



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 10:01 AM UTC

PDB ID : 5J0N / pdb_00005j0n
EMDB ID : EMD-3400
Title : Lambda excision HJ intermediate
Authors : Van Duyne, G.; Grigorieff, N.; Landy, A.
Deposited on : 2016-03-28
Resolution : 11.00 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

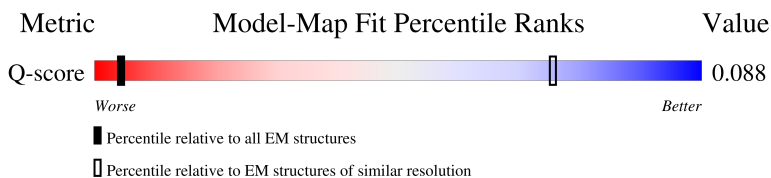
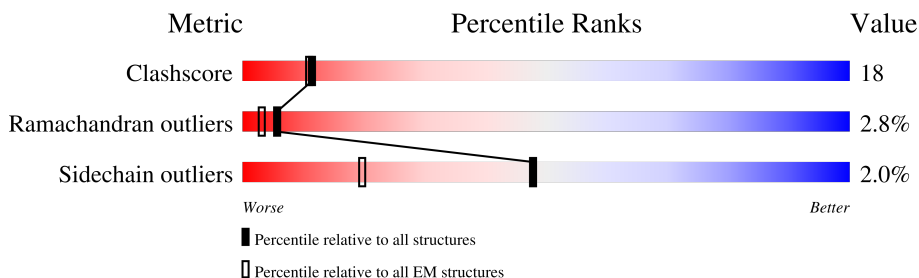
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

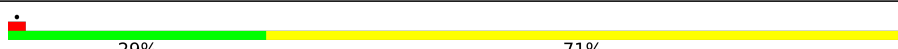
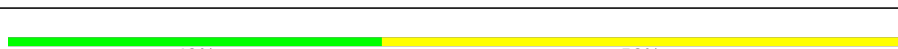
The reported resolution of this entry is 11.00 Å.

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	97 (10.50 - 11.50)

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	197	
2	B	139	
3	C	41	
4	D	99	

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Mol	Chain	Length	Quality of chain
5	E	356	
5	F	356	
5	G	356	
5	H	356	
6	I	96	
6	K	96	
7	J	94	
7	L	94	
8	M	55	
8	N	55	
8	O	55	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 29353 atoms, of which 4591 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a DNA chain called attP(-117 to +79).

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	197	Total	C	H	N	O	P	0	0
			4377	1944	345	693	1199	196		

- Molecule 2 is a DNA chain called attB(-21) to attP(+117).

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	139	Total	C	H	N	O	P	0	0
			3109	1367	259	535	810	138		

- Molecule 3 is a DNA chain called attB(-19 to +21).

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	41	Total	C	H	N	O	P	0	0
			915	401	79	148	247	40		

- Molecule 4 is a DNA chain called attP(-79) to attB(+19).

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	99	Total	C	H	N	O	P	0	0
			2211	974	183	364	592	98		

- Molecule 5 is a protein called Integrase.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	274	Total	C	H	N	O	S	0	0
			2661	1353	510	381	408	9		
5	F	356	Total	C	H	N	O	S	0	0
			3536	1768	703	524	529	12		
5	G	345	Total	C	H	N	O	S	0	0
			3413	1715	673	503	511	11		
5	H	356	Total	C	H	N	O	S	0	0
			3536	1768	703	524	529	12		

- Molecule 6 is a protein called Integration host factor subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	I	96	Total	C	H	N	O	S	0	0
			973	484	199	144	145	1		
6	K	96	Total	C	H	N	O	S	0	0
			973	484	199	144	145	1		

- Molecule 7 is a protein called Integration host factor subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	J	94	Total	C	H	N	O	S	0	0
			932	467	183	139	140	3		
7	L	94	Total	C	H	N	O	S	0	0
			932	467	183	139	140	3		

- Molecule 8 is a protein called Excisionase.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	M	53	Total	C	H	N	O	S	0	0
			581	292	120	90	78	1		
8	N	54	Total	C	H	N	O	S	0	0
			598	298	126	94	79	1		
8	O	55	Total	C	H	N	O	S	0	0
			606	303	126	95	81	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	28	SER	CYS	conflict	UNP P03699
N	28	SER	CYS	conflict	UNP P03699
O	28	SER	CYS	conflict	UNP P03699

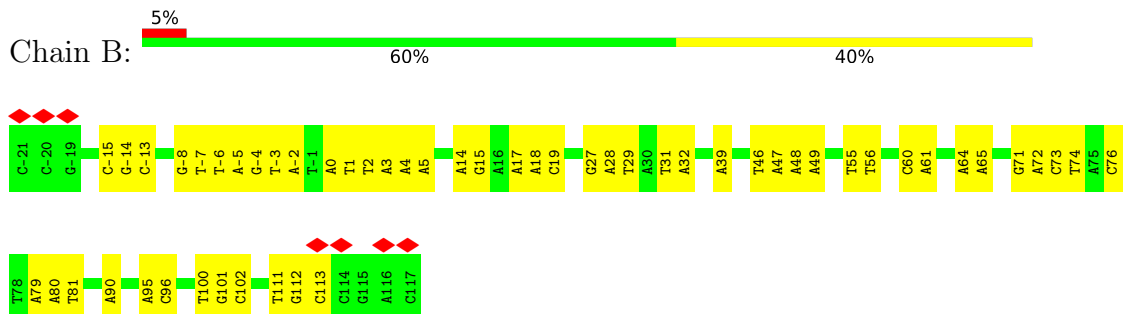
3 Residue-property plots

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.

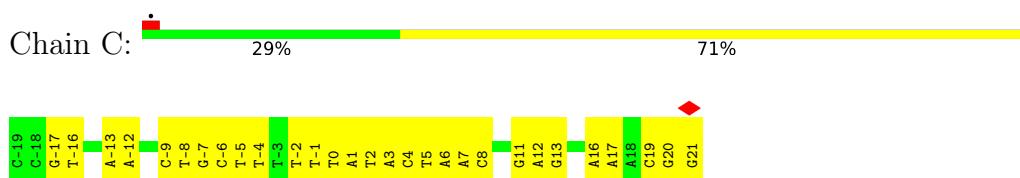
• Molecule 1: attP(-117 to +79)



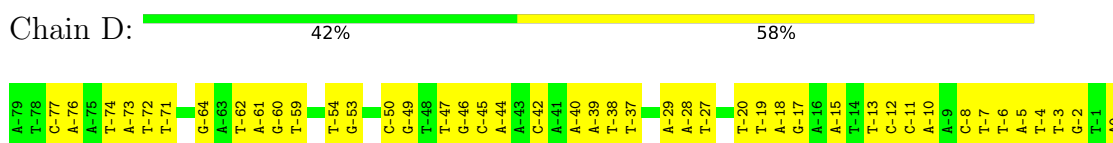
• Molecule 2: attB(-21) to attP(+117)

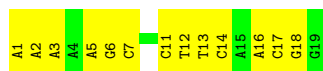


• Molecule 3: attB(-19 to +21)

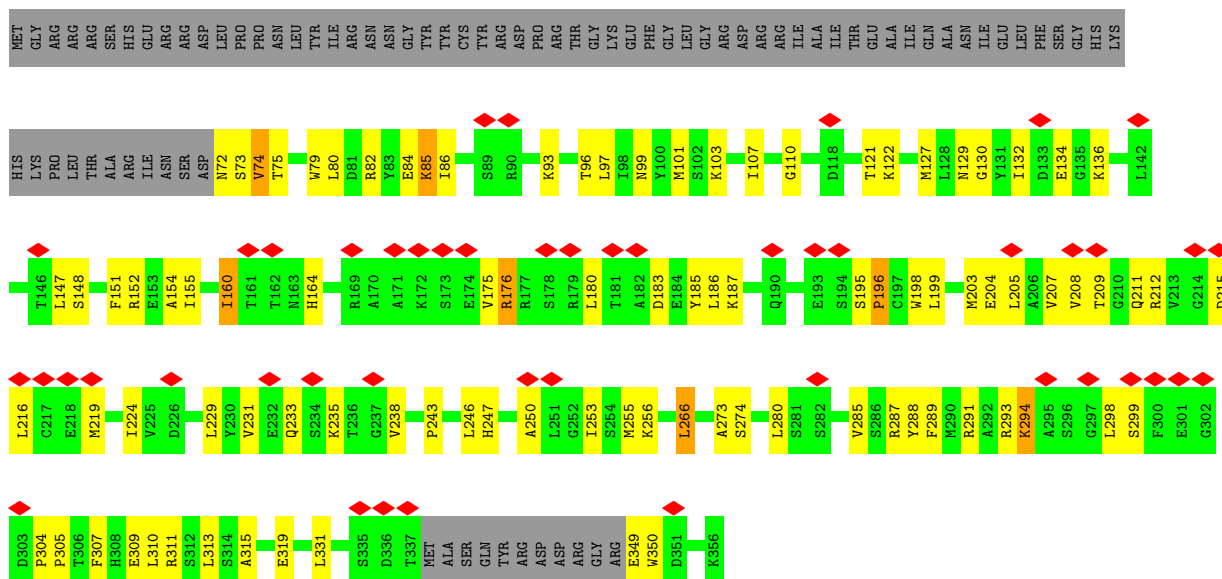


• Molecule 4: attP(-79) to attB(+19)

