



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 02:21 AM UTC

PDB ID : 9UJT / pdb_00009ujt
EMDB ID : EMD-64226
Title : RNA polymerase II elongation complex stalled at SHL(-0.5) of the H3-H4 octasome (tetrasome)
Authors : Ho, C.-H.; Nozawa, K.; Nishimura, M.; Oi, M.; Kujirai, T.; Ogasawara, M.; Ehara, H.; Sekine, S.; Takizawa, Y.; Kurumizaka, H.
Deposited on : 2025-04-17
Resolution : 6.54 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:

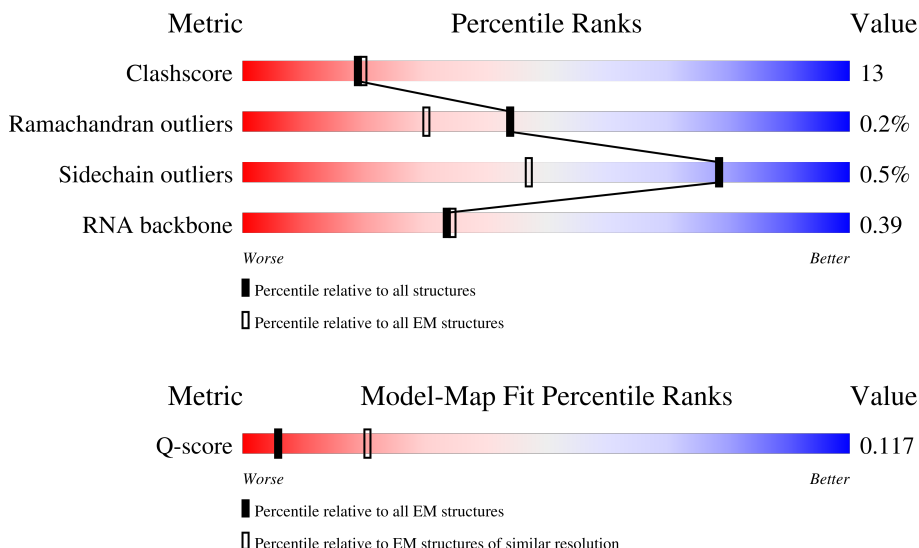
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 6.54 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	501 (6.04 - 7.04)

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

Mol	Chain	Length	Quality of chain
1	N	198	
2	T	198	
3	A	1743	

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Mol	Chain	Length	Quality of chain
4	B	1227	
5	C	304	
6	D	186	
7	E	214	
8	F	155	
9	G	171	
10	H	145	
11	I	115	
12	J	72	
13	K	118	
14	L	72	
15	P	11	
16	e	139	
16	g	139	
17	f	106	
17	h	106	

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 38099 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	100	Total	C	N	O	P	0	0
			2058	973	380	605	100		

- Molecule 2 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	109	Total	C	N	O	P	0	0
			2225	1053	417	646	109		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1404	Total	C	N	O	S	0	0
			11062	6979	1927	2086	70		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	1161	Total	C	N	O	S	0	0
			9261	5835	1636	1732	58		

- Molecule 5 is a protein called RNA polymerase II third largest subunit B44, part of central core.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	263	Total	C	N	O	S	0	0
			2098	1319	354	413	12		

- Molecule 6 is a protein called RNA polymerase II subunit B32.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	156	Total	C	N	O	S	0	0
			1210	753	210	245	2		

- Molecule 7 is a protein called RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	213	Total	C	N	O	S	0	0
			1740	1094	312	324	10		

- Molecule 8 is a protein called RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	84	Total	C	N	O	S	0	0
			677	429	114	131	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	171	Total	C	N	O	S	0	0
			1324	858	214	247	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	133	Total	C	N	O	S	0	0
			1052	671	169	208	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	111	Total	C	N	O	S	0	0
			917	565	161	180	11		

- Molecule 12 is a protein called RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	66	Total	C	N	O	S	0	0
			545	349	95	95	6		

- Molecule 13 is a protein called RNA polymerase II subunit B12.5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	113	Total	C	N	O	S	0	0
			932	599	160	169	4		

- Molecule 14 is a protein called RNA polymerase subunit ABC10-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	45	Total	C	N	O	S	0	0
			359	221	72	61	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	11	Total	C	N	O	P	0	0
			232	103	35	83	11		

- Molecule 16 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	e	76	Total	C	N	O	S	0	0
			619	392	115	108	4		
16	g	77	Total	C	N	O	S	0	0
			625	395	116	110	4		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	-3	GLY	-	expression tag	UNP P68431
e	-2	SER	-	expression tag	UNP P68431
e	-1	HIS	-	expression tag	UNP P68431
g	-3	GLY	-	expression tag	UNP P68431
g	-2	SER	-	expression tag	UNP P68431
g	-1	HIS	-	expression tag	UNP P68431

- Molecule 17 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	f	72	Total	C	N	O	S	0	0
			576	361	114	100	1		
17	h	73	Total	C	N	O	S	0	0
			587	367	118	101	1		

