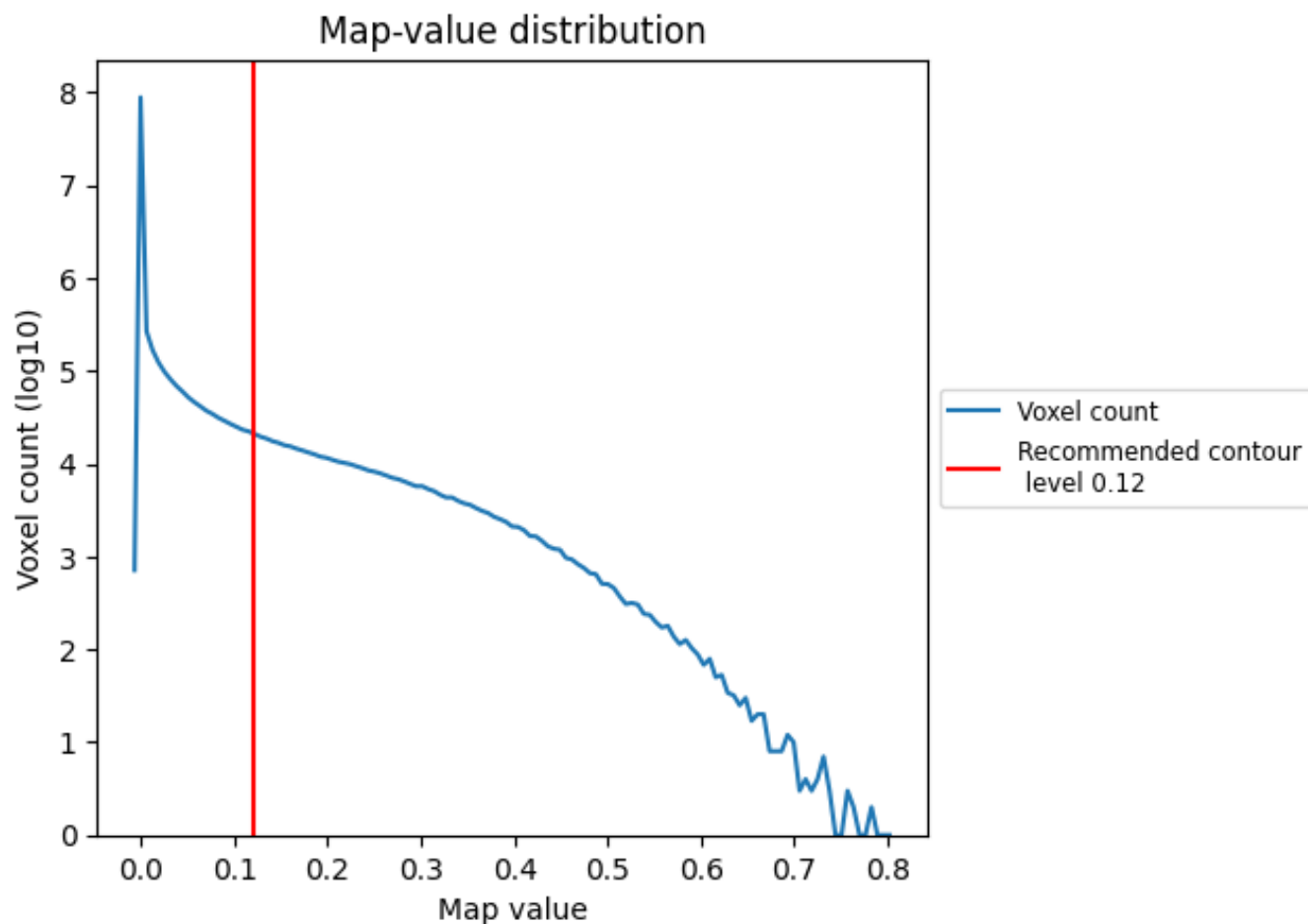
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