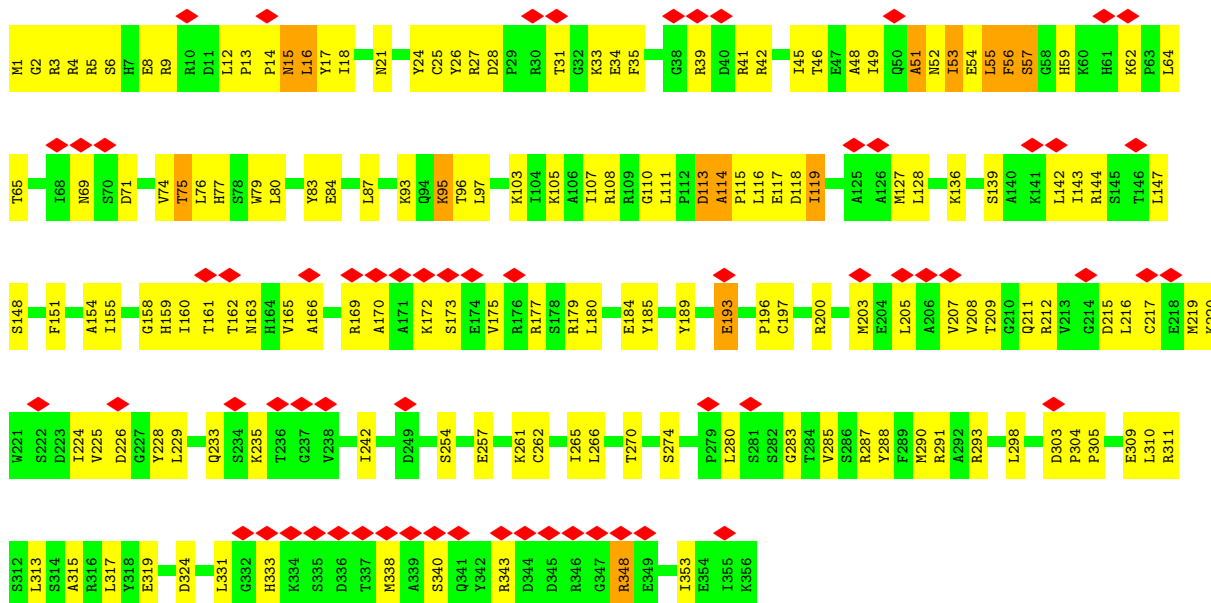




• Molecule 5: Integrase

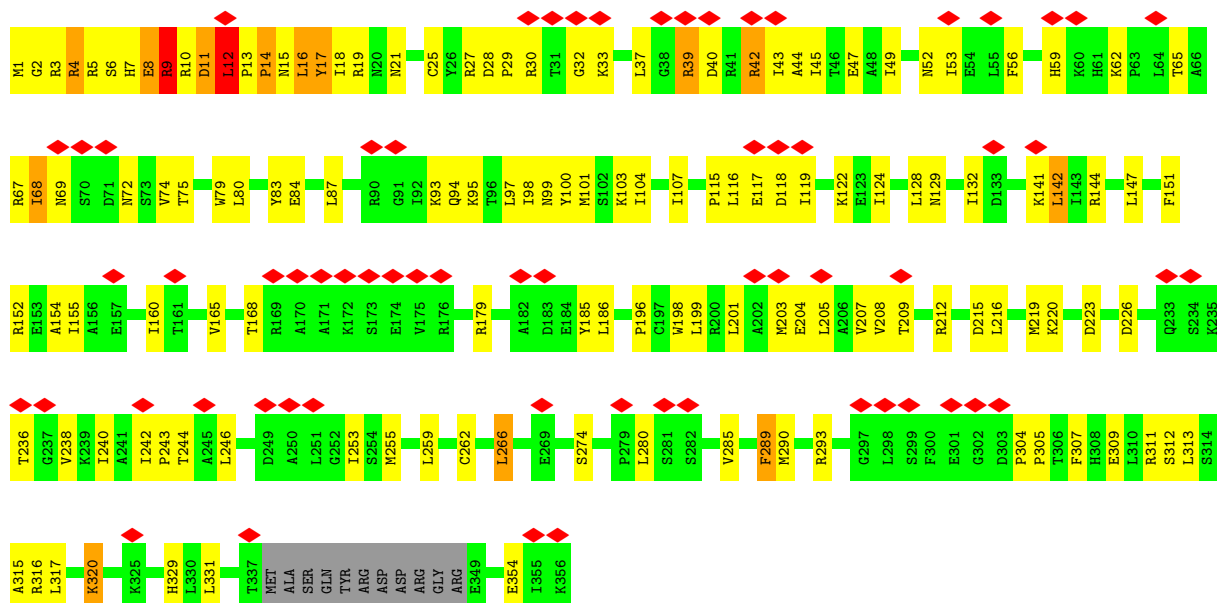


• Molecule 5: Integrase

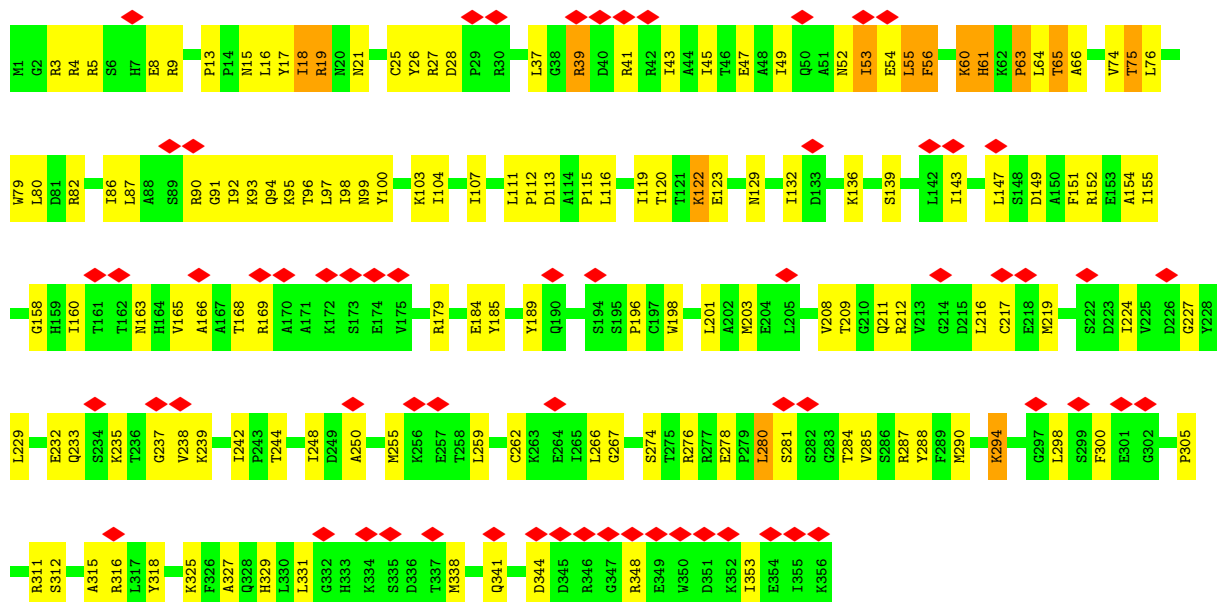


• Molecule 5: Integrase

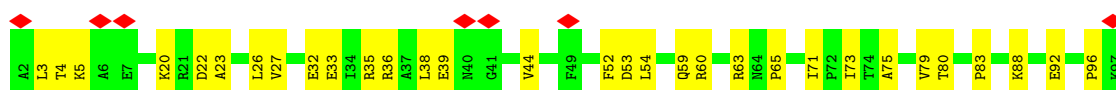




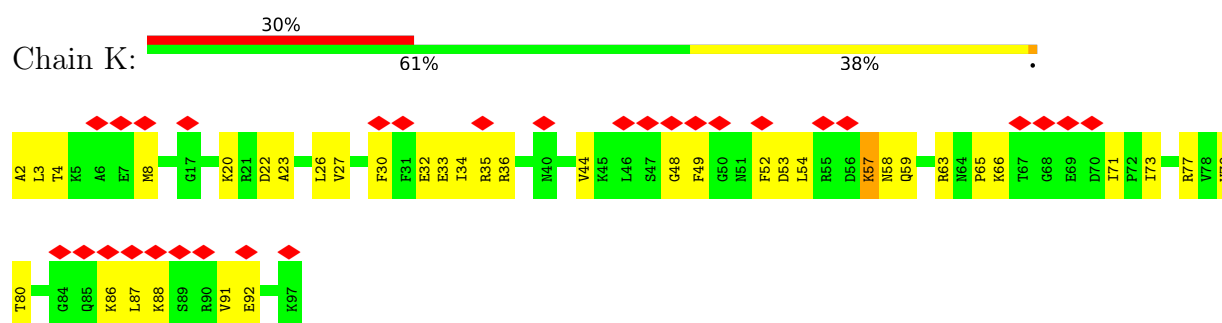
• Molecule 5: Integrase



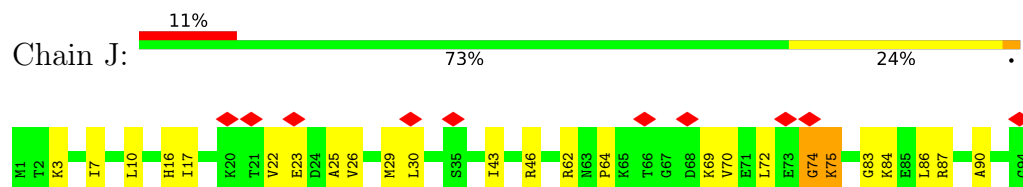
• Molecule 6: Integration host factor subunit alpha



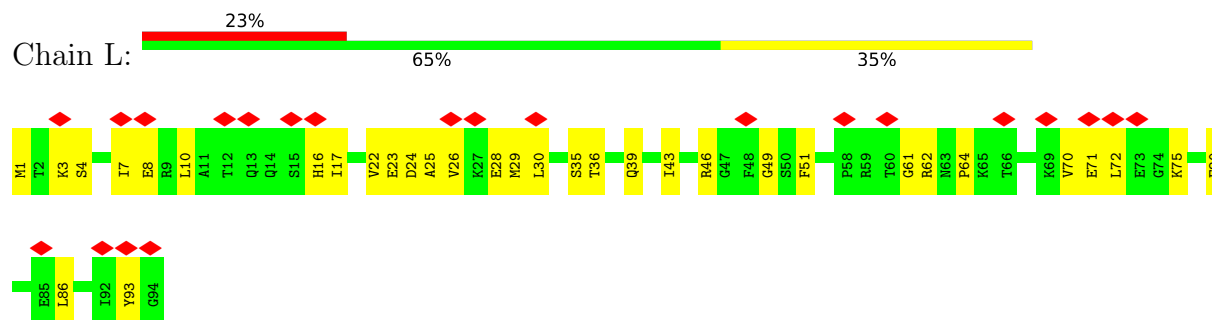
• Molecule 6: Integration host factor subunit alpha



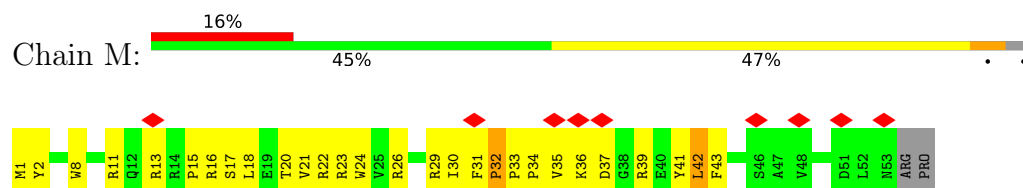
- Molecule 7: Integration host factor subunit beta



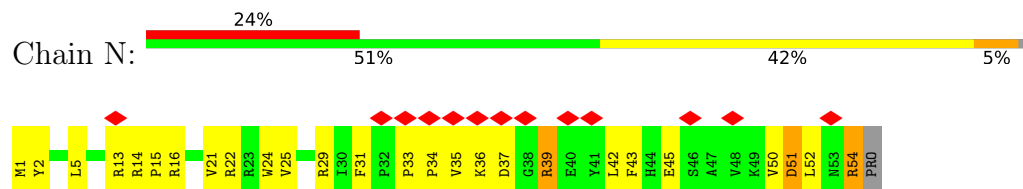
- Molecule 7: Integration host factor subunit beta



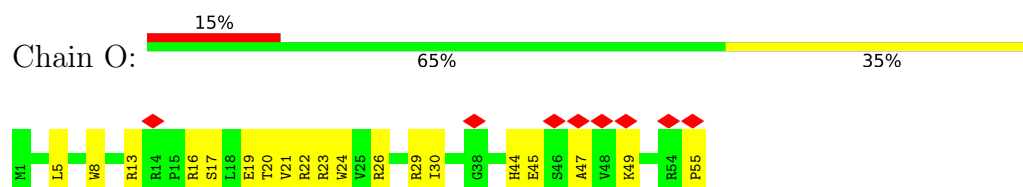
- Molecule 8: Excisionase



- Molecule 8: Excisionase



- Molecule 8: Excisionase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	10956	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Built-in correction in Frealign v9	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35.5	Depositor
Minimum defocus (nm)	1627.0	Depositor
Maximum defocus (nm)	4793.0	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	8.852	Depositor
Minimum map value	-1.882	Depositor
Average map value	-0.029	Depositor
Map value standard deviation	0.457	Depositor
Recommended contour level	2.32	Depositor
Map size ($\text{\AA}$)	358.4, 358.4, 358.4	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.8, 2.8, 2.8	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	0.25	0/4516	0.56	0/6971
2	B	0.25	0/3205	0.51	0/4942
3	C	0.25	0/936	0.51	0/1443
4	D	0.25	0/2275	0.53	0/3510
5	E	0.26	0/2185	0.69	0/2940
5	F	0.52	6/2882 (0.2%)	1.72	22/3875 (0.6%)
5	G	0.27	0/2787	0.74	4/3748 (0.1%)
5	H	0.26	0/2882	0.73	0/3875
6	I	0.25	0/785	0.69	0/1047
6	K	0.25	0/785	0.69	0/1047
7	J	0.27	0/763	0.69	0/1021
7	L	0.27	0/763	0.70	0/1021
8	M	0.29	0/473	0.77	2/639 (0.3%)
8	N	0.31	0/484	0.70	0/653
8	O	0.28	0/493	0.67	0/665
All	All	0.30	6/26214 (0.0%)	0.81	28/37397 (0.1%)

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
5	F	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	56	PHE	CG-CD1	9.65	1.59	1.38
5	F	56	PHE	CA-C	-9.31	1.40	1.52
5	F	55	LEU	C-O	-8.10	1.14	1.23
5	F	56	PHE	CG-CD2	8.01	1.55	1.38
5	F	56	PHE	CD1-CE1	6.61	1.58	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	55	LEU	C-N	-5.29	1.26	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	56	PHE	CE1-CZ-CE2	-63.52	5.67	120.00
5	F	56	PHE	CD1-CE1-CZ	-35.41	56.26	120.00
5	F	56	PHE	CZ-CE2-CD2	-33.58	59.56	120.00
5	F	56	PHE	CG-CD1-CE1	-22.27	82.83	120.70
5	F	56	PHE	CG-CD2-CE2	-22.01	83.28	120.70
5	F	56	PHE	CD1-CG-CD2	-17.02	93.07	118.60
5	F	56	PHE	CB-CA-C	-15.95	78.67	110.42
5	F	55	LEU	N-CA-C	-15.42	84.06	109.96
5	F	56	PHE	N-CA-C	-14.84	79.19	110.80
5	F	51	ALA	N-CA-C	-14.38	95.14	111.82
5	F	114	ALA	CA-C-N	-8.16	110.97	120.11
5	F	114	ALA	C-N-CA	-8.16	110.97	120.11
5	F	56	PHE	CB-CG-CD1	7.77	133.91	120.70
5	F	113	ASP	N-CA-C	-7.54	98.86	110.10
5	F	53	ILE	N-CA-C	-7.36	103.06	113.07
5	F	56	PHE	CB-CG-CD2	7.01	132.62	120.70
5	F	55	LEU	CA-C-O	6.98	128.95	120.92
5	F	15	ASN	N-CA-C	-6.66	101.93	110.53
5	F	56	PHE	N-CA-CB	6.66	121.74	110.49
5	G	11	ASP	N-CA-C	-6.55	103.97	112.23
5	F	62	LYS	CA-C-N	6.22	127.62	119.84
5	F	62	LYS	C-N-CA	6.22	127.62	119.84
5	G	9	ARG	N-CA-C	-6.12	105.62	114.12
5	G	12	LEU	N-CA-C	6.07	123.23	109.81
5	G	289	PHE	N-CA-C	-5.49	105.45	111.82
8	M	32	PRO	CA-C-N	5.33	123.55	119.66
8	M	32	PRO	C-N-CA	5.33	123.55	119.66
5	F	39	ARG	N-CA-C	-5.27	107.51	114.31

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	F	56	PHE	Sidechain

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	4032	345	2249	108	0
2	B	2850	259	1569	56	0
3	C	836	79	466	29	0
4	D	2028	183	1124	75	0
5	E	2151	510	2196	79	0
5	F	2833	703	2871	152	0
5	G	2740	673	2784	132	0
5	H	2833	703	2871	119	0
6	I	774	199	792	23	0
6	K	774	199	792	29	0
7	J	749	183	756	27	0
7	L	749	183	756	28	0
8	M	461	120	464	33	0
8	N	472	126	477	33	0
8	O	480	126	484	14	0
All	All	24762	4591	20651	812	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 18.