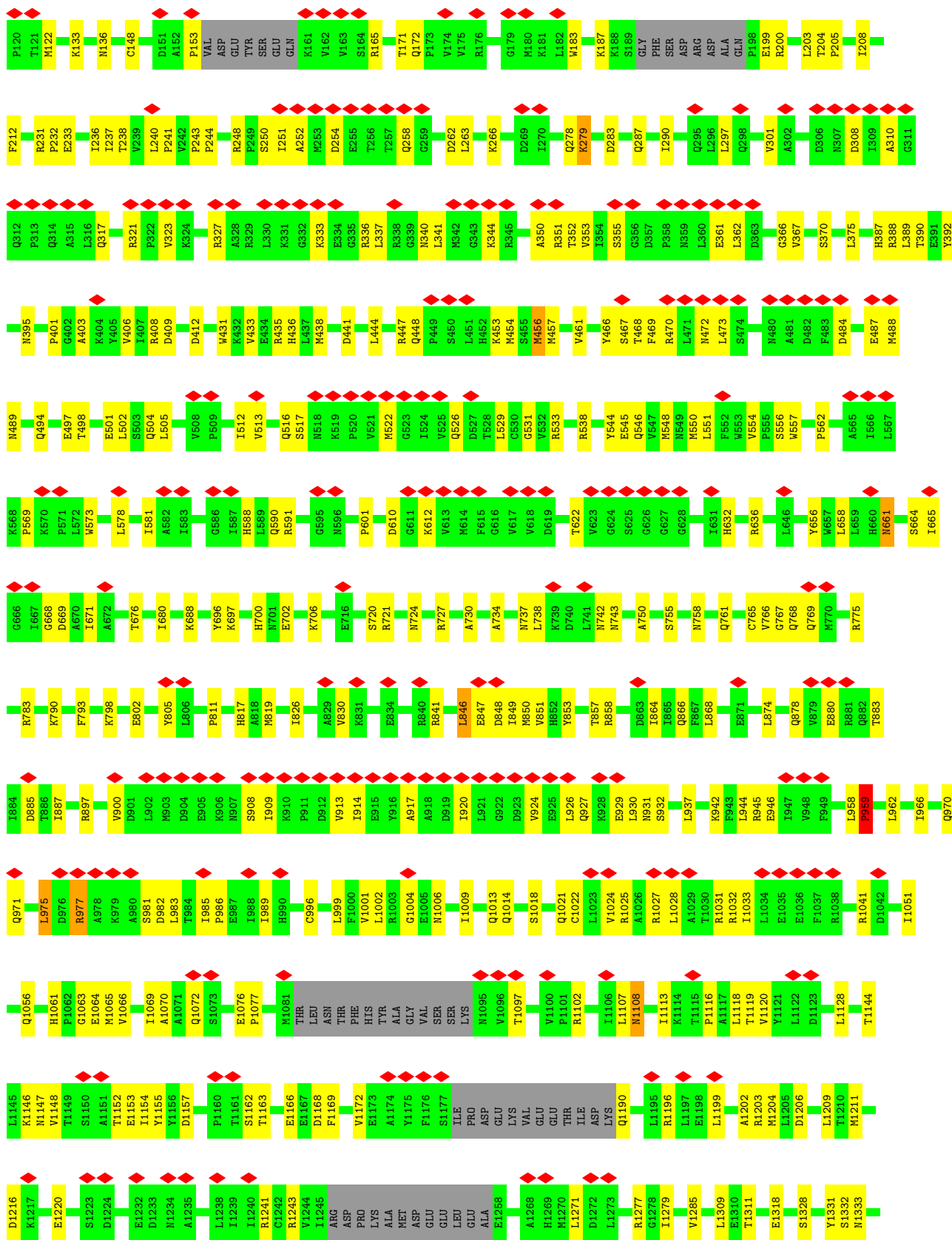
There are 6 discrepancies between the modelled and reference sequences:

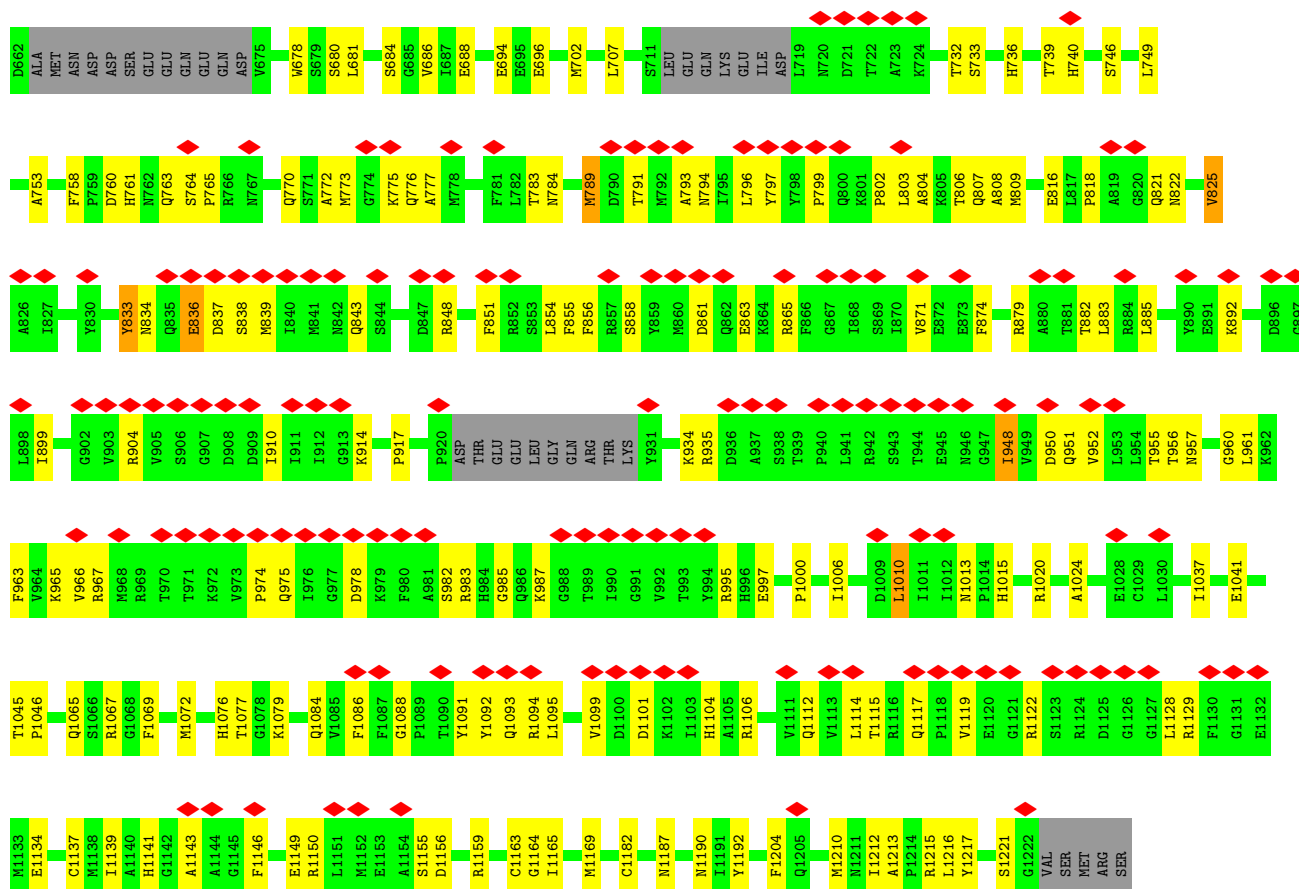
Chain	Residue	Modelled	Actual	Comment	Reference
f	-3	GLY	-	expression tag	UNP P62805
f	-2	SER	-	expression tag	UNP P62805