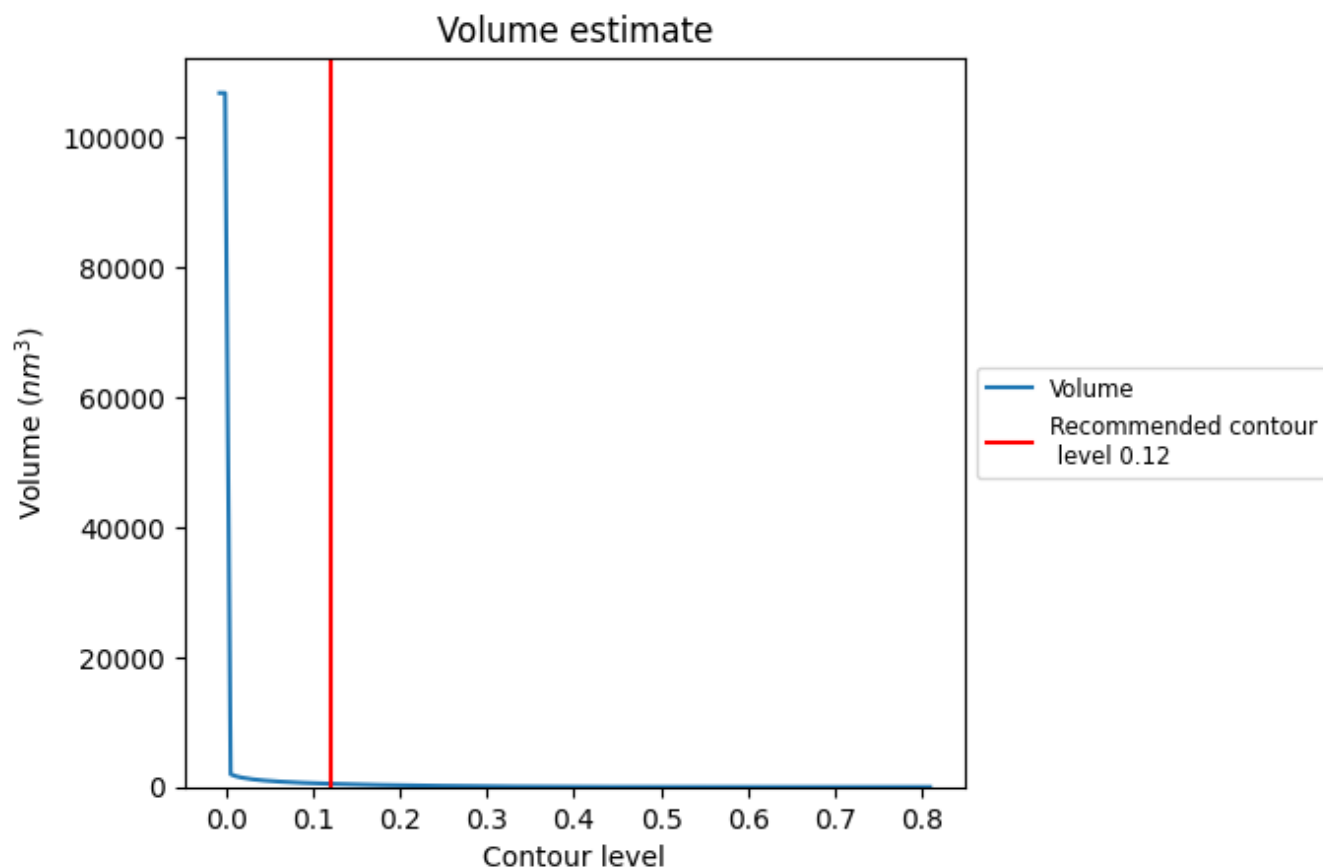
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