All (812) 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)
2:B:4:DA:H3'	5:E:93:LYS:HG3	1.32	1.11
1:A:48:DA:H2''	1:A:49:DC:H5''	1.33	1.10
1:A:-7:DG:H2''	1:A:-6:DC:H5''	1.33	1.10
2:B:0:DA:H2''	2:B:1:DT:H5''	1.39	1.03
1:A:11:DG:H2''	1:A:12:DG:H5''	1.43	1.00
4:D:-18:DA:H2''	4:D:-17:DG:H5''	1.43	0.99
4:D:2:DA:H2''	4:D:3:DA:H5''	1.44	0.99
2:B:95:DA:H2''	2:B:96:DC:H5''	1.43	0.97
2:B:72:DA:H2''	2:B:73:DC:H5'	1.46	0.96
1:A:-19:DG:H2''	1:A:-18:DT:H5''	1.48	0.93
4:D:-77:DC:H2''	4:D:-76:DA:H5'	1.49	0.93
5:F:49:ILE:HD11	8:N:31:PHE:CZ	2.05	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:54:GLU:HG3	5:H:55:LEU:H	1.33	0.92
1:A:-62:DA:H2''	1:A:-61:DT:H5''	1.48	0.91
1:A:6:DA:H2''	1:A:7:DA:H5''	1.51	0.91
2:B:28:DA:H2''	2:B:29:DT:H5'	1.52	0.91
4:D:-28:DA:H5'	7:J:70:VAL:HG11	1.55	0.89
2:B:60:DC:H2''	2:B:61:DA:H5''	1.53	0.89
3:C:0:DT:H2''	3:C:1:DA:H5''	1.52	0.88
5:F:116:LEU:HD13	5:F:160:ILE:HG12	1.56	0.88
4:D:1:DA:H2''	4:D:2:DA:H5'	1.56	0.88
2:B:4:DA:H2''	2:B:5:DA:H5''	1.56	0.86
1:A:-6:DC:O5'	5:E:136:LYS:HG2	1.75	0.86
1:A:-110:DT:H2''	1:A:-109:DA:H5'	1.58	0.85
5:F:115:PRO:HG2	5:F:118:ASP:HB2	1.58	0.85
5:G:103:LYS:HG3	5:G:142:LEU:HD12	1.59	0.83
1:A:46:DC:OP1	6:I:5:LYS:HE2	1.77	0.83
5:H:244:THR:HA	5:H:255:MET:HE2	1.60	0.83
5:G:244:THR:HA	5:G:255:MET:HE2	1.61	0.82
1:A:26:DC:H2''	1:A:27:DA:H5'	1.61	0.82
5:F:148:SER:HA	5:F:165:VAL:HG11	1.62	0.81
5:G:13:PRO:HG2	5:G:16:LEU:HG	1.60	0.81
5:F:76:LEU:HB3	5:F:114:ALA:O	1.79	0.80
1:A:71:DA:N3	5:G:2:GLY:HA3	1.96	0.80
4:D:-28:DA:H5''	7:J:70:VAL:HG21	1.61	0.80
5:F:76:LEU:HD13	5:F:116:LEU:HB3	1.63	0.80
3:C:20:DG:H2''	3:C:21:DG:H5''	1.62	0.79
5:F:13:PRO:HD3	5:F:45:ILE:HG13	1.66	0.78
5:G:11:ASP:O	5:G:12:LEU:HB2	1.83	0.78
5:G:40:ASP:HB2	5:G:43:ILE:HB	1.64	0.77
1:A:-53:DC:OP1	6:K:20:LYS:HE2	1.83	0.77
5:F:76:LEU:HD22	5:F:116:LEU:HA	1.66	0.77
5:G:203:MET:HE3	5:G:289:PHE:HE1	1.49	0.77
5:H:212:ARG:HA	5:H:311:ARG:HD2	1.67	0.77
1:A:48:DA:C2'	1:A:49:DC:H5''	2.14	0.77
5:H:155:ILE:HG12	5:H:160:ILE:HG13	1.65	0.77
2:B:81:DT:OP2	8:N:22:ARG:HD3	1.86	0.76
5:E:195:SER:HB3	5:E:199:LEU:HD22	1.68	0.76
2:B:48:DA:P	6:K:4:THR:HG21	2.26	0.75
5:E:274:SER:HB2	5:E:280:LEU:HD21	1.67	0.75
5:F:185:TYR:HE2	5:F:207:VAL:HG21	1.52	0.75
5:G:155:ILE:HG12	5:G:160:ILE:HG13	1.69	0.75
1:A:-29:DA:H2''	1:A:-28:DT:H72	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:212:ARG:HA	5:G:311:ARG:HD2	1.68	0.74
5:E:122:LYS:HB2	5:H:158:GLY:HA3	1.69	0.74
1:A:0:DT:H2''	1:A:1:DA:H5''	1.69	0.73
5:E:107:ILE:HD13	5:E:147:LEU:HD13	1.71	0.73
2:B:111:DT:H2''	2:B:112:DG:C8	2.22	0.73
4:D:-40:DA:H2''	4:D:-39:DA:H5'	1.71	0.73
5:F:5:ARG:HA	5:F:9:ARG:HD3	1.71	0.73
4:D:-11:DC:H2''	4:D:-10:DA:H5'	1.71	0.72
5:H:92:ILE:HG21	5:H:97:LEU:HB2	1.72	0.72
1:A:-42:DT:H2''	1:A:-41:DA:H5'	1.71	0.71
4:D:-62:DT:H2''	4:D:-61:DA:H5'	1.73	0.71
5:E:74:VAL:O	5:E:75:THR:HB	1.89	0.71
5:E:160:ILE:HD13	5:E:160:ILE:H	1.56	0.71
2:B:55:DT:H2''	2:B:56:DT:H72	1.72	0.71
5:H:216:LEU:HA	5:H:219:MET:HE2	1.72	0.71
1:A:-15:DC:H2''	1:A:-14:DT:H5'	1.72	0.70
5:F:74:VAL:HG22	5:F:75:THR:H	1.56	0.70
2:B:0:DA:C2'	2:B:1:DT:H5''	2.20	0.70
1:A:-45:DA:H4'	7:L:46:ARG:HD2	1.74	0.70
1:A:11:DG:C2'	1:A:12:DG:H5''	2.20	0.69
1:A:-7:DG:C2'	1:A:-6:DC:H5''	2.17	0.69
5:H:53:ILE:HG12	5:H:54:GLU:H	1.57	0.69
1:A:71:DA:C2	5:G:2:GLY:HA3	2.27	0.69
5:G:68:ILE:HG12	5:G:69:ASN:H	1.58	0.69
7:J:26:VAL:HA	7:J:29:MET:HE3	1.75	0.68
1:A:-77:DT:P	8:N:39:ARG:HG2	2.34	0.68
1:A:28:DT:O2	7:J:64:PRO:HB2	1.93	0.68
2:B:111:DT:H2''	2:B:112:DG:H8	1.56	0.68
4:D:-42:DC:H5'	7:J:46:ARG:HD3	1.74	0.68
5:H:107:ILE:HD13	5:H:147:LEU:HD13	1.75	0.68
8:M:42:LEU:HD23	8:M:42:LEU:H	1.56	0.68
4:D:2:DA:C2'	4:D:3:DA:H5''	2.22	0.67
5:E:209:THR:HG22	5:E:255:MET:HE1	1.75	0.67
8:N:31:PHE:CZ	8:N:50:VAL:HG11	2.29	0.67
5:G:274:SER:HB2	5:G:280:LEU:HD21	1.77	0.67
5:H:212:ARG:NH1	5:H:235:LYS:HB3	2.10	0.67
5:H:287:ARG:O	5:H:290:MET:HG2	1.95	0.66
1:A:7:DA:H5'	5:F:95:LYS:HG2	1.77	0.66
5:F:311:ARG:HH22	5:F:331:LEU:HB3	1.59	0.66
1:A:-30:DT:H5''	7:L:70:VAL:HG21	1.78	0.66
1:A:-5:DT:H5'	5:E:176:ARG:HH21	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:DA:C2'	2:B:96:DC:H5''	2.21	0.66
5:G:14:PRO:HG2	5:G:52:ASN:ND2	2.11	0.66
5:H:54:GLU:HG3	5:H:55:LEU:N	2.09	0.66
5:F:311:ARG:NH2	5:F:331:LEU:HB3	2.10	0.66
2:B:27:DG:H2''	2:B:28:DA:H5'	1.77	0.66
5:F:163:ASN:HD22	5:F:166:ALA:HB2	1.61	0.66
6:K:34:ILE:HA	7:L:1:MET:HE1	1.77	0.66
4:D:-6:DT:H71	5:F:142:LEU:HD11	1.78	0.65
5:H:13:PRO:HD2	5:H:16:LEU:HD23	1.79	0.65
5:G:6:SER:O	5:G:9:ARG:HG2	1.96	0.65
1:A:-77:DT:H4'	8:N:39:ARG:HD3	1.79	0.65
1:A:73:DT:H2''	1:A:74:DA:N7	2.12	0.65
1:A:-30:DT:H5'	7:L:70:VAL:HG11	1.78	0.64
5:E:203:MET:HE3	5:E:289:PHE:HE1	1.61	0.64
5:G:315:ALA:HB2	5:G:331:LEU:HD11	1.78	0.64
5:E:212:ARG:HH11	5:E:235:LYS:HB3	1.63	0.63
5:H:224:ILE:HG12	5:H:229:LEU:HG	1.80	0.63
5:G:8:GLU:O	5:G:18:ILE:HD12	1.99	0.63
7:L:26:VAL:HA	7:L:29:MET:HE3	1.81	0.63
1:A:7:DA:OP2	5:F:93:LYS:HG2	1.99	0.63
3:C:-9:DC:H2''	3:C:-8:DT:H5'	1.80	0.63
4:D:-7:DT:H2''	4:D:-6:DT:H5''	1.81	0.63
5:G:208:VAL:HG13	5:G:209:THR:HG23	1.81	0.62
5:G:84:GLU:HG2	5:G:104:ILE:HD13	1.80	0.62
1:A:-19:DG:C2'	1:A:-18:DT:H5''	2.25	0.62
6:I:33:GLU:HB2	7:J:10:LEU:HD21	1.82	0.62
4:D:-7:DT:OP2	5:F:136:LYS:HG3	1.99	0.62
1:A:-62:DA:C2'	1:A:-61:DT:H5''	2.25	0.62
1:A:61:DT:O2	5:F:2:GLY:HA3	2.00	0.61
5:G:93:LYS:HE2	5:G:93:LYS:HA	1.80	0.61
5:H:184:GLU:OE2	5:H:298:LEU:HD22	2.00	0.61
5:F:212:ARG:HH12	5:F:235:LYS:HD3	1.65	0.61
2:B:4:DA:H2'	5:E:96:THR:OG1	2.00	0.61
1:A:-31:DA:C8	7:L:64:PRO:HD3	2.36	0.61
1:A:46:DC:P	6:I:5:LYS:HE2	2.41	0.61
5:E:349:GLU:HG3	5:E:350:TRP:H	1.66	0.60
5:F:116:LEU:HD12	5:F:117:GLU:N	2.16	0.60
4:D:-60:DG:N2	5:F:3:ARG:HD3	2.16	0.60
5:G:124:ILE:HD13	5:G:165:VAL:HG22	1.81	0.60
5:F:161:THR:HG23	5:F:162:THR:HG23	1.82	0.60
5:H:45:ILE:O	5:H:49:ILE:HG12	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:93:LYS:HA	5:E:93:LYS:HE2	1.82	0.60
4:D:-18:DA:C2'	4:D:-17:DG:H5''	2.26	0.60
5:F:333:HIS:NE2	5:F:338:MET:HB2	2.16	0.60
1:A:-86:DA:H5'	8:M:39:ARG:HH22	1.66	0.60
1:A:-31:DA:H4'	7:L:72:LEU:CD2	2.31	0.60
5:G:101:MET:HA	5:G:104:ILE:HD12	1.84	0.60
8:N:29:ARG:HD3	8:N:51:ASP:HA	1.84	0.60
5:F:288:TYR:HA	5:F:291:ARG:HD3	1.82	0.60
1:A:6:DA:H2'	5:F:96:THR:OG1	2.02	0.59
4:D:-72:DT:O2	5:G:1:MET:HG2	2.02	0.59
5:E:212:ARG:NH1	5:E:235:LYS:HB3	2.18	0.59
4:D:-60:DG:H21	5:F:3:ARG:HE	1.50	0.59
5:F:54:GLU:O	5:F:54:GLU:HG3	2.00	0.59
5:H:208:VAL:HG13	5:H:209:THR:HG23	1.83	0.59
1:A:65:DA:H4'	4:D:-62:DT:H4'	1.84	0.59
5:G:305:PRO:HB3	5:G:309:GLU:HG3	1.84	0.59
5:F:77:HIS:HB2	5:F:113:ASP:OD1	2.02	0.59
5:G:40:ASP:HB3	5:G:43:ILE:HD13	1.83	0.59
4:D:-59:DT:H5'	5:F:6:SER:OG	2.02	0.59
5:H:122:LYS:HE3	5:H:122:LYS:HA	1.85	0.59
6:K:33:GLU:HB2	7:L:10:LEU:HD21	1.84	0.59
7:L:61:GLY:O	7:L:62:ARG:HG2	2.02	0.59
2:B:31:DT:H2''	2:B:32:DA:N7	2.18	0.58
1:A:-6:DC:H2'	1:A:-5:DT:H71	1.84	0.58
6:K:88:LYS:O	6:K:92:GLU:HG3	2.04	0.58
5:G:74:VAL:HG22	5:G:75:THR:H	1.69	0.58
5:H:315:ALA:HB2	5:H:331:LEU:HD21	1.84	0.58
6:K:44:VAL:HB	6:K:52:PHE:HB2	1.85	0.58
1:A:-47:DT:H2''	1:A:-46:DA:N7	2.18	0.58
1:A:54:DA:N7	5:F:21:ASN:OD1	2.37	0.58
5:F:111:LEU:HD13	5:F:119:ILE:HD13	1.85	0.58
4:D:5:DA:N6	5:G:99:ASN:ND2	2.51	0.58
1:A:-117:DG:H2''	1:A:-116:DT:H71	1.85	0.58
2:B:64:DA:H2''	2:B:65:DA:C8	2.38	0.58
1:A:-77:DT:O5'	8:N:39:ARG:HG2	2.04	0.58
4:D:-74:DT:H2''	4:D:-73:DA:C8	2.38	0.57
5:F:79:TRP:HE1	5:F:154:ALA:HB2	1.68	0.57
4:D:-42:DC:H5'	7:J:46:ARG:CD	2.33	0.57
4:D:-38:DT:H2'	4:D:-37:DT:H71	1.87	0.57
5:H:79:TRP:NE1	5:H:154:ALA:HB2	2.18	0.57
5:H:248:ILE:HG22	5:H:250:ALA:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:205:LEU:HA	5:E:208:VAL:HG12	1.86	0.57
5:F:116:LEU:HB2	5:F:160:ILE:HD11	1.86	0.57
8:N:13:ARG:HD3	8:N:13:ARG:N	2.19	0.57
5:E:176:ARG:H	5:E:176:ARG:HD3	1.69	0.57
1:A:6:DA:C2'	1:A:7:DA:H5''	2.30	0.57
4:D:-60:DG:H21	5:F:3:ARG:NE	2.02	0.57
5:H:65:THR:HG23	5:H:66:ALA:H	1.70	0.57
5:H:224:ILE:HD13	5:H:259:LEU:HD11	1.85	0.57
3:C:6:DA:H2''	3:C:7:DA:H5''	1.87	0.57
1:A:65:DA:H2''	1:A:66:DG:H5'	1.86	0.57
5:F:8:GLU:HB3	5:F:18:ILE:CG2	2.35	0.57
5:G:152:ARG:HD3	5:H:169:ARG:CZ	2.35	0.57
8:N:5:LEU:HA	8:N:43:PHE:CE2	2.40	0.57
5:E:79:TRP:NE1	5:E:154:ALA:HB2	2.20	0.56
5:G:242:ILE:N	5:G:242:ILE:HD12	2.19	0.56
5:H:53:ILE:HG12	5:H:54:GLU:N	2.19	0.56
5:G:16:LEU:HD22	5:G:18:ILE:HG13	1.87	0.56
1:A:-73:DG:H2''	1:A:-72:DT:H5''	1.86	0.56
1:A:0:DT:C2'	1:A:1:DA:H5''	2.35	0.56
5:E:211:GLN:HB2	5:E:216:LEU:HD21	1.85	0.56
5:F:26:TYR:HE1	5:F:35:PHE:HB2	1.70	0.56
5:H:16:LEU:HD12	5:H:25:CYS:O	2.05	0.56
5:F:115:PRO:CG	5:F:118:ASP:HB2	2.33	0.56
8:N:31:PHE:CE1	8:N:50:VAL:HG11	2.40	0.56
5:E:195:SER:CB	5:E:199:LEU:HD22	2.35	0.56
4:D:-60:DG:H21	5:F:3:ARG:HD3	1.70	0.56
5:F:105:LYS:HA	5:F:108:ARG:NH1	2.21	0.56
8:N:5:LEU:HA	8:N:43:PHE:HE2	1.69	0.56
5:F:49:ILE:HA	5:F:52:ASN:HB2	1.87	0.56
8:M:20:THR:HA	8:M:23:ARG:HD3	1.87	0.56
5:F:2:GLY:C	5:F:3:ARG:HD2	2.30	0.56
5:F:205:LEU:HA	5:F:208:VAL:HG12	1.88	0.56
5:H:179:ARG:HH21	5:H:316:ARG:HB2	1.71	0.56
1:A:-31:DA:H2'	1:A:-30:DT:H72	1.88	0.55
3:C:6:DA:H1'	3:C:7:DA:O4'	2.06	0.55
5:E:294:LYS:HE3	5:E:294:LYS:HA	1.87	0.55
5:H:262:CYS:HB3	5:H:266:LEU:HD12	1.89	0.55
5:F:55:LEU:HB3	5:F:57:SER:HB3	1.88	0.55
8:N:52:LEU:HD23	8:N:52:LEU:H	1.72	0.55
5:F:16:LEU:HD21	5:F:24:TYR:HB3	1.88	0.55
5:F:280:LEU:N	5:F:280:LEU:HD12	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:144:ARG:HE	5:G:168:THR:HG23	1.72	0.55
1:A:-4:DT:OP1	5:E:175:VAL:HG13	2.06	0.55
4:D:-3:DT:H2''	4:D:-2:DG:H5'	1.88	0.55
5:E:155:ILE:HG12	5:E:160:ILE:HG12	1.88	0.55
5:G:204:GLU:HG2	5:G:253:ILE:HD13	1.88	0.55
5:H:92:ILE:HD11	5:H:96:THR:HG21	1.89	0.55
5:F:293:ARG:NH1	5:F:304:PRO:HB2	2.21	0.55
6:I:35:ARG:HG2	7:J:86:LEU:HD13	1.88	0.55
5:E:199:LEU:HD21	5:E:288:TYR:HB3	1.87	0.54
5:F:31:THR:HG23	5:F:33:LYS:H	1.72	0.54
5:G:79:TRP:HE1	5:G:154:ALA:HB2	1.71	0.54
7:J:16:HIS:ND1	7:J:17:ILE:HG13	2.22	0.54
7:L:7:ILE:HG12	7:L:26:VAL:HG21	1.88	0.54
8:N:21:VAL:HA	8:N:24:TRP:CE3	2.42	0.54
5:G:129:ASN:HA	5:G:132:ILE:HD12	1.89	0.54
5:G:19:ARG:NH1	5:G:21:ASN:H	2.05	0.54
5:H:39:ARG:H	5:H:39:ARG:HE	1.54	0.54
1:A:-88:DT:H2''	1:A:-87:DT:H72	1.90	0.54
2:B:4:DA:C2'	2:B:5:DA:H5''	2.34	0.54
5:F:16:LEU:HA	5:F:26:TYR:HA	1.90	0.54
1:A:74:DA:H61	4:D:-74:DT:H3	1.56	0.54
4:D:-60:DG:H2''	4:D:-59:DT:OP2	2.07	0.54
8:O:5:LEU:HD22	8:O:22:ARG:HE	1.72	0.54
4:D:-45:DC:H2''	4:D:-44:DA:N7	2.22	0.54
3:C:12:DA:H2''	3:C:13:DG:C8	2.43	0.54
8:N:13:ARG:HD3	8:N:13:ARG:H	1.73	0.54
6:I:39:GLU:HA	7:J:90:ALA:HA	1.90	0.53
5:G:100:TYR:O	5:G:104:ILE:HG13	2.08	0.53
3:C:-7:DG:H2''	3:C:-6:DC:O5'	2.08	0.53
5:E:287:ARG:HG2	5:E:291:ARG:HH12	1.73	0.53
5:E:305:PRO:HB3	5:E:309:GLU:HG3	1.89	0.53
5:F:49:ILE:HD11	8:N:31:PHE:CE1	2.42	0.53
5:H:19:ARG:HH12	5:H:21:ASN:HD22	1.54	0.53
5:H:184:GLU:HG2	5:H:300:PHE:HZ	1.72	0.53
8:N:31:PHE:CE2	8:N:50:VAL:HG11	2.43	0.53
5:G:80:LEU:HD11	5:G:104:ILE:HG23	1.90	0.53
5:G:290:MET:HG3	5:G:293:ARG:NH2	2.23	0.53
4:D:-60:DG:H21	5:F:3:ARG:CD	2.21	0.53
4:D:-28:DA:C5'	7:J:70:VAL:HG21	2.33	0.53
5:G:290:MET:HG3	5:G:293:ARG:HH21	1.73	0.53
5:G:329:HIS:NE2	5:H:353:ILE:HG12	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:92:GLU:HA	7:J:75:LYS:HG3	1.90	0.53
1:A:64:DC:OP2	5:G:21:ASN:HB3	2.08	0.53
2:B:112:DG:H2'	2:B:113:DC:C5	2.44	0.53
5:F:46:THR:HG22	5:F:46:THR:O	2.09	0.53
5:G:141:LYS:O	5:G:141:LYS:HD3	2.09	0.53
5:H:179:ARG:HE	5:H:316:ARG:HD2	1.74	0.53
5:F:216:LEU:HA	5:F:219:MET:HE2	1.90	0.53
5:H:92:ILE:HG13	5:H:93:LYS:H	1.74	0.53
5:F:49:ILE:O	5:F:52:ASN:HB2	2.09	0.53
5:H:13:PRO:HD3	5:H:45:ILE:HG23	1.90	0.53
5:E:215:ASP:O	5:E:219:MET:HG3	2.09	0.53
5:E:288:TYR:HA	5:E:291:ARG:HH11	1.73	0.53
8:M:42:LEU:HD23	8:M:42:LEU:N	2.22	0.53
5:F:49:ILE:C	5:F:52:ASN:HB2	2.34	0.53