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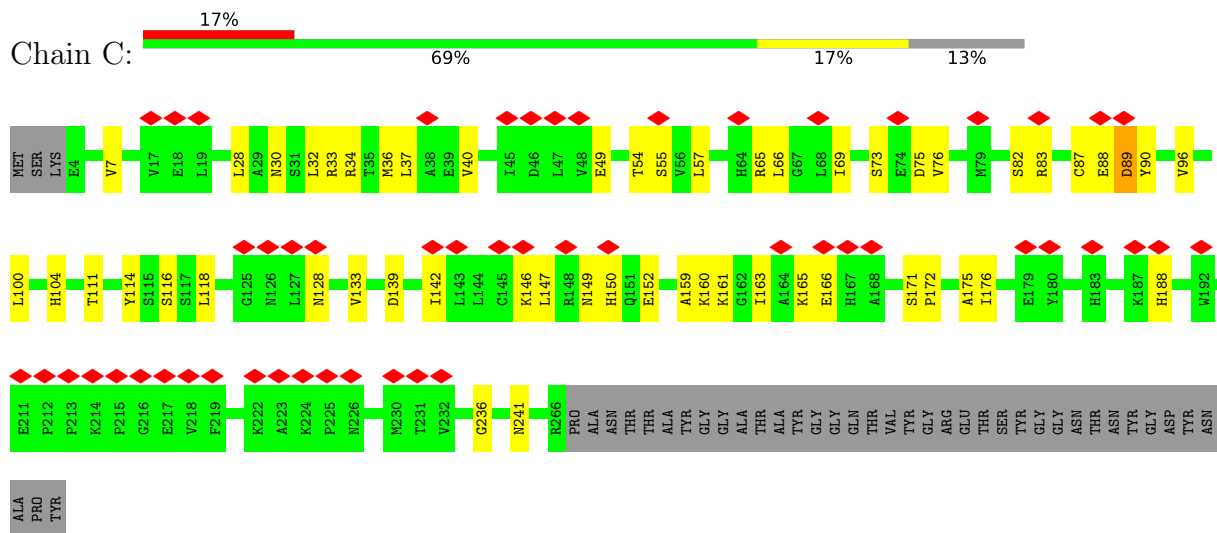
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Chain	Residue	Modelled	Actual	Comment	Reference
f	-1	HIS	-	expression tag	UNP P62805
h	-3	GLY	-	expression tag	UNP P62805
h	-2	SER	-	expression tag	UNP P62805
h	-1	HIS	-	expression tag	UNP P62805