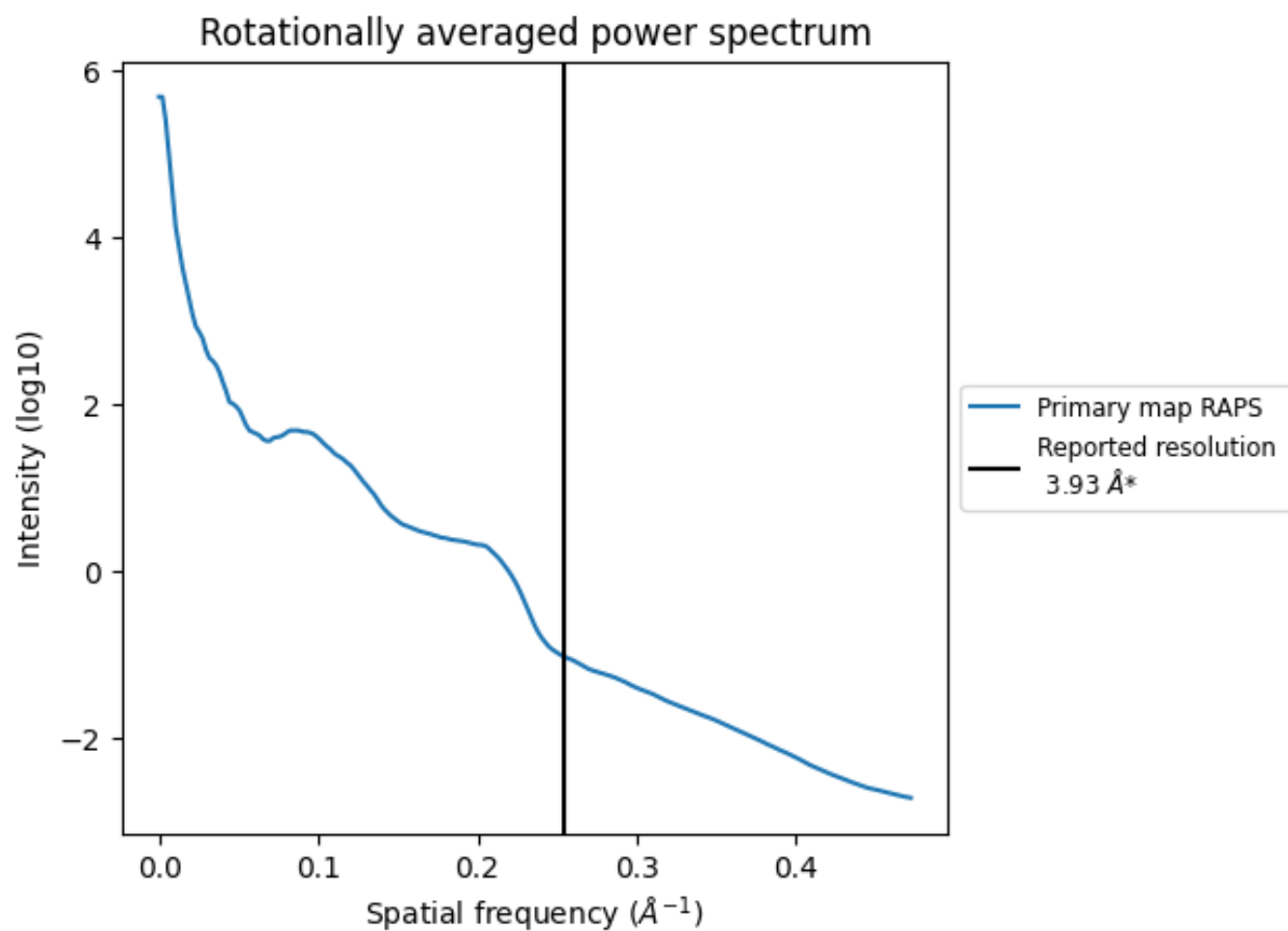
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 490 nm^3 ; this corresponds to an approximate mass of 443 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 0.254 Å⁻¹

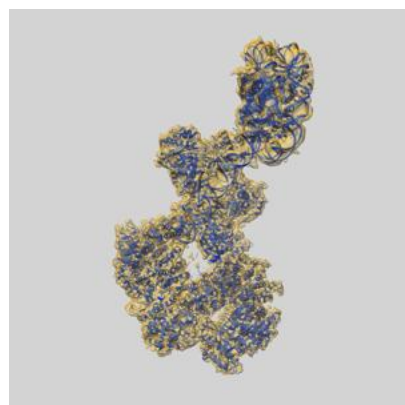
8 Fourier-Shell correlation

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

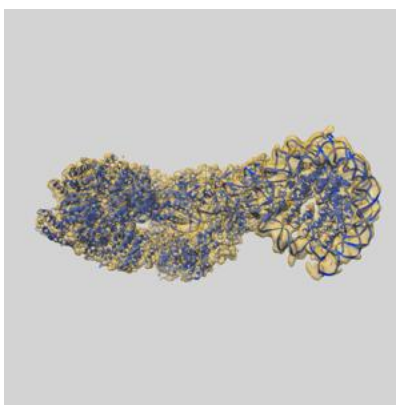
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-74444 and PDB model 9ZNC. Per-residue inclusion information can be found in section 3 on page 6.