5:F:315:ALA:HB2	5:F:331:LEU:HD21	1.90	0.53
7:L:71:GLU:O	7:L:72:LEU:HD23	2.09	0.53
2:B:-15:DC:H2''	2:B:-14:DG:C8	2.44	0.52
5:E:196:PRO:HB2	5:E:198:TRP:CD1	2.43	0.52
5:F:15:ASN:O	5:F:16:LEU:HB3	2.09	0.52
5:F:17:TYR:HE2	5:F:27:ARG:HD3	1.73	0.52
5:H:92:ILE:CG1	5:H:96:THR:HB	2.39	0.52
5:F:24:TYR:OH	5:F:41:ARG:HG2	2.09	0.52
5:F:115:PRO:HG2	5:F:118:ASP:CB	2.35	0.52
1:A:-96:DG:OP2	8:M:20:THR:HG21	2.10	0.52
5:H:185:TYR:CE1	5:H:203:MET:HE3	2.43	0.52
1:A:-31:DA:H4'	7:L:72:LEU:HD21	1.92	0.52
2:B:60:DC:C2'	2:B:61:DA:H5''	2.33	0.52
2:B:79:DA:H2''	2:B:80:DA:C8	2.43	0.52
3:C:7:DA:H62	5:H:99:ASN:ND2	2.08	0.52
5:F:274:SER:N	5:F:280:LEU:HD11	2.24	0.52
6:I:38:LEU:HD13	6:I:79:VAL:HG11	1.92	0.52
5:E:96:THR:HA	5:E:99:ASN:HD22	1.74	0.52
5:E:315:ALA:O	5:E:319:GLU:HG3	2.10	0.52
5:F:254:SER:HB3	5:F:257:GLU:HB3	1.92	0.52
1:A:63:DT:H2''	1:A:64:DC:C5	2.45	0.52
5:E:233:GLN:OE1	5:E:238:VAL:HB	2.10	0.52
5:F:26:TYR:CE1	5:F:35:PHE:HB2	2.44	0.52
5:G:6:SER:H	5:G:9:ARG:HD3	1.73	0.52
5:G:13:PRO:HB3	5:G:45:ILE:HG13	1.91	0.52
5:H:13:PRO:HD2	5:H:16:LEU:CD2	2.40	0.52
2:B:90:DA:H5'	8:M:39:ARG:HD2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:5:ARG:HE	8:N:54:ARG:HH21	1.57	0.52
5:F:64:LEU:O	5:F:65:THR:HB	2.10	0.52
1:A:-2:DA:H2''	1:A:-1:DA:C8	2.45	0.52
5:G:151:PHE:O	5:G:155:ILE:HG13	2.10	0.52
1:A:-70:DT:H2''	1:A:-69:DG:C8	2.46	0.51
1:A:-55:DA:H2''	1:A:-54:DT:H72	1.93	0.51
4:D:-74:DT:H2''	4:D:-73:DA:N7	2.25	0.51
4:D:7:DC:OP1	5:G:307:PHE:HB3	2.10	0.51
5:E:121:THR:HG22	5:E:164:HIS:HB3	1.90	0.51
4:D:-13:DT:H2''	4:D:-12:DC:C5	2.45	0.51
6:I:83:PRO:O	6:I:88:LYS:HE3	2.10	0.51
5:E:74:VAL:O	5:E:75:THR:CB	2.59	0.51
5:F:27:ARG:HG3	5:F:28:ASP:H	1.75	0.51
5:F:172:LYS:HD3	5:F:173:SER:O	2.11	0.51
5:F:353:ILE:HD12	5:F:353:ILE:N	2.25	0.51
5:G:37:LEU:HD21	5:G:47:GLU:HB2	1.91	0.51
5:H:75:THR:HG22	5:H:113:ASP:O	2.10	0.51
6:K:2:ALA:O	6:K:4:THR:HG23	2.11	0.51
5:F:197:CYS:SG	5:F:265:ILE:HG21	2.50	0.51
5:H:139:SER:O	5:H:143:ILE:HG13	2.10	0.51
1:A:55:DG:N7	5:F:21:ASN:ND2	2.59	0.51
2:B:39:DA:H5'	6:K:73:ILE:HG23	1.93	0.51
5:F:13:PRO:HG2	5:F:15:ASN:O	2.11	0.51
5:G:13:PRO:HG2	5:G:16:LEU:CG	2.36	0.51
2:B:-14:DG:OP2	5:H:288:TYR:OH	2.29	0.51
2:B:18:DA:H2''	2:B:19:DC:H5'	1.92	0.51
2:B:48:DA:OP2	6:K:4:THR:HG21	2.11	0.51
5:F:16:LEU:HD13	5:F:16:LEU:C	2.36	0.51
5:F:207:VAL:HG22	5:F:310:LEU:HB3	1.91	0.51
8:O:23:ARG:HG2	8:O:26:ARG:HH21	1.76	0.51
1:A:49:DC:H2''	1:A:50:DG:C8	2.46	0.51
2:B:-14:DG:H2''	2:B:-13:DC:H5'	1.93	0.51
5:H:280:LEU:HD13	5:H:281:SER:N	2.26	0.51
1:A:64:DC:H42	4:D:-64:DG:H1	1.59	0.51
5:G:74:VAL:HG22	5:G:75:THR:N	2.24	0.51
5:E:224:ILE:HD12	5:E:224:ILE:N	2.26	0.51
8:N:36:LYS:NZ	8:N:39:ARG:HA	2.25	0.51
2:B:46:DT:H2''	2:B:47:DA:N7	2.25	0.51
4:D:-19:DT:H2''	4:D:-18:DA:C8	2.45	0.51
7:L:16:HIS:ND1	7:L:17:ILE:HG13	2.26	0.51
8:O:21:VAL:HA	8:O:24:TRP:CE3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:11:ASP:HB3	5:G:16:LEU:HD11	1.93	0.50
7:J:3:LYS:HE3	7:J:30:LEU:HD12	1.94	0.50
5:G:12:LEU:N	5:G:13:PRO:HD2	2.26	0.50
5:F:110:GLY:HA3	5:F:127:MET:SD	2.51	0.50
5:F:217:CYS:SG	5:F:285:VAL:HG21	2.52	0.50
5:G:198:TRP:HZ3	5:G:285:VAL:HG22	1.76	0.50
8:M:36:LYS:HB2	8:M:41:TYR:CE1	2.47	0.50
1:A:66:DG:O6	5:G:19:ARG:NH2	2.45	0.50
3:C:-9:DC:H2''	3:C:-8:DT:C5'	2.40	0.50
5:E:130:GLY:O	5:E:134:GLU:HG3	2.12	0.50
5:F:208:VAL:HG13	5:F:209:THR:HG23	1.93	0.50
5:H:151:PHE:O	5:H:155:ILE:HG13	2.12	0.50
8:M:2:TYR:HB2	8:N:14:ARG:HH12	1.76	0.50
5:E:186:LEU:HD13	5:E:186:LEU:O	2.11	0.50
5:G:5:ARG:HA	5:G:9:ARG:HE	1.77	0.50
5:G:79:TRP:NE1	5:G:154:ALA:HB2	2.26	0.50
5:H:274:SER:HB3	5:H:280:LEU:HD23	1.94	0.50
8:O:20:THR:HA	8:O:23:ARG:HH11	1.77	0.50
2:B:112:DG:H2'	2:B:113:DC:C6	2.47	0.50
4:D:-7:DT:C2'	4:D:-6:DT:H5''	2.41	0.50
4:D:5:DA:H2'	5:G:95:LYS:NZ	2.26	0.50
4:D:13:DT:H2''	4:D:14:DC:C5	2.47	0.50
4:D:-61:DA:O4'	5:F:1:MET:HG2	2.12	0.50
5:G:16:LEU:HD23	5:G:17:TYR:H	1.76	0.50
5:G:94:GLN:O	5:G:98:ILE:HG12	2.11	0.50
5:H:92:ILE:HG13	5:H:96:THR:HB	1.94	0.50
7:J:22:VAL:O	7:J:26:VAL:HG23	2.11	0.50
3:C:1:DA:H2'	3:C:2:DT:H71	1.93	0.49
5:H:129:ASN:HA	5:H:132:ILE:HD12	1.94	0.49
5:H:211:GLN:NE2	5:H:242:ILE:HD11	2.27	0.49
1:A:-73:DG:C2'	1:A:-72:DT:H5''	2.41	0.49
3:C:-2:DT:H2''	3:C:-1:DT:H5'	1.93	0.49
4:D:11:DC:H1'	4:D:12:DT:H5'	1.93	0.49
8:M:37:ASP:HB2	8:M:42:LEU:HD22	1.94	0.49
5:F:211:GLN:NE2	5:F:242:ILE:HD11	2.27	0.49
5:H:198:TRP:HZ3	5:H:285:VAL:HG22	1.76	0.49
1:A:29:DT:H2''	1:A:30:DG:N7	2.28	0.49
1:A:72:DA:H2''	1:A:73:DT:H72	1.94	0.49
5:H:87:LEU:HD12	5:H:90:ARG:HD3	1.95	0.49
6:K:87:LEU:O	6:K:91:VAL:HG23	2.12	0.49
5:E:72:ASN:O	5:F:65:THR:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:219:MET:HE1	5:E:229:LEU:HD21	1.93	0.49
5:F:160:ILE:HG22	5:F:162:THR:H	1.78	0.49
3:C:19:DC:H2''	3:C:20:DG:C8	2.48	0.49
3:C:16:DA:H2''	3:C:17:DA:C8	2.47	0.49
5:E:293:ARG:NH1	5:E:304:PRO:HB2	2.27	0.49
5:G:5:ARG:HA	5:G:9:ARG:NE	2.27	0.49
5:G:6:SER:N	5:G:9:ARG:HD3	2.26	0.49
5:G:243:PRO:HD3	5:H:353:ILE:O	2.13	0.49
5:F:348:ARG:HA	5:F:348:ARG:CZ	2.43	0.49
5:G:9:ARG:C	5:G:11:ASP:H	2.21	0.49
5:H:208:VAL:HG21	5:H:255:MET:HB2	1.94	0.49
5:H:217:CYS:SG	5:H:285:VAL:HG21	2.53	0.49
6:K:22:ASP:O	6:K:26:LEU:HG	2.12	0.49
7:L:3:LYS:HE3	7:L:30:LEU:HD12	1.95	0.49
5:E:199:LEU:O	5:E:203:MET:HG3	2.13	0.49
5:E:208:VAL:HG13	5:E:209:THR:HG23	1.94	0.49
2:B:90:DA:H4'	8:M:39:ARG:O	2.13	0.48
5:F:27:ARG:HA	5:F:34:GLU:HB3	1.95	0.48
5:F:41:ARG:O	5:F:45:ILE:HG22	2.13	0.48
5:G:203:MET:HE3	5:G:289:PHE:CE1	2.39	0.48
5:H:280:LEU:HD11	5:H:284:THR:HB	1.94	0.48
4:D:-60:DG:C2	5:F:3:ARG:HD3	2.47	0.48
5:E:224:ILE:HD12	5:E:224:ILE:H	1.78	0.48
5:G:37:LEU:HD23	5:G:44:ALA:HB1	1.95	0.48
5:H:259:LEU:C	5:H:259:LEU:HD23	2.37	0.48
7:J:7:ILE:HG21	7:J:23:GLU:HA	1.95	0.48
8:N:29:ARG:HG2	8:N:51:ASP:H	1.78	0.48
3:C:6:DA:H4'	5:H:235:LYS:HG3	1.94	0.48
4:D:-61:DA:N3	5:F:1:MET:HB3	2.28	0.48
5:H:92:ILE:HG13	5:H:93:LYS:N	2.28	0.48
2:B:71:DG:H2''	2:B:72:DA:O5'	2.14	0.48
3:C:-5:DT:H1'	3:C:-4:DT:H5''	1.95	0.48
5:E:298:LEU:HD13	5:E:299:SER:N	2.28	0.48
1:A:-73:DG:H1'	1:A:-72:DT:H5''	1.95	0.48
5:G:30:ARG:HD3	5:G:30:ARG:N	2.29	0.48
6:I:3:LEU:HB3	7:J:43:ILE:HG12	1.95	0.48
2:B:-3:DT:H1'	2:B:-2:DA:H5'	1.94	0.48
5:F:83:TYR:CE2	5:F:87:LEU:HD11	2.48	0.48
5:G:16:LEU:CD2	5:G:17:TYR:H	2.26	0.48
5:G:19:ARG:HH11	5:G:21:ASN:H	1.61	0.48
1:A:-110:DT:C2'	1:A:-109:DA:H5'	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:74:VAL:HB	5:H:115:PRO:HB3	1.96	0.48
7:J:25:ALA:O	7:J:29:MET:HG3	2.13	0.48
6:K:63:ARG:O	6:K:65:PRO:HD3	2.14	0.48
2:B:101:DG:H2''	2:B:102:DC:C6	2.49	0.48
4:D:0:DA:H2''	4:D:1:DA:C8	2.48	0.48
5:G:205:LEU:HA	5:G:208:VAL:HG12	1.96	0.48
6:I:63:ARG:O	6:I:65:PRO:HD3	2.13	0.48
8:N:2:TYR:HB2	8:O:13:ARG:HD3	1.96	0.48
8:O:19:GLU:HG3	8:O:23:ARG:NH1	2.29	0.48
1:A:10:DT:H3	4:D:-10:DA:H61	1.60	0.48
5:G:10:ARG:HG3	5:G:10:ARG:HH11	1.79	0.48
5:G:83:TYR:O	5:G:87:LEU:HG	2.14	0.48
5:E:110:GLY:HA3	5:E:127:MET:SD	2.54	0.48
5:H:318:TYR:HB3	5:H:327:ALA:HB2	1.96	0.48
5:E:93:LYS:HB2	5:E:96:THR:OG1	2.13	0.47
5:F:116:LEU:HD12	5:F:117:GLU:H	1.78	0.47
5:F:340:SER:HA	5:F:343:ARG:HH12	1.79	0.47
5:H:287:ARG:HA	5:H:290:MET:HE2	1.96	0.47
6:I:63:ARG:HA	6:I:71:ILE:H	1.78	0.47
8:N:5:LEU:HD23	8:N:5:LEU:O	2.13	0.47
1:A:-53:DC:P	6:K:20:LYS:HE2	2.54	0.47
1:A:-41:DA:H1'	1:A:-40:DT:H5''	1.96	0.47
3:C:8:DC:H41	5:H:95:LYS:NZ	2.12	0.47
5:F:331:LEU:N	5:F:331:LEU:HD12	2.29	0.47
5:H:43:ILE:O	5:H:47:GLU:HG3	2.14	0.47
5:H:341:GLN:HA	5:H:344:ASP:OD2	2.14	0.47
1:A:7:DA:H2'	5:F:95:LYS:HZ3	1.79	0.47
3:C:-2:DT:H2''	3:C:-1:DT:C5'	2.44	0.47
5:E:85:LYS:NZ	5:E:85:LYS:HB3	2.29	0.47
8:M:23:ARG:HG2	8:M:26:ARG:HH21	1.79	0.47
5:E:160:ILE:HD13	5:E:160:ILE:N	2.26	0.47
6:K:58:ASN:ND2	6:K:59:GLN:H	2.13	0.47
1:A:20:DA:H2''	1:A:21:DA:C5'	2.45	0.47
5:E:176:ARG:HD3	5:E:176:ARG:N	2.29	0.47
5:G:68:ILE:O	5:G:69:ASN:HB2	2.14	0.47
5:G:240:ILE:HD12	5:G:242:ILE:HD11	1.97	0.47
8:M:31:PHE:HA	8:M:32:PRO:C	2.38	0.47
1:A:6:DA:C8	5:F:96:THR:HG23	2.50	0.47
1:A:20:DA:H2''	1:A:21:DA:H5''	1.97	0.47
1:A:27:DA:H61	4:D:-27:DT:H3	1.63	0.47
2:B:17:DA:H2''	2:B:18:DA:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:20:DG:C2'	3:C:21:DG:H5''	2.39	0.47
5:F:8:GLU:HB3	5:F:18:ILE:HG21	1.95	0.47
5:G:97:LEU:O	5:G:101:MET:HG3	2.15	0.47
5:H:136:LYS:N	5:H:136:LYS:HD2	2.30	0.47
7:L:43:ILE:HB	7:L:51:PHE:HB2	1.97	0.47
8:N:5:LEU:HD23	8:N:5:LEU:C	2.39	0.47
2:B:-4:DG:H2'	5:H:338:MET:SD	2.54	0.47
5:F:229:LEU:HB3	5:F:242:ILE:HB	1.96	0.47
5:H:280:LEU:CD1	5:H:284:THR:HB	2.45	0.47
6:I:59:GLN:N	6:I:75:ALA:HB2	2.30	0.47
8:N:36:LYS:HZ2	8:N:39:ARG:HA	1.80	0.47
1:A:64:DC:H5	5:G:21:ASN:ND2	2.13	0.47
5:F:16:LEU:HD13	5:F:17:TYR:N	2.29	0.47
5:G:313:LEU:O	5:G:317:LEU:HG	2.14	0.47
6:I:23:ALA:O	6:I:27:VAL:HG23	2.15	0.47
8:M:35:VAL:O	8:M:42:LEU:HD23	2.15	0.47
1:A:3:DA:N1	4:D:-3:DT:O2	2.48	0.47
5:F:177:ARG:HH21	5:F:303:ASP:HB3	1.80	0.47
5:G:4:ARG:HG2	5:G:5:ARG:HG3	1.96	0.47
5:G:19:ARG:HH12	5:G:21:ASN:ND2	2.13	0.47
1:A:-107:DT:H5''	5:H:3:ARG:HE	1.79	0.46
3:C:7:DA:H2''	3:C:8:DC:O5'	2.14	0.46
5:E:151:PHE:O	5:E:155:ILE:HG13	2.14	0.46
5:G:165:VAL:O	5:G:168:THR:HG22	2.14	0.46
5:G:216:LEU:HD12	5:G:219:MET:SD	2.55	0.46
5:G:255:MET:O	5:G:259:LEU:HG	2.16	0.46
5:H:8:GLU:HB3	5:H:18:ILE:HG21	1.96	0.46
8:M:17:SER:O	8:M:21:VAL:HG23	2.15	0.46
4:D:6:DG:H1'	4:D:7:DC:H5''	1.96	0.46
5:H:26:TYR:HB2	5:H:37:LEU:HD21	1.97	0.46
5:H:189:TYR:HA	5:H:203:MET:HE1	1.98	0.46
8:M:1:MET:HE3	8:M:1:MET:HA	1.96	0.46
8:M:21:VAL:HA	8:M:24:TRP:CE3	2.51	0.46
8:M:21:VAL:HA	8:M:24:TRP:HE3	1.80	0.46
2:B:-8:DG:H2'	2:B:-7:DT:H72	1.98	0.46
5:E:243:PRO:HG2	5:E:246:LEU:CD1	2.45	0.46
5:F:151:PHE:O	5:F:155:ILE:HG13	2.15	0.46
5:G:39:ARG:CZ	5:G:39:ARG:H	2.28	0.46
5:G:116:LEU:HA	5:G:119:ILE:HD13	1.96	0.46
4:D:-29:DA:O3'	7:J:72:LEU:HD21	2.15	0.46
5:F:340:SER:HA	5:F:343:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:68:ILE:HG23	5:G:69:ASN:CG	2.39	0.46
5:H:115:PRO:O	5:H:119:ILE:HG13	2.15	0.46
5:H:119:ILE:HA	5:H:123:GLU:OE2	2.16	0.46
5:H:179:ARG:NH1	5:H:312:SER:HB3	2.31	0.46
1:A:45:DG:H5''	6:I:4:THR:HG22	1.98	0.46
5:G:117:GLU:HG2	5:G:160:ILE:HG22	1.96	0.46
8:M:18:LEU:O	8:M:22:ARG:HG3	2.15	0.46
1:A:-87:DT:H4'	8:M:39:ARG:CD	2.46	0.46
1:A:2:DC:H2''	1:A:3:DA:C5'	2.46	0.46
1:A:3:DA:H61	4:D:-3:DT:H3	1.62	0.46
2:B:48:DA:H1'	2:B:49:DA:C8	2.50	0.46
4:D:-39:DA:H1'	4:D:-38:DT:H5''	1.97	0.46
5:G:124:ILE:O	5:G:128:LEU:HG	2.16	0.46
5:H:18:ILE:HG23	5:H:18:ILE:O	2.16	0.46
4:D:-7:DT:P	5:F:136:LYS:HG3	2.54	0.46
5:F:160:ILE:HG22	5:F:161:THR:N	2.29	0.46
5:H:92:ILE:HD11	5:H:96:THR:CG2	2.45	0.46
1:A:12:DG:H2''	1:A:13:DA:C8	2.50	0.46
3:C:3:DA:H2''	3:C:4:DC:C6	2.51	0.46
5:H:98:ILE:HD12	5:H:98:ILE:N	2.31	0.46
7:L:22:VAL:O	7:L:26:VAL:HG23	2.16	0.46
2:B:2:DT:O4	2:B:3:DA:N6	2.49	0.46
5:G:29:PRO:C	5:G:30:ARG:HD3	2.41	0.46
8:N:1:MET:O	8:N:45:GLU:HB3	2.15	0.46
5:F:79:TRP:NE1	5:F:154:ALA:HB2	2.31	0.46
5:G:19:ARG:NH1	5:G:21:ASN:HD22	2.14	0.46
7:L:25:ALA:O	7:L:29:MET:HG3	2.16	0.46
5:G:13:PRO:HD3	5:G:45:ILE:HG13	1.98	0.45
5:G:7:HIS:C	5:G:9:ARG:H	2.22	0.45
5:G:243:PRO:HG2	5:G:246:LEU:CD1	2.47	0.45
5:H:227:GLY:O	5:H:244:THR:HG23	2.17	0.45
1:A:-11:DT:H2''	1:A:-10:DT:C6	2.52	0.45
2:B:100:DT:H2''	2:B:101:DG:C8	2.51	0.45
5:E:180:LEU:O	5:E:313:LEU:HD13	2.16	0.45
5:F:27:ARG:HG3	5:F:28:ASP:N	2.30	0.45
5:F:103:LYS:O	5:F:107:ILE:HG13	2.16	0.45
5:G:274:SER:HB2	5:G:280:LEU:CD2	2.45	0.45
6:K:63:ARG:HA	6:K:71:ILE:H	1.81	0.45
8:O:8:TRP:CH2	8:O:30:ILE:HD12	2.52	0.45
2:B:-7:DT:H2''	2:B:-6:DT:H5''	1.99	0.45
5:E:203:MET:O	5:E:207:VAL:HG23	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:17:TYR:HD2	5:H:25:CYS:HB2	1.82	0.45
8:M:36:LYS:HB2	8:M:41:TYR:HE1	1.80	0.45
4:D:-61:DA:C4'	5:F:1:MET:HE3	2.46	0.45
5:E:311:ARG:NH2	5:E:331:LEU:HB3	2.31	0.45
5:F:107:ILE:HD13	5:F:147:LEU:HD13	1.97	0.45
6:I:32:GLU:O	6:I:36:ARG:HG3	2.16	0.45