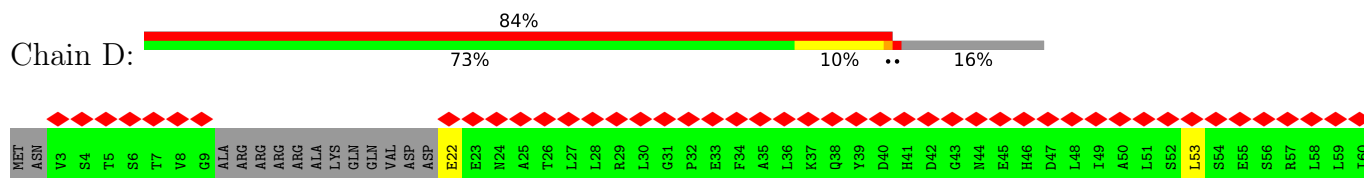




- Molecule 5: RNA polymerase II third largest subunit B44, part of central core

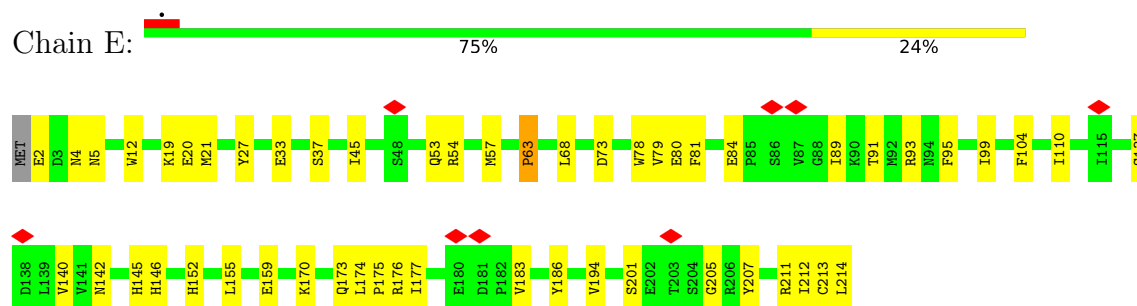


- Molecule 6: RNA polymerase II subunit B32

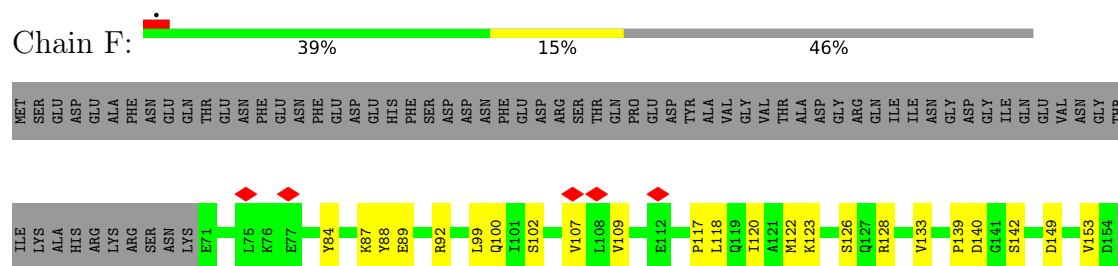




- Molecule 7: RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III



- Molecule 8: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III

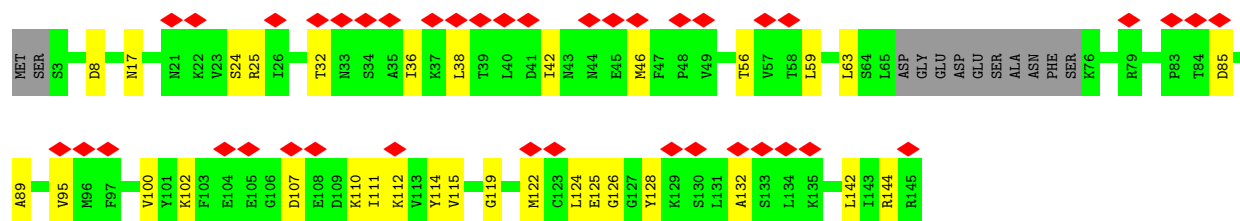


- Molecule 9: RNA polymerase II subunit

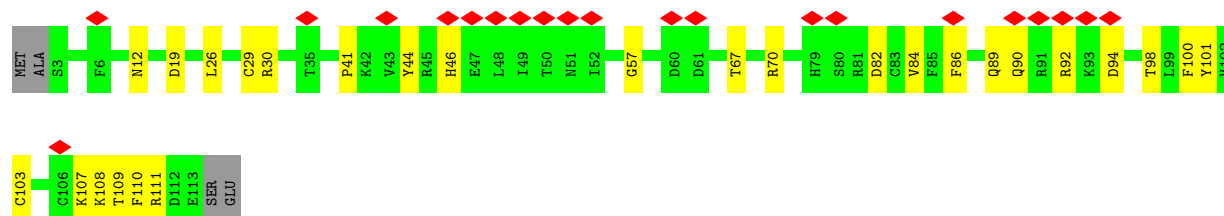


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3





• Molecule 11: DNA-directed RNA polymerase subunit



• Molecule 12: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III



• Molecule 13: RNA polymerase II subunit B12.5



• Molecule 14: RNA polymerase subunit ABC10-alpha



• Molecule 15: RNA (5'-R(P*CP*UP*UP*GP*GP*GP*UP*GP*UP*UP*U)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.017	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	N	0.27	0/2307	0.52	0/3559
2	T	0.29	0/2496	0.55	1/3846 (0.0%)
3	A	0.62	1/11266 (0.0%)	0.85	9/15221 (0.1%)
4	B	0.64	1/9441 (0.0%)	0.90	6/12732 (0.0%)
5	C	0.65	0/2139	0.91	2/2895 (0.1%)
6	D	0.22	0/1221	0.51	0/1648
7	E	0.57	0/1772	0.79	1/2385 (0.0%)
8	F	0.54	0/687	0.75	0/931
9	G	0.25	0/1353	0.61	2/1837 (0.1%)
10	H	0.58	0/1069	0.79	0/1444
11	I	0.40	0/934	0.82	0/1257
12	J	0.75	0/554	0.98	0/742
13	K	0.53	0/953	0.77	0/1291
14	L	0.52	0/365	0.86	0/484
15	P	0.27	0/257	0.61	0/398
16	e	0.10	0/626	0.30	0/839
16	g	0.11	0/632	0.31	0/846
17	f	0.15	0/581	0.38	0/778
17	h	0.10	0/592	0.28	0/792
All	All	0.54	2/39245 (0.0%)	0.78	21/53925 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	8
4	B	0	8
5	C	0	3
7	E	0	2
11	I	0	1
12	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	23

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	789	MET	CA-CB	-8.07	1.41	1.53
3	A	3	GLN	C-N	-5.38	1.26	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	504	GLN	CA-C-N	-6.37	111.95	122.79
3	A	504	GLN	C-N-CA	-6.37	111.95	122.79
2	T	37	DC	O3'-P-O5'	-6.26	94.61	104.00
9	G	133	ASN	CA-C-N	6.06	133.12	121.54
9	G	133	ASN	C-N-CA	6.06	133.12	121.54
3	A	977	ARG	CA-CB-CG	5.85	125.80	114.10
3	A	279	LYS	N-CA-C	5.82	119.48	112.38
4	B	833	TYR	CA-C-N	-5.53	113.89	122.67
4	B	833	TYR	C-N-CA	-5.53	113.89	122.67
3	A	279	LYS	CB-CA-C	5.52	121.97	110.32
4	B	500	LYS	CA-C-N	5.33	128.27	120.71
4	B	500	LYS	C-N-CA	5.33	128.27	120.71
7	E	173	GLN	N-CA-C	5.30	119.38	113.02
5	C	89	ASP	CA-C-N	5.29	131.65	121.54
5	C	89	ASP	C-N-CA	5.29	131.65	121.54
3	A	1004	GLY	N-CA-C	-5.29	105.50	111.85
3	A	513	VAL	CA-C-N	-5.23	114.34	121.61
3	A	513	VAL	C-N-CA	-5.23	114.34	121.61
4	B	256	GLY	CA-C-N	5.07	129.25	121.19
4	B	256	GLY	C-N-CA	5.07	129.25	121.19
3	A	456	MET	N-CA-C	-5.05	100.06	108.34