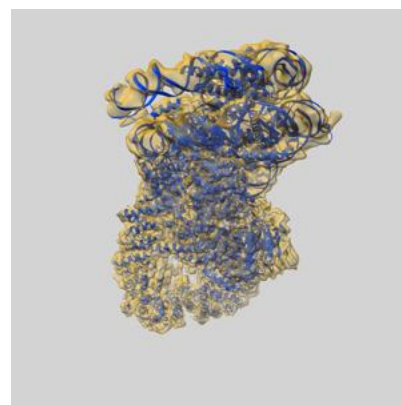
9.1 Map-model overlay [i](#)



X



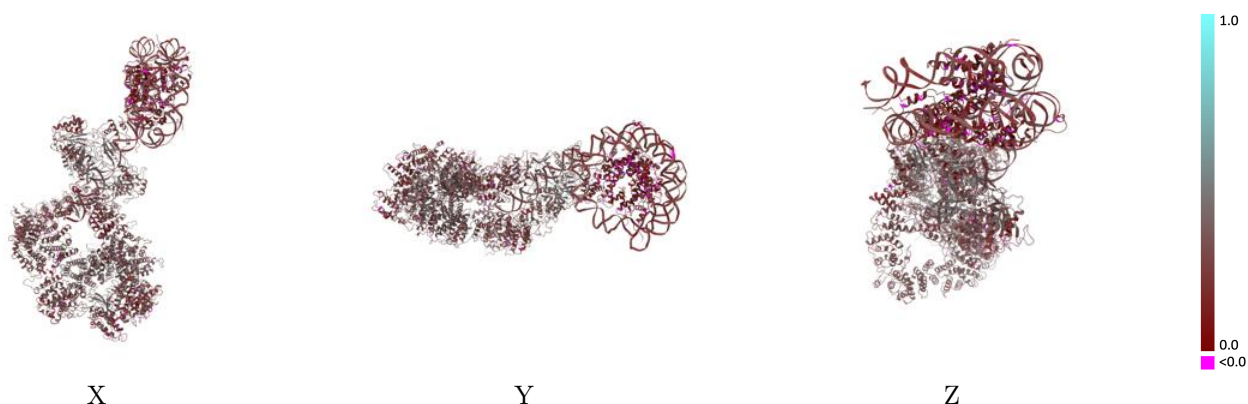
Y



Z

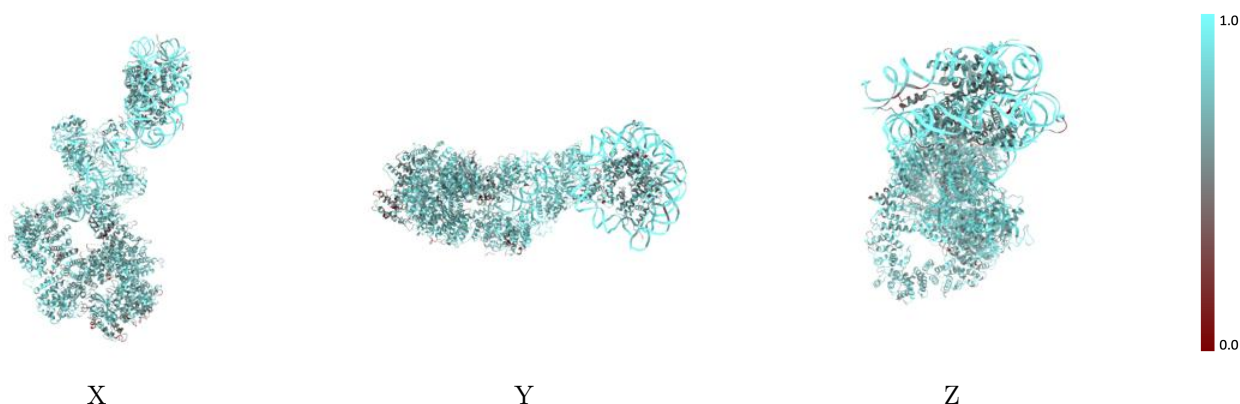
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