8:M:8:TRP:HH2	8:M:30:ILE:HD12	1.81	0.45
8:O:8:TRP:NE1	8:O:47:ALA:HB3	2.31	0.45
1:A:-52:DT:H2''	1:A:-51:DA:C8	2.52	0.45
1:A:64:DC:H4'	5:F:1:MET:HE1	1.98	0.45
5:E:243:PRO:O	5:E:246:LEU:HD13	2.16	0.45
5:F:290:MET:HG3	5:F:293:ARG:NH2	2.32	0.45
5:G:119:ILE:N	5:G:119:ILE:HD12	2.31	0.45
5:G:201:LEU:HD13	5:G:262:CYS:SG	2.57	0.45
5:H:331:LEU:N	5:H:331:LEU:HD12	2.32	0.45
6:K:35:ARG:HG2	7:L:86:LEU:HD13	1.99	0.45
1:A:-12:DG:H2''	1:A:-11:DT:H5'	1.98	0.45
1:A:7:DA:H2'	5:F:95:LYS:NZ	2.32	0.45
1:A:65:DA:H2''	1:A:66:DG:C5'	2.47	0.45
4:D:-8:DC:H2'	4:D:-7:DT:H72	1.99	0.45
5:E:80:LEU:O	5:E:84:GLU:HG3	2.16	0.45
5:F:158:GLY:HA3	5:G:122:LYS:HB2	1.99	0.45
5:F:180:LEU:O	5:F:313:LEU:HD13	2.16	0.45
5:H:163:ASN:HD22	5:H:166:ALA:HB2	1.81	0.45
8:M:34:PRO:HB3	8:M:43:PHE:CG	2.51	0.45
2:B:28:DA:C2'	2:B:29:DT:H5'	2.35	0.45
5:F:220:LYS:HA	5:F:270:THR:HA	1.99	0.45
5:G:199:LEU:O	5:G:203:MET:HG3	2.17	0.45
8:O:5:LEU:HD22	8:O:22:ARG:NE	2.31	0.45
5:F:212:ARG:NH1	5:F:235:LYS:HD3	2.31	0.45
5:G:5:ARG:HG2	5:G:9:ARG:HH21	1.81	0.45
5:G:236:THR:OG1	5:G:238:VAL:HG23	2.17	0.45
5:G:320:LYS:HE2	5:G:320:LYS:HB2	1.82	0.45
5:H:111:LEU:HD13	5:H:112:PRO:N	2.31	0.45
5:H:201:LEU:HB3	5:H:262:CYS:SG	2.57	0.45
7:J:7:ILE:HG12	7:J:26:VAL:HG21	1.99	0.45
8:N:31:PHE:N	8:N:31:PHE:CD2	2.82	0.45
8:N:50:VAL:HG23	8:N:51:ASP:N	2.32	0.45
4:D:-47:DT:H2''	4:D:-46:DG:C8	2.52	0.45
4:D:-29:DA:H4'	7:J:72:LEU:CD2	2.47	0.45
2:B:76:DC:H2''	2:B:77:DA:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:7:DA:H62	5:H:99:ASN:HD21	1.64	0.44
5:E:198:TRP:HZ3	5:E:285:VAL:HG22	1.80	0.44
5:E:274:SER:HB2	5:E:280:LEU:CD2	2.40	0.44
5:F:12:LEU:HD21	5:F:24:TYR:HE2	1.82	0.44
5:G:39:ARG:HE	5:G:40:ASP:N	2.15	0.44
1:A:-40:DT:H6	1:A:-39:DT:H72	1.82	0.44
4:D:-54:DT:H1'	4:D:-53:DG:C8	2.52	0.44
5:G:42:ARG:C	5:G:43:ILE:HD12	2.42	0.44
6:K:3:LEU:HB2	7:L:36:THR:HG21	1.99	0.44
8:M:11:ARG:HA	8:M:11:ARG:NE	2.32	0.44
1:A:14:DA:N6	4:D:-15:DA:N6	2.66	0.44
5:E:136:LYS:N	5:E:136:LYS:HD2	2.32	0.44
5:F:274:SER:HB2	5:F:280:LEU:HD11	1.99	0.44
5:H:41:ARG:O	5:H:45:ILE:HG13	2.17	0.44
1:A:62:DA:N3	5:F:1:MET:HA	2.33	0.44
5:H:294:LYS:HB2	5:H:294:LYS:NZ	2.31	0.44
8:M:16:ARG:HG3	8:M:24:TRP:HH2	1.83	0.44
1:A:18:DT:H2''	1:A:19:DA:C8	2.53	0.44
2:B:90:DA:H5'	8:M:39:ARG:CD	2.48	0.44
5:E:185:TYR:CE2	5:E:207:VAL:HG21	2.53	0.44
5:F:49:ILE:CA	5:F:52:ASN:HB2	2.47	0.44
6:K:92:GLU:HG2	7:L:75:LYS:HD2	1.99	0.44
5:F:193:GLU:HA	5:F:200:ARG:HH21	1.82	0.44
4:D:-60:DG:N3	5:F:3:ARG:HD3	2.33	0.44
5:F:262:CYS:HB3	5:F:266:LEU:HD12	1.99	0.44
5:G:107:ILE:HD13	5:G:147:LEU:HD13	1.99	0.44
5:H:63:PRO:C	5:H:64:LEU:HD22	2.42	0.44
1:A:-86:DA:H5'	8:M:39:ARG:NH2	2.32	0.44
5:F:18:ILE:HD12	5:F:24:TYR:CZ	2.53	0.44
5:F:42:ARG:NH2	8:O:55:PRO:O	2.50	0.44
5:F:136:LYS:H	5:F:136:LYS:HD2	1.83	0.44
5:F:184:GLU:OE2	5:F:298:LEU:HD21	2.17	0.44
1:A:-87:DT:H1'	8:M:39:ARG:NH1	2.32	0.44
2:B:72:DA:C2'	2:B:73:DC:H5'	2.34	0.44
5:F:136:LYS:HD2	5:F:136:LYS:N	2.33	0.44
5:F:257:GLU:HG2	5:F:261:LYS:NZ	2.33	0.44
5:G:17:TYR:CD2	5:G:25:CYS:HB2	2.52	0.44
5:H:103:LYS:O	5:H:107:ILE:HG13	2.17	0.44
6:I:20:LYS:HA	6:I:23:ALA:HB3	1.99	0.44
6:K:54:LEU:HB3	6:K:77:ARG:HE	1.82	0.44
3:C:0:DT:C2'	3:C:1:DA:H5''	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:80:LEU:O	5:F:84:GLU:HG3	2.18	0.43
5:G:30:ARG:HG2	5:G:30:ARG:HH11	1.83	0.43
3:C:-5:DT:H2''	3:C:-4:DT:H5''	2.00	0.43
4:D:-50:DC:H2''	4:D:-49:DG:C8	2.53	0.43
5:F:189:TYR:HD2	5:F:203:MET:HE3	1.83	0.43
5:G:33:LYS:HD2	5:G:33:LYS:N	2.33	0.43
5:F:3:ARG:HD2	5:F:3:ARG:N	2.33	0.43
5:G:13:PRO:CG	5:G:45:ILE:HG13	2.49	0.43
1:A:-73:DG:H2''	1:A:-72:DT:C5'	2.47	0.43
5:F:13:PRO:HG3	5:F:48:ALA:O	2.18	0.43
5:G:179:ARG:NH2	5:G:312:SER:HB3	2.34	0.43
7:L:7:ILE:HG21	7:L:23:GLU:HA	1.99	0.43
2:B:64:DA:H2''	2:B:65:DA:N7	2.34	0.43
4:D:-71:DT:OP2	5:G:27:ARG:NH2	2.52	0.43
4:D:-5:DA:H2''	4:D:-4:DT:H5''	2.00	0.43
5:F:16:LEU:HA	5:F:25:CYS:O	2.19	0.43
5:G:220:LYS:HB2	5:G:223:ASP:OD1	2.19	0.43
2:B:-5:DA:H2''	2:B:-4:DG:H5'	1.99	0.43
3:C:-13:DA:H2''	3:C:-12:DA:O5'	2.19	0.43
5:F:16:LEU:HD11	5:F:24:TYR:HD2	1.83	0.43
5:H:239:LYS:HD2	5:H:239:LYS:N	2.33	0.43
6:K:44:VAL:HG22	7:L:1:MET:HE2	1.99	0.43
8:O:17:SER:O	8:O:21:VAL:HG23	2.18	0.43
4:D:5:DA:H2'	5:G:95:LYS:HZ1	1.81	0.43
5:E:204:GLU:HG2	5:E:253:ILE:HD13	2.00	0.43
5:G:11:ASP:HB3	5:G:13:PRO:HD2	2.01	0.43
5:H:17:TYR:CZ	5:H:27:ARG:HB2	2.53	0.43
3:C:4:DC:H2''	3:C:5:DT:O5'	2.19	0.43
5:E:208:VAL:HG22	5:E:255:MET:HE2	2.00	0.43
5:E:349:GLU:HG3	5:E:350:TRP:N	2.34	0.43
5:F:139:SER:O	5:F:143:ILE:HG13	2.19	0.43
5:G:115:PRO:HB2	5:G:118:ASP:OD2	2.19	0.43
5:H:76:LEU:O	5:H:80:LEU:HG	2.19	0.43
5:H:165:VAL:O	5:H:168:THR:HG22	2.18	0.43
6:I:22:ASP:O	6:I:26:LEU:HG	2.16	0.43
6:K:32:GLU:O	6:K:36:ARG:HG3	2.19	0.43
5:E:82:ARG:O	5:E:86:ILE:HG13	2.19	0.42
5:G:11:ASP:C	5:G:13:PRO:HD2	2.44	0.42
5:H:5:ARG:O	5:H:9:ARG:HB3	2.19	0.42
5:H:116:LEU:N	5:H:116:LEU:HD12	2.34	0.42
2:B:73:DC:H2''	2:B:74:DT:H71	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:-17:DG:H2''	3:C:-16:DT:H71	2.01	0.42
5:H:27:ARG:HG2	5:H:28:ASP:N	2.33	0.42
5:H:64:LEU:HD22	5:H:64:LEU:N	2.34	0.42
5:H:325:LYS:HE3	5:H:329:HIS:CE1	2.54	0.42
6:K:48:GLY:HA2	6:K:86:LYS:HD3	2.01	0.42
6:K:57:LYS:NZ	6:K:57:LYS:HB3	2.34	0.42
7:L:49:GLY:HA3	7:L:80:PHE:CZ	2.54	0.42
8:M:13:ARG:C	8:M:15:PRO:HD3	2.45	0.42
5:E:97:LEU:HD23	5:E:97:LEU:O	2.18	0.42
5:F:51:ALA:C	5:F:53:ILE:H	2.26	0.42
5:H:100:TYR:O	5:H:104:ILE:HG13	2.19	0.42
5:H:232:GLU:O	5:H:232:GLU:HG2	2.19	0.42
5:H:233:GLN:OE1	5:H:238:VAL:HB	2.19	0.42
7:L:16:HIS:HD1	7:L:17:ILE:HG13	1.84	0.42
2:B:1:DT:H2''	2:B:2:DT:O5'	2.20	0.42
4:D:1:DA:C2'	4:D:2:DA:H5'	2.38	0.42
6:I:38:LEU:HD12	7:J:86:LEU:HD11	2.01	0.42
5:E:183:ASP:O	5:E:187:LYS:HG2	2.19	0.42
5:F:45:ILE:O	5:F:49:ILE:HB	2.19	0.42
5:F:155:ILE:HG23	5:F:160:ILE:O	2.19	0.42
5:G:1:MET:HB3	5:G:2:GLY:H	1.59	0.42
5:G:3:ARG:O	5:G:5:ARG:N	2.52	0.42
5:H:184:GLU:HG2	5:H:300:PHE:CZ	2.54	0.42
5:H:262:CYS:O	5:H:266:LEU:HB2	2.19	0.42
6:K:4:THR:O	6:K:8:MET:HG3	2.19	0.42
5:F:74:VAL:HG13	5:F:75:THR:N	2.34	0.42
5:G:49:ILE:O	5:G:53:ILE:HG12	2.19	0.42
1:A:-41:DA:H2	6:K:66:LYS:HE2	1.85	0.42
4:D:-42:DC:C5'	7:J:46:ARG:HD3	2.45	0.42
4:D:-11:DC:C2'	4:D:-10:DA:H5'	2.46	0.42
1:A:70:DA:H2	5:G:3:ARG:HE	1.68	0.42
4:D:-42:DC:OP2	7:J:84:LYS:HB2	2.20	0.42
5:E:266:LEU:HD13	5:E:273:ALA:H	1.84	0.42
5:F:128:LEU:C	5:F:128:LEU:HD13	2.45	0.42
5:G:28:ASP:HB3	5:G:30:ARG:HE	1.84	0.42
5:G:103:LYS:O	5:G:107:ILE:HG13	2.19	0.42
5:H:201:LEU:HD13	5:H:262:CYS:SG	2.60	0.42
5:H:232:GLU:H	5:H:232:GLU:CD	2.28	0.42
1:A:-41:DA:C2'	1:A:-40:DT:H5''	2.50	0.42
1:A:51:DA:H2''	1:A:52:DA:C8	2.55	0.42
2:B:14:DA:H2''	2:B:15:DG:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:76:LEU:CB	5:F:114:ALA:O	2.57	0.42
5:F:224:ILE:HA	5:F:228:TYR:O	2.19	0.42
5:H:15:ASN:OD1	5:H:27:ARG:HB3	2.20	0.42
6:I:36:ARG:HA	6:I:39:GLU:OE2	2.20	0.42
1:A:26:DC:C2'	1:A:27:DA:H5'	2.40	0.42
2:B:18:DA:H2''	2:B:19:DC:C5'	2.49	0.42
3:C:-5:DT:C2'	3:C:-4:DT:H5''	2.50	0.42
5:F:97:LEU:HD23	5:F:97:LEU:O	2.20	0.42
5:G:14:PRO:HG2	5:G:52:ASN:HD22	1.83	0.42
5:G:27:ARG:CZ	5:G:32:GLY:HA2	2.49	0.42
5:H:19:ARG:HH12	5:H:21:ASN:HB2	1.85	0.42
5:F:116:LEU:HD22	5:F:160:ILE:HG13	2.02	0.41
5:F:319:GLU:HG3	5:F:324:ASP:OD1	2.20	0.41
7:J:74:GLY:O	7:J:75:LYS:HB3	2.20	0.41
8:M:29:ARG:HE	8:M:29:ARG:HA	1.85	0.41
8:M:32:PRO:HA	8:M:33:PRO:HD3	1.82	0.41
2:B:90:DA:O3'	8:M:39:ARG:O	2.39	0.41
5:E:103:LYS:O	5:E:107:ILE:HG13	2.20	0.41
5:E:219:MET:HE3	5:E:231:VAL:HG22	2.01	0.41
5:F:105:LYS:HA	5:F:108:ARG:HH12	1.84	0.41
5:F:313:LEU:O	5:F:317:LEU:HG	2.20	0.41
5:G:313:LEU:HA	5:G:316:ARG:NH2	2.35	0.41
5:H:37:LEU:HB3	5:H:47:GLU:OE1	2.20	0.41
5:H:82:ARG:O	5:H:86:ILE:HG13	2.20	0.41
6:I:44:VAL:HB	6:I:52:PHE:HB2	2.01	0.41
7:L:4:SER:O	7:L:8:GLU:HG3	2.19	0.41
8:M:29:ARG:HA	8:M:29:ARG:NE	2.35	0.41
1:A:-116:DT:H2''	1:A:-115:DC:C6	2.54	0.41
5:F:116:LEU:HD21	5:F:159:HIS:HB3	2.02	0.41
5:H:229:LEU:N	5:H:229:LEU:HD12	2.35	0.41
6:K:23:ALA:O	6:K:27:VAL:HG23	2.20	0.41
6:K:53:ASP:HB2	6:K:80:THR:OG1	2.20	0.41
1:A:-54:DT:H2''	1:A:-53:DC:C6	2.55	0.41
5:F:225:VAL:HG12	5:F:226:ASP:OD2	2.20	0.41
5:F:283:GLY:O	5:F:287:ARG:HB2	2.20	0.41
8:N:37:ASP:CG	8:N:42:LEU:HD12	2.46	0.41
1:A:-31:DA:C2	7:L:62:ARG:HB2	2.56	0.41
2:B:46:DT:H2''	2:B:47:DA:C8	2.56	0.41
4:D:17:DC:H2''	4:D:18:DG:C8	2.56	0.41
5:E:198:TRP:HB3	5:E:266:LEU:HD21	2.03	0.41
5:G:141:LYS:HD3	5:G:141:LYS:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:5:ARG:HB2	5:H:5:ARG:NH2	2.34	0.41
5:H:233:GLN:O	5:H:237:GLY:HA2	2.21	0.41
6:I:60:ARG:NH1	6:I:73:ILE:HD12	2.36	0.41
1:A:-90:DT:H2'	1:A:-89:DT:H71	2.02	0.41
4:D:-61:DA:H5''	5:F:1:MET:HE3	2.03	0.41
6:I:53:ASP:HB2	6:I:80:THR:OG1	2.21	0.41
6:I:54:LEU:CD2	6:I:79:VAL:HG22	2.51	0.41
5:E:212:ARG:O	5:E:216:LEU:HG	2.21	0.41
5:G:242:ILE:HD12	5:G:242:ILE:H	1.86	0.41
5:H:107:ILE:HG21	5:H:147:LEU:HD13	2.02	0.41
7:J:62:ARG:NE	7:J:69:LYS:HG2	2.35	0.41
8:N:39:ARG:NH2	8:O:16:ARG:HH12	2.18	0.41
5:E:79:TRP:HE1	5:E:154:ALA:HB2	1.86	0.41
5:E:152:ARG:HH11	5:F:169:ARG:NH2	2.17	0.41
5:E:198:TRP:CZ3	5:E:285:VAL:HG22	2.56	0.41
5:G:185:TYR:CE2	5:G:207:VAL:HG21	2.55	0.41
5:H:149:ASP:HA	5:H:152:ARG:HH11	1.86	0.41
7:J:62:ARG:CD	7:J:69:LYS:HG2	2.51	0.41
6:K:54:LEU:CD2	6:K:79:VAL:HG22	2.51	0.41
8:N:33:PRO:HA	8:N:34:PRO:HD3	1.85	0.41
2:B:73:DC:H2''	2:B:74:DT:OP2	2.20	0.41
3:C:6:DA:O3'	5:H:235:LYS:HA	2.21	0.41
3:C:11:DG:H2'	3:C:12:DA:C8	2.55	0.41
5:F:144:ARG:HD3	5:F:170:ALA:HB2	2.03	0.41
5:F:179:ARG:HA	5:F:309:GLU:CD	2.46	0.41
5:G:215:ASP:O	5:G:219:MET:HG3	2.20	0.41
5:G:304:PRO:HA	5:G:305:PRO:HD3	1.88	0.41
5:H:76:LEU:CD2	5:H:111:LEU:HD12	2.50	0.41
6:K:30:PHE:O	6:K:34:ILE:HG13	2.21	0.41
8:N:25:VAL:HG13	8:N:34:PRO:HD2	2.02	0.41
5:E:307:PHE:CE1	5:E:310:LEU:HD12	2.56	0.41
5:H:52:ASN:O	5:H:53:ILE:HB	2.20	0.41
5:H:55:LEU:HB3	5:H:56:PHE:H	1.57	0.41
5:H:276:ARG:O	5:H:278:GLU:HG2	2.21	0.41
4:D:-20:DT:H1'	4:D:-19:DT:H5'	2.03	0.40
4:D:16:DA:H2''	4:D:17:DC:C6	2.55	0.40
5:E:129:ASN:HA	5:E:132:ILE:HD12	2.02	0.40
5:F:215:ASP:CG	5:F:233:GLN:HA	2.46	0.40
5:G:186:LEU:O	5:G:186:LEU:HD13	2.21	0.40
5:G:198:TRP:HB3	5:G:266:LEU:HD21	2.02	0.40
7:J:83:GLY:O	7:J:87:ARG:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:15:PRO:C	8:N:16:ARG:HD2	2.46	0.40
4:D:13:DT:H2''	4:D:14:DC:C6	2.56	0.40
5:F:4:ARG:HB3	5:F:5:ARG:HD3	2.03	0.40
7:L:24:ASP:O	7:L:28:GLU:HG2	2.21	0.40
8:N:13:ARG:H	8:N:13:ARG:CD	2.34	0.40
1:A:-97:DT:H2'	8:M:23:ARG:NH2	2.36	0.40
1:A:2:DC:H2''	1:A:3:DA:H5'	2.03	0.40
5:E:97:LEU:O	5:E:101:MET:HG3	2.21	0.40
7:L:35:SER:O	7:L:39:GLN:HG3	2.21	0.40
8:O:24:TRP:HD1	8:O:29:ARG:HD3	1.86	0.40
4:D:-38:DT:H2'	4:D:-38:DT:H6	1.73	0.40
5:E:148:SER:O	5:E:152:ARG:HG3	2.21	0.40
5:G:7:HIS:O	5:G:8:GLU:HB2	2.21	0.40
5:G:19:ARG:NH1	5:G:21:ASN:ND2	2.69	0.40
5:G:39:ARG:H	5:G:39:ARG:NE	2.18	0.40
5:G:68:ILE:HG12	5:G:69:ASN:N	2.31	0.40
5:H:120:THR:HG23	5:H:123:GLU:H	1.87	0.40
2:B:-7:DT:H1'	2:B:-6:DT:H5''	2.04	0.40
4:D:-5:DA:H2''	4:D:-4:DT:C5'	2.51	0.40
5:G:246:LEU:HD12	5:G:246:LEU:N	2.37	0.40
8:O:44:HIS:ND1	8:O:45:GLU:N	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	270/356 (76%)	249 (92%)	16 (6%)	5 (2%)	6	32
5	F	354/356 (99%)	303 (86%)	40 (11%)	11 (3%)	3	22
5	G	341/356 (96%)	288 (84%)	38 (11%)	15 (4%)	2	17
5	H	354/356 (99%)	299 (84%)	41 (12%)	14 (4%)	2	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	I	94/96 (98%)	87 (93%)	6 (6%)	1 (1%)	11	46
6	K	94/96 (98%)	86 (92%)	7 (7%)	1 (1%)	11	46
7	J	92/94 (98%)	85 (92%)	5 (5%)	2 (2%)	5	29
7	L	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
8	M	51/55 (93%)	45 (88%)	6 (12%)	0	100	100
8	N	52/55 (94%)	42 (81%)	8 (15%)	2 (4%)	2	19
8	O	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
All	All	1847/1969 (94%)	1621 (88%)	175 (10%)	51 (3%)	6	24