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	1108	ASN	Peptide
3	A	46	GLN	Peptide
3	A	466	TYR	Peptide
3	A	846	LEU	Peptide

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Mol	Chain	Res	Type	Group
3	A	920	ILE	Peptide
3	A	959	PRO	Peptide
3	A	975	LEU	Peptide
3	A	977	ARG	Peptide
4	B	1086	PHE	Peptide
4	B	175	LEU	Peptide
4	B	393	HIS	Peptide
4	B	458	ASN	Peptide
4	B	508	HIS	Peptide
4	B	64	HIS	Peptide
4	B	836	GLU	Peptide
4	B	910	ILE	Peptide
5	C	87	CYS	Peptide
5	C	88	GLU	Peptide
5	C	89	ASP	Peptide
7	E	170	LYS	Peptide
7	E	63	PRO	Peptide
11	I	94	ASP	Peptide
12	J	63	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	2058	0	1124	94	0
2	T	2225	0	1218	92	0
3	A	11062	0	11108	279	0
4	B	9261	0	9267	272	0
5	C	2098	0	2061	37	0
6	D	1210	0	1205	17	0
7	E	1740	0	1754	48	0
8	F	677	0	693	18	0
9	G	1324	0	1342	27	0
10	H	1052	0	1050	19	0
11	I	917	0	872	17	0
12	J	545	0	564	27	0
13	K	932	0	944	34	0
14	L	359	0	362	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	P	232	0	116	19	0
16	e	619	0	649	23	0
16	g	625	0	654	31	0
17	f	576	0	618	18	0
17	h	587	0	631	29	0
All	All	38099	0	36232	944	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 13.