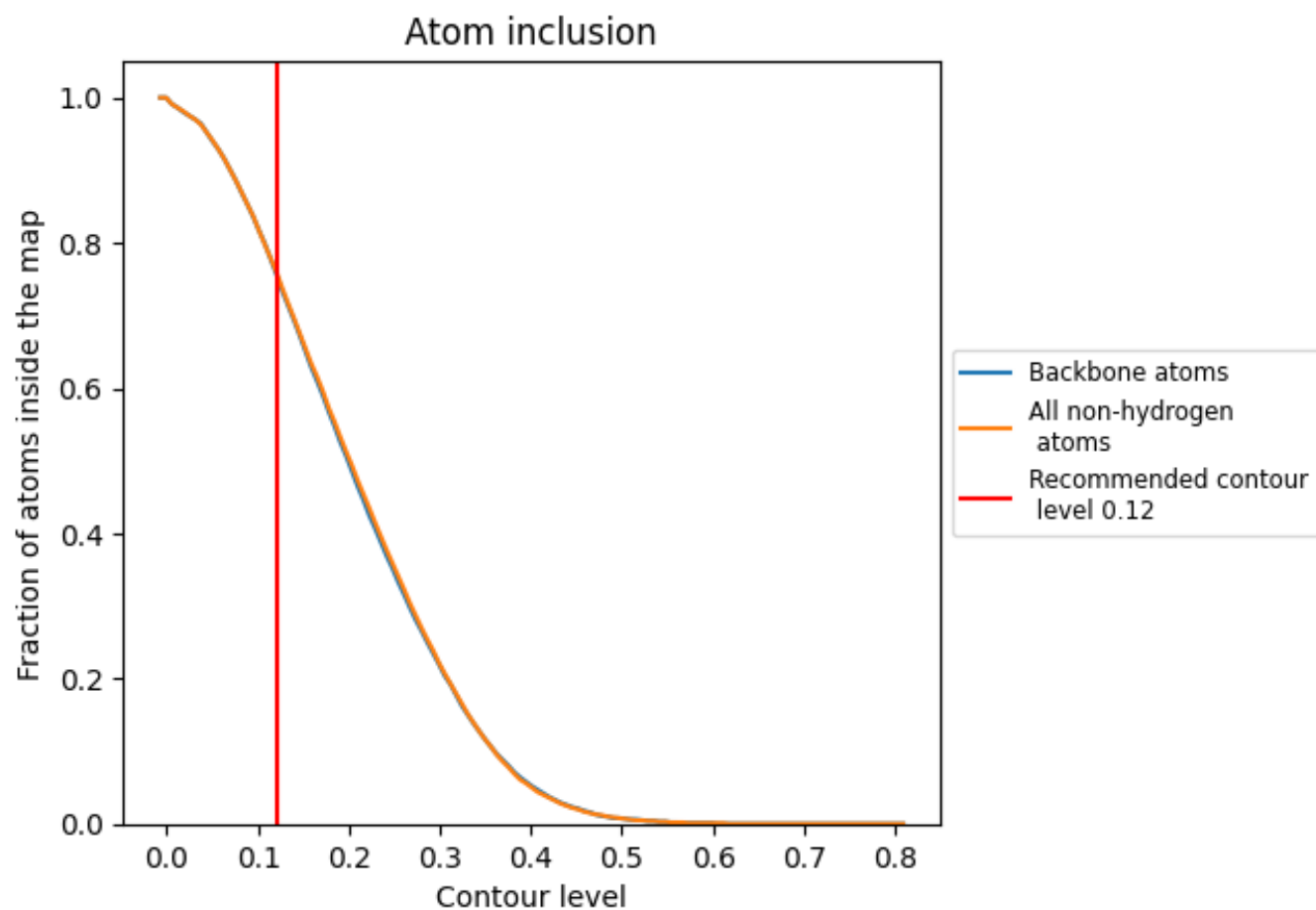
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7610	0.2900
A	0.6510	0.1430
B	0.6810	0.1470
C	0.6810	0.1830
D	0.6910	0.1560
E	0.6920	0.1660
F	0.6310	0.1400
G	0.7080	0.1810
H	0.6820	0.1630
I	0.9210	0.2620
J	0.9210	0.2660
K	0.8480	0.3530
L	0.8110	0.3520
M	0.7370	0.3070
N	0.8710	0.3930