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	75	THR
5	G	12	LEU
5	H	18	ILE
5	H	55	LEU
5	H	60	LYS
5	H	63	PRO
5	E	196	PRO
5	E	266	LEU
5	F	57	SER
5	F	95	LYS
5	G	68	ILE
5	H	19	ARG
5	H	53	ILE
5	E	250	ALA
5	F	69	ASN
5	G	4	ARG
5	G	59	HIS
5	G	65	THR
5	G	67	ARG
5	G	72	ASN
5	G	226	ASP
5	G	266	LEU
5	H	94	GLN
5	H	305	PRO
8	N	51	ASP
5	E	73	SER
5	F	59	HIS
5	F	71	ASP

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Mol	Chain	Res	Type
5	F	305	PRO
5	G	15	ASN
5	G	17	TYR
5	H	4	ARG
5	H	91	GLY
5	H	267	GLY
5	F	175	VAL
5	G	56	PHE
5	G	62	LYS
5	H	56	PHE
5	H	61	HIS
7	J	75	LYS
6	K	49	PHE
8	N	35	VAL
5	F	16	LEU
6	I	96	PRO
5	E	74	VAL
5	F	196	PRO
5	G	196	PRO
5	G	14	PRO
5	H	196	PRO
5	F	119	ILE
7	J	74	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	230/300 (77%)	224 (97%)	6 (3%)	40	62
5	F	300/300 (100%)	297 (99%)	3 (1%)	68	78
5	G	291/300 (97%)	283 (97%)	8 (3%)	39	61
5	H	300/300 (100%)	291 (97%)	9 (3%)	36	57
6	I	83/83 (100%)	83 (100%)	0	100	100
6	K	83/83 (100%)	82 (99%)	1 (1%)	63	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	J	79/79 (100%)	79 (100%)	0	100	100
7	L	79/79 (100%)	78 (99%)	1 (1%)	61	74
8	M	50/52 (96%)	49 (98%)	1 (2%)	48	66
8	N	51/52 (98%)	49 (96%)	2 (4%)	28	49
8	O	52/52 (100%)	51 (98%)	1 (2%)	50	67
All	All	1598/1680 (95%)	1566 (98%)	32 (2%)	48	66