All (944) 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)
1:N:-13:DA:P	7:E:89:ILE:HG21	1.46	1.55
1:N:-13:DA:OP1	7:E:89:ILE:CG1	1.76	1.30
1:N:-13:DA:OP1	7:E:89:ILE:HG12	1.04	1.19
2:T:30:DA:OP2	3:A:333:LYS:NZ	1.82	1.11
1:N:-13:DA:P	7:E:89:ILE:CG2	2.40	1.09
2:T:33:DC:P	4:B:1122:ARG:HB2	1.96	1.05
3:A:497:GLU:OE1	9:G:64:GLY:HA2	1.57	1.05
3:A:1202:ALA:O	3:A:1206:ASP:HB2	1.60	1.02
4:B:471:GLY:HA3	15:P:7:G:H5'	1.42	0.98
3:A:1448:ILE:HG22	9:G:59:GLY:H	1.24	0.96
2:T:33:DC:OP1	4:B:1122:ARG:HB2	1.65	0.95
1:N:-14:DA:O3'	7:E:89:ILE:HG21	1.66	0.95
2:T:33:DC:OP1	4:B:1122:ARG:CB	2.15	0.94
4:B:549:ASN:O	4:B:553:GLU:HB2	1.67	0.93
3:A:1450:GLU:OE1	9:G:58:LYS:HE2	1.67	0.92
1:N:-19:DG:H22	2:T:19:DC:H1'	1.32	0.92
1:N:-13:DA:OP1	7:E:89:ILE:HG21	1.71	0.89
2:T:33:DC:P	4:B:1122:ARG:CB	2.60	0.88
1:N:-13:DA:OP1	7:E:89:ILE:CG2	2.22	0.87
4:B:471:GLY:HA3	15:P:7:G:C5'	2.05	0.87
4:B:776:GLN:NE2	15:P:9:U:O2'	2.12	0.82
2:T:25:DG:OP1	3:A:310:ALA:HB2	1.78	0.82
1:N:-13:DA:OP1	7:E:89:ILE:CB	2.27	0.81
2:T:33:DC:H2'	2:T:34:DA:H8	1.47	0.79
2:T:-53:DG:OP2	4:B:335:GLY:HA2	1.84	0.78
3:A:1448:ILE:HG22	9:G:59:GLY:N	2.01	0.75
4:B:83:TYR:HB2	4:B:116:TYR:HB2	1.65	0.75
4:B:471:GLY:CA	15:P:7:G:H5'	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:-19:DG:N1	2:T:19:DC:O2	2.18	0.75
8:F:128:ARG:HH21	8:F:153:VAL:H	1.35	0.74
16:e:109:LEU:HD21	16:g:129:ARG:HE	1.52	0.74
9:G:106:LEU:HG	9:G:157:ILE:HD11	1.70	0.74
4:B:1187:ASN:HD21	4:B:1190:ASN:HB3	1.52	0.74
1:N:-6:DG:H2'	1:N:-5:DG:C8	2.23	0.73
1:N:-13:DA:OP2	7:E:89:ILE:HG21	1.89	0.72
2:T:33:DC:OP2	4:B:1122:ARG:HB2	1.88	0.72
3:A:819:MET:SD	4:B:509:ASN:ND2	2.61	0.71
12:J:10:CYS:SG	12:J:11:GLY:N	2.64	0.71
4:B:205:ALA:HB3	4:B:491:THR:HG22	1.72	0.70
10:H:56:THR:HB	10:H:144:ARG:HB3	1.74	0.70
17:f:64:ASN:OD1	17:f:67:ARG:NH1	2.24	0.70
16:e:75:ALA:HB1	16:e:82:LEU:HD11	1.74	0.70
14:L:49:ARG:HA	14:L:56:ARG:HA	1.73	0.70
3:A:89:PRO:HB3	3:A:238:THR:HG22	1.75	0.69
4:B:74:ARG:HB2	4:B:124:PHE:HB2	1.73	0.69
1:N:-14:DA:C3'	7:E:89:ILE:CG2	2.71	0.69
4:B:770:GLN:HE22	4:B:1093:GLN:HE22	1.41	0.69
5:C:49:GLU:HG2	14:L:68:GLN:HG2	1.74	0.69
1:N:-14:DA:C3'	7:E:89:ILE:HG21	2.22	0.68
9:G:132:SER:HB2	9:G:135:GLU:HB2	1.74	0.68
11:I:70:ARG:HA	11:I:84:VAL:HA	1.75	0.68
3:A:1006:ASN:H	3:A:1009:ILE:HD12	1.58	0.68
4:B:66:ASN:HB3	4:B:69:ASP:H	1.59	0.68
4:B:789:MET:HE3	4:B:967:ARG:HB2	1.75	0.68
1:N:-47:DC:N4	2:T:46:DA:N1	2.42	0.68
3:A:588:HIS:HB3	3:A:590:GLN:HE22	1.59	0.67
2:T:-22:DA:H2''	2:T:-21:DC:C6	2.29	0.67
3:A:351:ARG:NH2	3:A:487:GLU:OE1	2.27	0.67
5:C:28:LEU:HD21	13:K:98:LEU:HD21	1.77	0.67
11:I:29:CYS:SG	11:I:30:ARG:N	2.68	0.67
2:T:30:DA:H2'	2:T:31:DA:H8	1.59	0.67
4:B:1163:CYS:SG	4:B:1187:ASN:ND2	2.67	0.67
2:T:16:DA:H2'	2:T:17:DA:C8	2.30	0.67
15:P:2:U:H2'	15:P:3:G:C8	2.28	0.67
3:A:352:THR:OG1	3:A:353:VAL:N	2.24	0.67
3:A:841:ARG:HH22	3:A:1108:ASN:HD21	1.43	0.67
6:D:169:VAL:C	6:D:171:LEU:H	2.01	0.66
12:J:1:MET:N	12:J:53:VAL:O	2.28	0.66
3:A:588:HIS:NE2	3:A:971:GLN:OE1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1448:ILE:CG2	9:G:59:GLY:H	2.04	0.66
6:D:169:VAL:HG12	6:D:170:ASN:N	2.11	0.66
3:A:883:THR:O	3:A:1027:ARG:NH2	2.28	0.65
3:A:1436:LEU:HD22	9:G:63:PRO:HG2	1.79	0.65
1:N:-14:DA:H2''	1:N:-13:DA:H5'	1.78	0.65
2:T:7:DC:H2''	2:T:8:DC:C5	2.31	0.65
2:T:33:DC:OP1	4:B:1122:ARG:CG	2.43	0.65
1:N:-48:DC:H2''	1:N:-47:DC:C5	2.31	0.65
16:e:113:HIS:NE2	16:g:123:ASP:OD1	2.30	0.65
3:A:562:PRO:HG2	3:A:573:TRP:HE1	1.61	0.65
1:N:-14:DA:O3'	7:E:89:ILE:CG2	2.43	0.65
11:I:70:ARG:HG2	11:I:84:VAL:HG12	1.79	0.65
3:A:883:THR:OG1	3:A:1027:ARG:NH2	2.30	0.65
1:N:-41:DT:H2''	1:N:-40:DC:C5	2.32	0.64
3:A:113:LEU:O	3:A:165:ARG:NH2	2.30	0.64
4:B:995:ARG:NH2	13:K:39:ASP:OD2	2.31	0.64
9:G:89:ALA:HB2	9:G:103:VAL:HG22	1.79	0.64
1:N:-37:DG:H1'	4:B:419:ARG:NH1	2.13	0.64
2:T:-50:DC:OP1	16:e:72:ARG:NH1	2.22	0.64
2:T:33:DC:OP1	4:B:1122:ARG:HG3	1.98	0.64
3:A:1413:PHE:O	3:A:1417:ALA:HB2	1.97	0.64
4:B:105:ARG:O	4:B:965:LYS:NZ	2.31	0.64
3:A:848:ASP:OD1	3:A:848:ASP:N	2.30	0.64
16:g:76:GLN:HA	16:g:80:THR:HA	1.80	0.64
3:A:996:CYS:SG	3:A:1025:ARG:NH1	2.71	0.63
4:B:1112:GLN:NE2	15:P:3:G:OP1	2.32	0.63
3:A:203:LEU:HB3	3:A:208:ILE:HD11	1.79	0.63
2:T:24:DA:H2'	2:T:25:DG:C8	2.33	0.63
3:A:1119:THR:HB	3:A:1331:TYR:HB3	1.81	0.63
1:N:45:DT:H1'	1:N:46:DG:C8	2.34	0.63
4:B:193:TYR:OH	4:B:478:ARG:NH2	2.32	0.63
1:N:21:DG:H2''	1:N:22:DT:H73	1.80	0.63
3:A:1457:PRO:O	9:G:20:PRO:HB3	1.99	0.63
4:B:190:MET:SD	4:B:190:MET:N	2.71	0.63
4:B:688:GLU:OE2	4:B:740:HIS:NE2	2.32	0.63
16:g:86:SER:HA	16:g:89:VAL:HB	1.80	0.63
2:T:23:DA:H2'	2:T:24:DA:C8	2.33	0.63
17:h:33:ALA:HA	17:h:36:ARG:HE	1.63	0.62
3:A:1448:ILE:N	9:G:59:GLY:O	2.32	0.62
2:T:-25:DA:H2''	2:T:-24:DG:C8	2.35	0.62
11:I:98:THR:OG1	11:I:111:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:33:DC:OP2	4:B:1122:ARG:CB	2.48	0.62
4:B:574:PHE:HB2	4:B:618:LYS:HG2	1.80	0.62
16:g:100:LEU:HD21	17:h:37:LEU:HD13	1.80	0.62
3:A:327:ARG:HG3	3:A:1409:VAL:HG21	1.82	0.62
1:N:34:DC:H2''	1:N:35:DT:H71	1.80	0.62
1:N:-7:DG:C8	1:N:-7:DG:H5'	2.35	0.61
16:g:116:ARG:NH2	16:g:123:ASP:OD2	2.33	0.61
4:B:586:PRO:HG2	4:B:610:ARG:HH21	1.65	0.61
1:N:21:DG:H2''	1:N:22:DT:C7	2.30	0.61
3:A:874:LEU:HD13	3:A:959:PRO:HG3	1.81	0.61
4:B:791:THR:HA	4:B:858:SER:H	1.65	0.61
4:B:1065:GLN:OE1	4:B:1069:PHE:N	2.32	0.61
5:C:175:ALA:HB2	12:J:10:CYS:HB2	1.82	0.61
16:g:132:GLY:O	16:g:134:ARG:NH2	2.33	0.61
2:T:34:DA:H2'	2:T:35:DC:C6	2.35	0.61
4:B:635:ASP:N	4:B:635:ASP:OD1	2.31	0.61
13:K:20:LYS:HB3	13:K:34:LYS:HB3	1.83	0.61
3:A:366:GLY:HA3	3:A:470:ARG:HB2	1.82	0.61
3:A:944:LEU:HD11	3:A:1022:CYS:HB3	1.82	0.61
1:N:-14:DA:H3'	7:E:89:ILE:CG2	2.31	0.61
4:B:761:HIS:HB2	4:B:1024:ALA:HB2	1.83	0.61
2:T:16:DA:H2'	2:T:17:DA:H8	1.65	0.61
5:C:76:VAL:O	5:C:161:LYS:NZ	2.33	0.61
2:T:18:DC:H2'	2:T:19:DC:C2	2.36	0.60
3:A:966:ILE:HD11	3:A:1028:LEU:HD21	1.83	0.60
4:B:579:TRP:NE1	4:B:581:GLY:O	2.32	0.60
4:B:833:TYR:O	4:B:838:SER:OG	2.18	0.60
4:B:590:VAL:HG21	4:B:610:ARG:HD2	1.82	0.60
4:B:807:GLN:H	4:B:1045:THR:HG1	1.47	0.60
5:C:65:ARG:NH2	12:J:3:ILE:O	2.33	0.60
2:T:33:DC:P	4:B:1122:ARG:HB3	2.40	0.60
3:A:999:LEU:O	3:A:1013:GLN:NE2	2.35	0.60
2:T:45:DC:H2''	2:T:46:DA:C5	2.37	0.60
3:A:664:SER:OG	3:A:665:ILE:N	2.30	0.60
3:A:279:LYS:O	3:A:283:ASP:OD1	2.19	0.60
1:N:7:DC:H2''	1:N:8:DG:H5'	1.84	0.60
3:A:453:LYS:O	4:B:1141:HIS:NE2	2.35	0.60
3:A:308:ASP:OD2	3:A:327:ARG:NH1	2.35	0.59
4:B:109:LEU:O	4:B:198:GLY:N	2.34	0.59
4:B:807:GLN:N	4:B:1045:THR:OG1	2.28	0.59
3:A:435:ARG:NH1	3:A:436:HIS:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1166:GLU:HA	3:A:1169:PHE:HB2	1.84	0.59
3:A:336:ARG:O	3:A:340:ASN:HB2	2.01	0.59
12:J:44:CYS:SG	12:J:45:CYS:N	2.75	0.59
16:e:61:LEU:HD23	17:f:36:ARG:HB3	1.83	0.59
3:A:340:ASN:O	4:B:1117:GLN:NE2	2.34	0.59
4:B:794:ASN:HD21	4:B:855:PHE:HD1	1.51	0.59
13:K:57:THR:H	13:K:77:THR:HA	1.67	0.59
17:f:67:ARG:O	17:f:71:THR:N	2.32	0.59
3:A:1157:ASP:OD2	3:A:1241:ARG:NH2	2.35	0.59