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	85	LYS
5	E	160	ILE
5	E	176	ARG
5	E	247	HIS
5	E	256	LYS
5	E	294	LYS
5	F	14	PRO
5	F	193	GLU
5	F	348	ARG
5	G	8	GLU
5	G	9	ARG
5	G	16	LEU
5	G	39	ARG
5	G	42	ARG
5	G	142	LEU
5	G	320	LYS
5	G	354	GLU
5	H	39	ARG
5	H	60	LYS
5	H	61	HIS
5	H	65	THR
5	H	75	THR
5	H	122	LYS
5	H	280	LEU
5	H	294	LYS
5	H	348	ARG
6	K	57	LYS
7	L	93	TYR
8	M	42	LEU
8	N	39	ARG

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Mol	Chain	Res	Type
8	N	54	ARG
8	O	49	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	99	ASN
5	E	159	HIS
5	E	164	HIS
5	E	211	GLN
5	E	247	HIS
5	E	308	HIS
5	E	328	GLN
5	F	50	GLN
5	F	99	ASN
5	F	159	HIS
5	F	163	ASN
5	F	164	HIS
5	F	211	GLN
5	F	233	GLN
5	F	308	HIS
5	G	21	ASN
5	G	52	ASN
5	G	69	ASN
5	G	99	ASN
5	G	190	GLN
5	G	328	GLN
5	H	21	ASN
5	H	59	HIS
5	H	77	HIS
5	H	99	ASN
5	H	159	HIS
5	H	329	HIS
6	I	93	ASN
7	J	14	GLN
7	J	39	GLN
6	K	58	ASN
6	K	93	ASN
8	M	44	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.

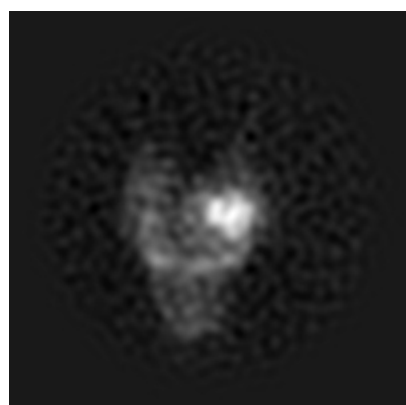
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3400. These allow visual inspection of the internal detail of the map and identification of artifacts.

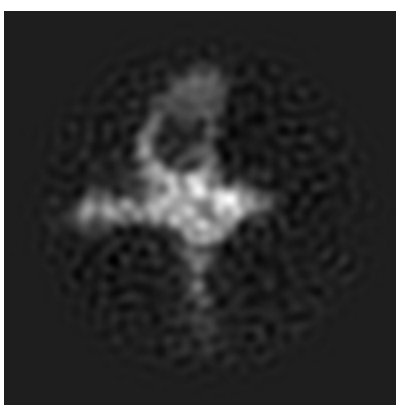
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

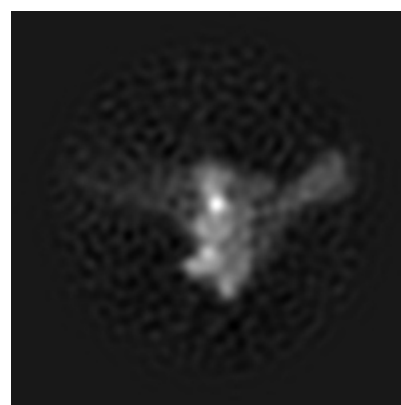
6.1.1 Primary map



X



Y

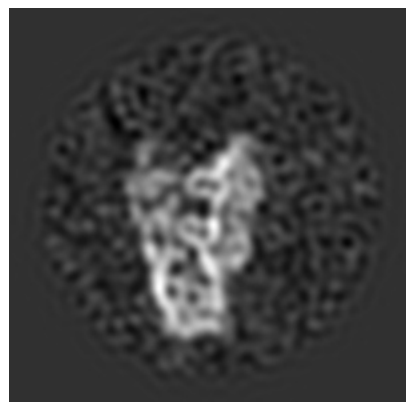


Z

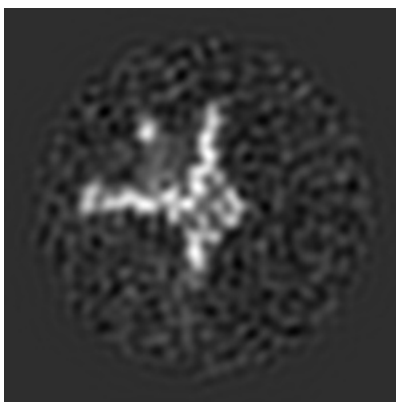
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 64



Y Index: 64

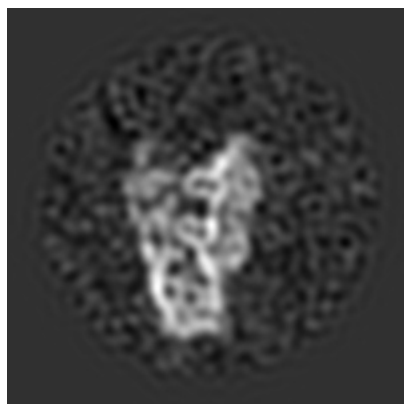


Z Index: 64

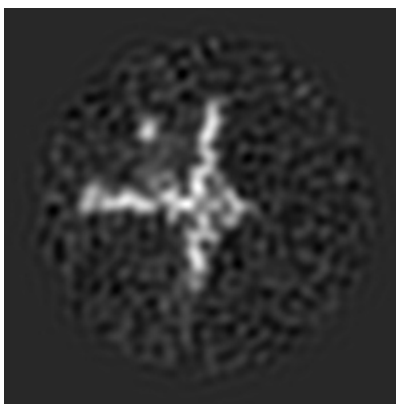
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

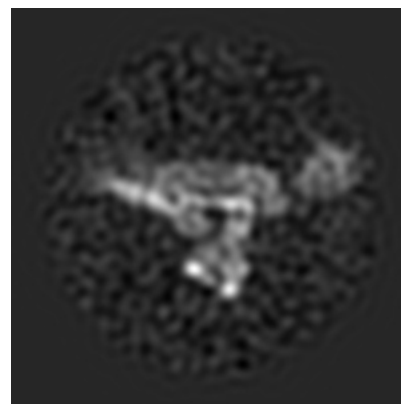
6.3.1 Primary map



X Index: 64



Y Index: 65

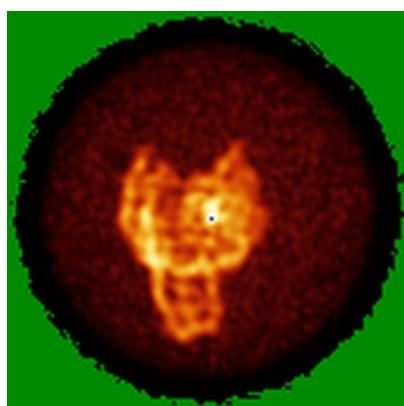


Z Index: 62

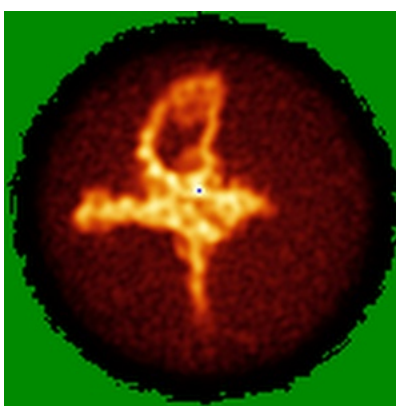
The images above show the largest variance slices of the map in three orthogonal directions.

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

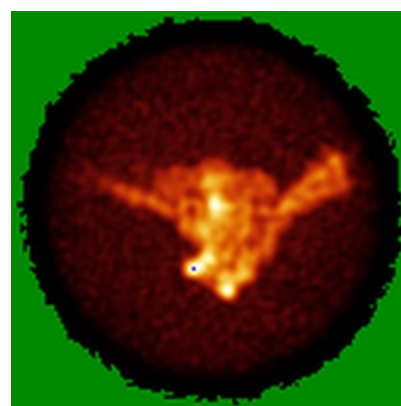
6.4.1 Primary map



X



Y

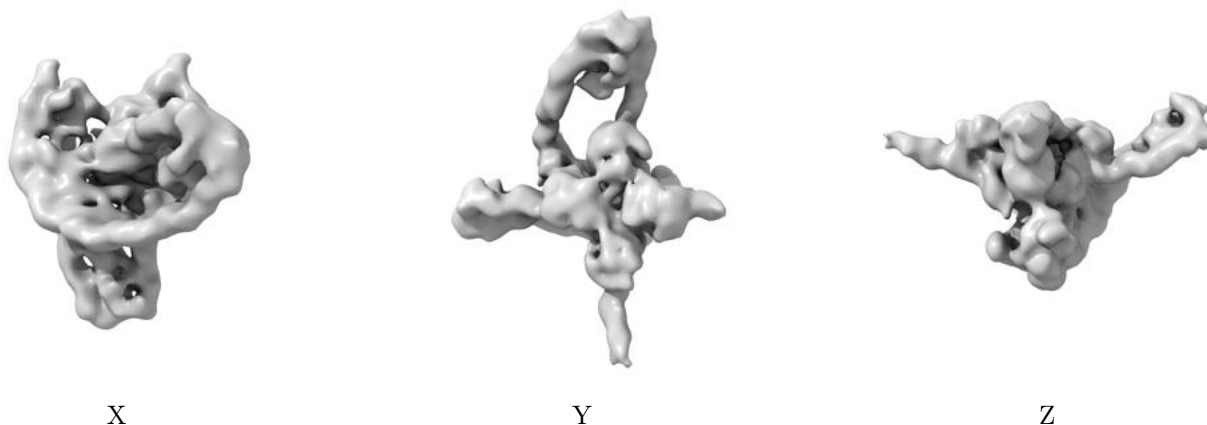


Z

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



The images above show the 3D surface view of the map at the recommended contour level 2.32. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

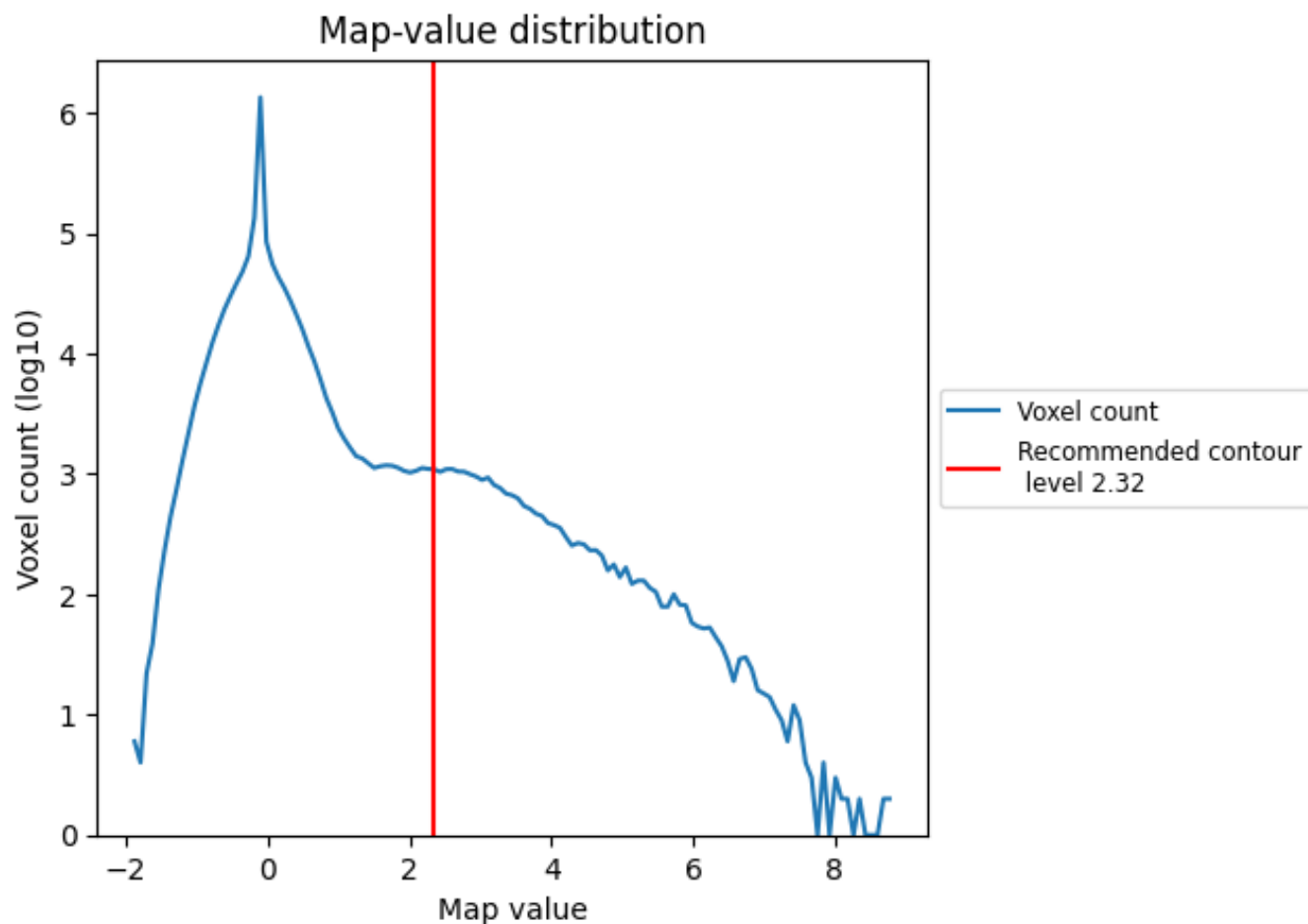
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

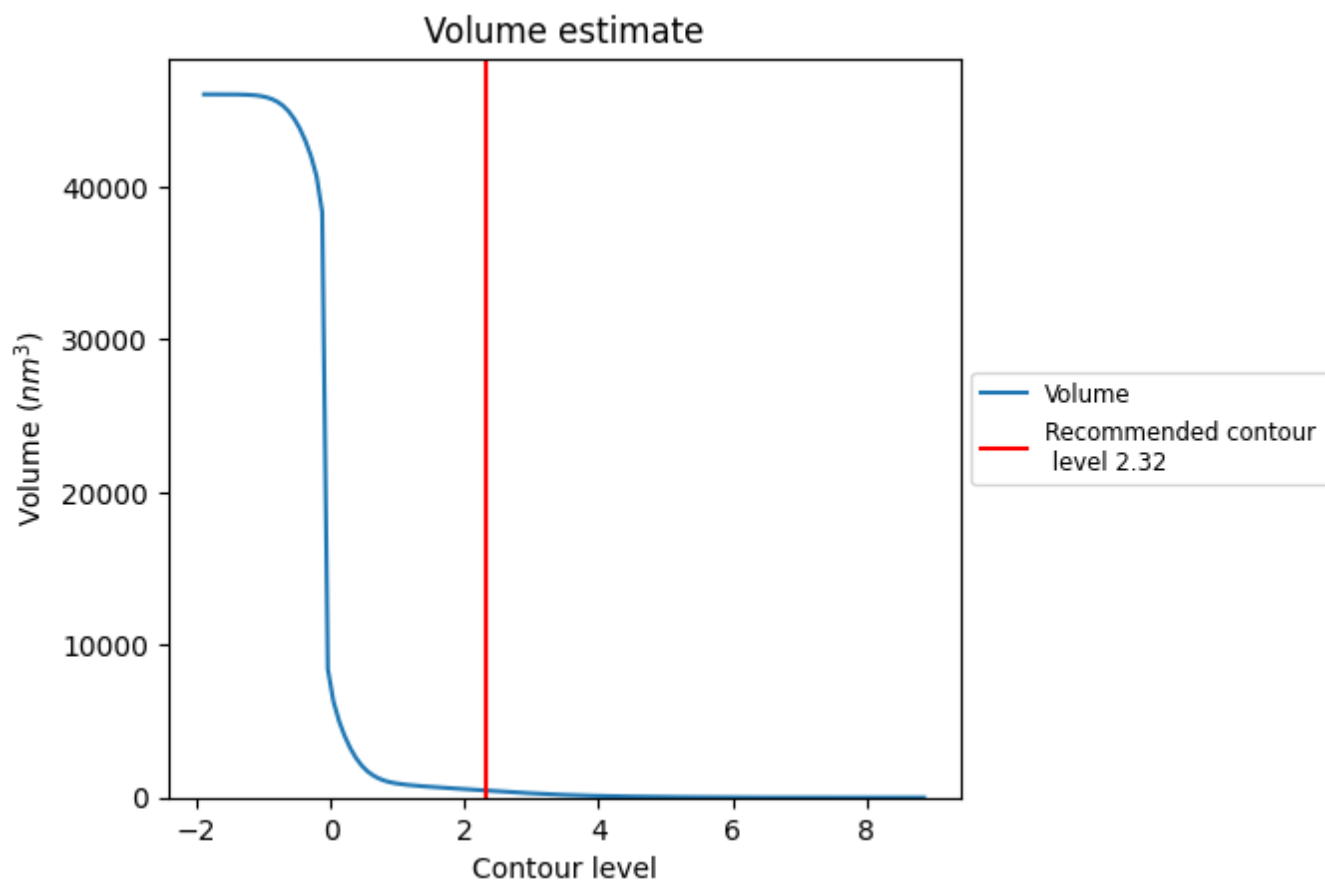
This section contains the results of statistical analysis of the map.

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.

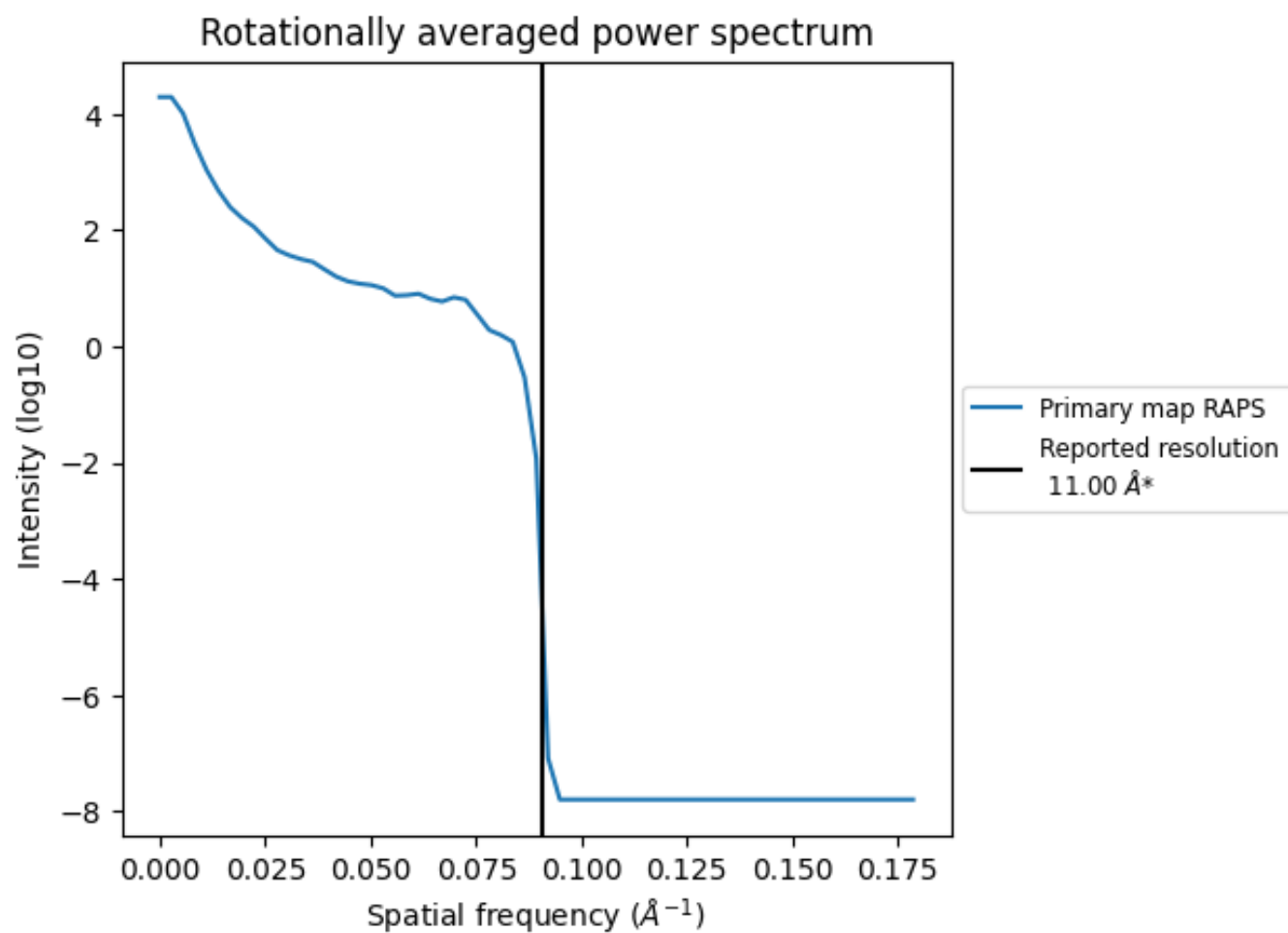
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 464 nm³; this corresponds to an approximate mass of 419 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 0.091 $\text{\AA}^{-1}$

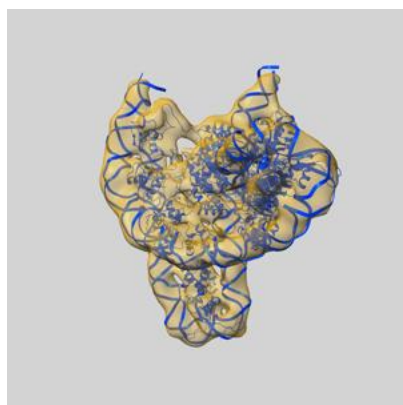
8 Fourier-Shell correlation ⓘ

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

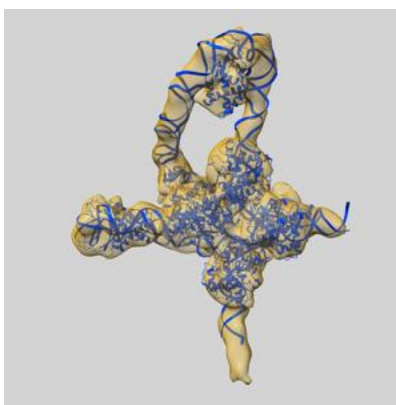
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3400 and PDB model 5J0N. Per-residue inclusion information can be found in section [3](#) on page [6](#).

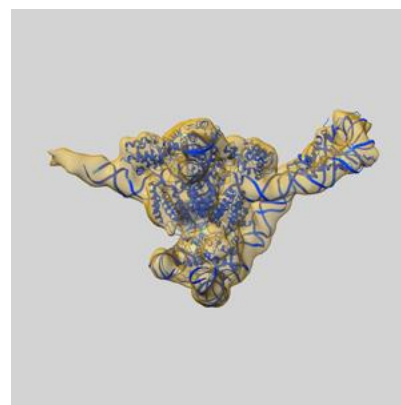
9.1 Map-model overlay [i](#)



X



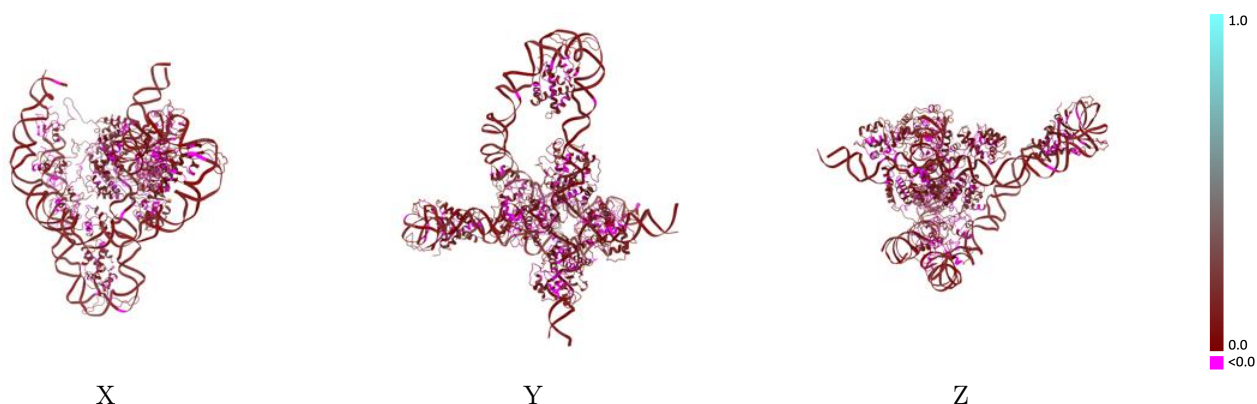
Y



Z

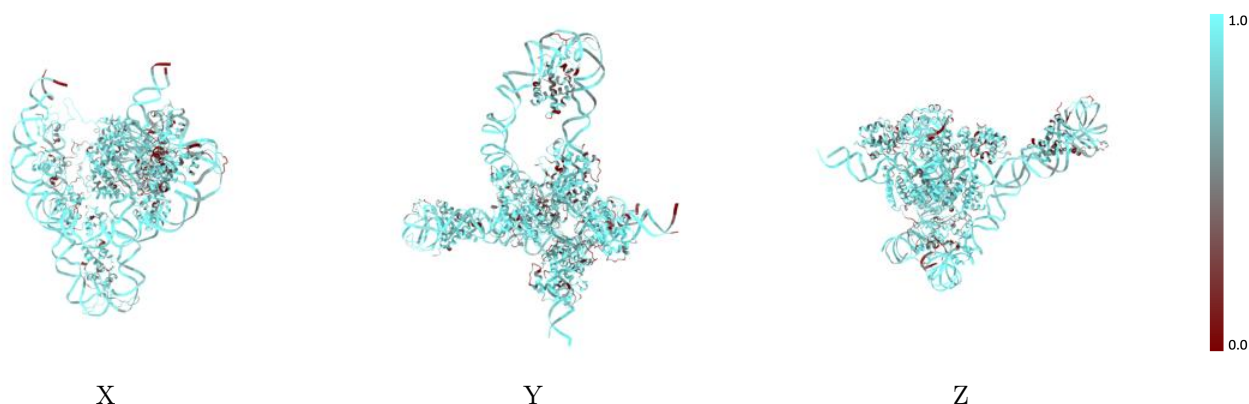
The images above show the 3D surface view of the map at the recommended contour level 2.32 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



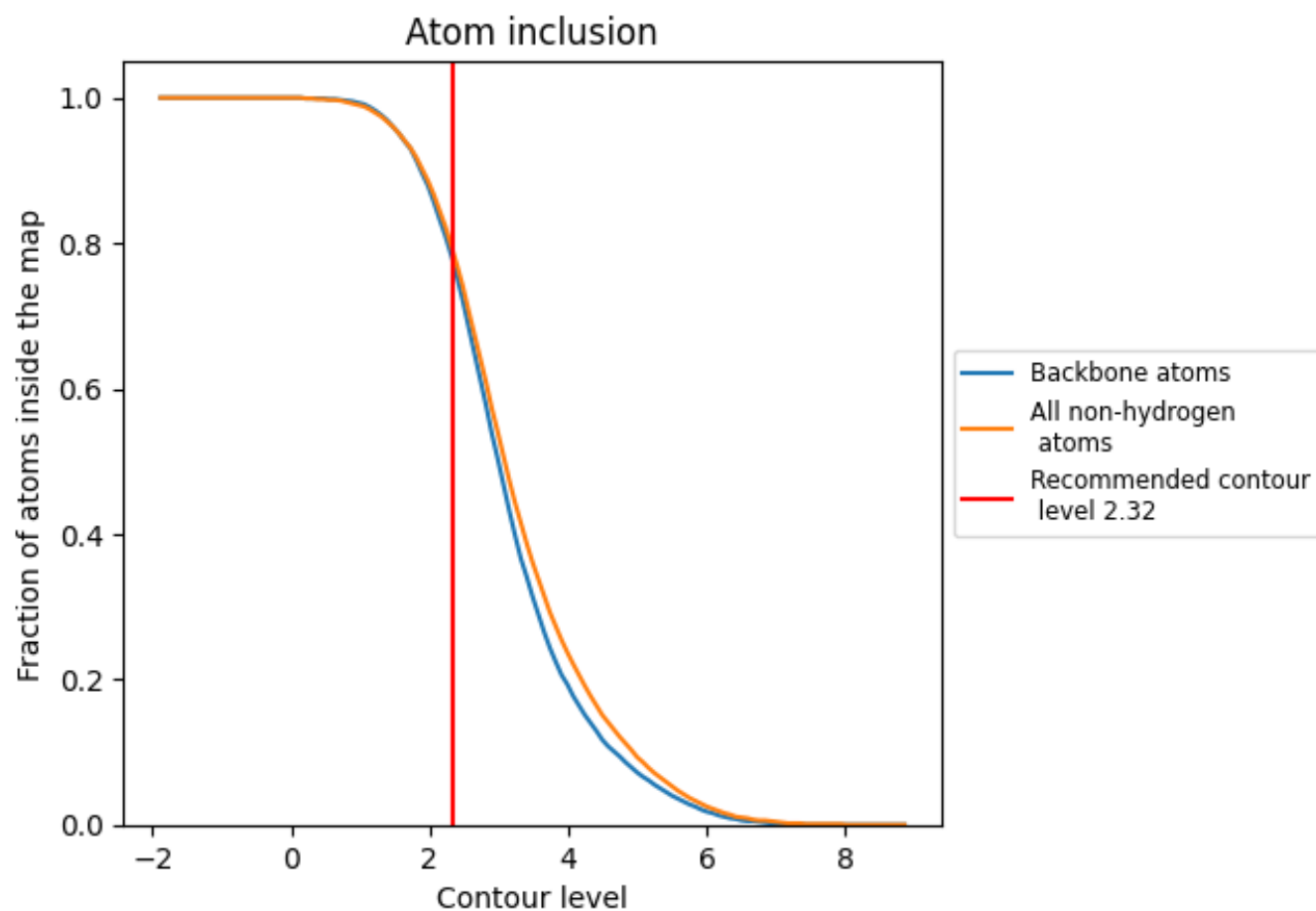
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.32).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 79% 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 (2.32) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7940	0.0880
A	0.8490	0.1010
B	0.8390	0.1230
C	0.8670	0.1090
D	0.8770	0.0970
E	0.7600	0.0830
F	0.7870	0.0690
G	0.7390	0.0760
H	0.7700	0.0790
I	0.8250	0.0750
J	0.8140	0.0930
K	0.6020	0.0740
L	0.6620	0.1000
M	0.7810	0.0640
N	0.7340	0.0260
O	0.8070	0.0810