11:I:70:ARG:NH2	11:I:82:ASP:OD1	2.35	0.59
5:C:146:LYS:NZ	12:J:57:GLU:OE2	2.35	0.59
1:N:14:DT:OP2	17:h:32:PRO:HB2	2.02	0.59
4:B:821:GLN:HE22	4:B:851:PHE:H	1.50	0.59
5:C:114:TYR:OH	12:J:19:ASP:OD2	2.20	0.59
3:A:18:GLN:HB3	4:B:1215:ARG:HB2	1.85	0.59
3:A:231:ARG:HD2	3:A:232:PRO:HD2	1.85	0.58
3:A:351:ARG:NH1	3:A:489:ASN:OD1	2.35	0.58
8:F:118:LEU:HG	8:F:122:MET:HE2	1.84	0.58
4:B:680:SER:O	4:B:684:SER:HB3	2.03	0.58
5:C:33:ARG:HG3	5:C:176:ILE:HG21	1.85	0.58
4:B:153:GLY:N	4:B:436:ASN:O	2.37	0.58
4:B:822:ASN:O	12:J:47:ARG:NH1	2.36	0.58
4:B:837:ASP:OD2	4:B:1020:ARG:NH2	2.36	0.58
2:T:33:DC:H2'	2:T:34:DA:C8	2.33	0.58
3:A:1120:VAL:HB	3:A:1309:LEU:HB2	1.86	0.58
16:g:128:ARG:HH22	17:h:60:VAL:HG11	1.67	0.58
4:B:635:ASP:HB3	4:B:739:THR:HA	1.84	0.58
4:B:843:GLN:HG2	13:K:6:ARG:HH22	1.68	0.58
6:D:84:ILE:HG23	6:D:85:ASP:H	1.68	0.58
13:K:50:LEU:HD11	13:K:87:LEU:HD13	1.84	0.58
3:A:467:SER:OG	13:K:2:ASN:ND2	2.37	0.58
3:A:847:GLU:OE2	3:A:1428:SER:OG	2.22	0.58
3:A:92:HIS:NE2	4:B:1210:MET:O	2.29	0.57
3:A:962:LEU:HD22	3:A:1051:ILE:HG12	1.85	0.57
16:e:124:ILE:HG13	16:e:128:ARG:HE	1.67	0.57
7:E:19:LYS:NZ	7:E:33:GLU:O	2.37	0.57
4:B:1101:ASP:O	4:B:1122:ARG:NH1	2.37	0.57
2:T:21:DC:H4'	2:T:22:DC:OP1	2.03	0.57
3:A:468:THR:OG1	3:A:470:ARG:NH1	2.38	0.57
4:B:279:ARG:HG2	4:B:284:VAL:HA	1.85	0.57
1:N:13:DT:H4'	1:N:14:DT:OP1	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:279:ARG:NH2	4:B:286:ASP:OD1	2.38	0.57
4:B:303:LEU:HA	4:B:306:LEU:HD12	1.87	0.57
1:N:7:DC:N4	1:N:8:DG:O6	2.38	0.57
4:B:167:SER:OG	4:B:170:CYS:N	2.38	0.57
13:K:5:ASP:HB2	13:K:8:GLU:HG2	1.87	0.57
3:A:996:CYS:O	3:A:1021:GLN:NE2	2.38	0.57
5:C:166:GLU:OE2	14:L:72:ARG:NH2	2.37	0.57
3:A:153:PRO:HD3	3:A:165:ARG:HD2	1.87	0.57
4:B:793:ALA:HB3	4:B:856:PHE:HB2	1.86	0.57
1:N:42:DA:H2''	1:N:43:DA:C8	2.39	0.57
4:B:243:SER:HB2	4:B:266:PRO:HG3	1.87	0.57
2:T:42:DC:H2''	2:T:43:DA:C8	2.40	0.57
3:A:351:ARG:HB2	4:B:1128:LEU:HD11	1.86	0.57
4:B:489:ARG:NH2	4:B:533:SER:O	2.38	0.57
4:B:505:ARG:NH1	4:B:526:CYS:O	2.37	0.57
3:A:546:GLN:OE1	4:B:1079:LYS:NZ	2.38	0.56
6:D:169:VAL:HG13	6:D:171:LEU:CB	2.34	0.56
7:E:174:LEU:HD12	7:E:212:ILE:HD12	1.86	0.56
3:A:1144:THR:OG1	3:A:1147:ASN:N	2.37	0.56
4:B:225:ILE:O	4:B:252:ARG:NH2	2.37	0.56
4:B:955:THR:OG1	4:B:956:THR:N	2.38	0.56
1:N:-46:DT:H2''	1:N:-45:DG:C8	2.40	0.56
2:T:11:DG:C8	2:T:11:DG:H5'	2.40	0.56
2:T:43:DA:H2''	2:T:44:DC:C5	2.40	0.56
6:D:61:ARG:NH1	6:D:86:ASP:OD1	2.39	0.56
16:g:128:ARG:HH11	17:h:57:VAL:HG13	1.70	0.56
3:A:87:ALA:HB2	3:A:278:GLN:HE21	1.70	0.56
4:B:13:THR:N	4:B:16:ASP:OD2	2.35	0.56
7:E:27:TYR:HA	7:E:63:PRO:HA	1.87	0.56
16:e:131:ARG:NH1	16:g:131:ARG:O	2.33	0.56
2:T:-15:DA:H2''	2:T:-14:DA:N7	2.20	0.56
4:B:300:TRP:HA	4:B:303:LEU:HB2	1.86	0.56
5:C:75:ASP:OD2	5:C:128:ASN:N	2.38	0.56
15:P:9:U:H2'	15:P:10:U:C6	2.39	0.56
3:A:86:LEU:HD22	3:A:297:LEU:HD21	1.88	0.56
4:B:110:THR:HG22	4:B:112:SER:HB3	1.88	0.56
9:G:121:TYR:CE2	9:G:123:PRO:HG3	2.41	0.56
3:A:31:SER:OG	3:A:32:VAL:N	2.39	0.56
17:h:44:LYS:HE3	17:h:45:ARG:HG3	1.87	0.56
1:N:-1:DA:H2''	1:N:0:DG:C8	2.41	0.56
3:A:406:VAL:HG22	3:A:433:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1154:ILE:HD12	11:I:44:TYR:HB3	1.88	0.56
12:J:7:CYS:SG	12:J:8:PHE:N	2.78	0.56
1:N:19:DC:H1'	1:N:20:DG:H5'	1.87	0.56
5:C:163:ILE:HG13	5:C:165:LYS:H	1.71	0.56
3:A:738:LEU:HB3	3:A:742:ASN:HD22	1.70	0.55
3:A:761:GLN:HG2	3:A:766:VAL:HA	1.87	0.55
4:B:300:TRP:O	4:B:304:GLU:HB2	2.05	0.55
3:A:601:PRO:HA	10:H:25:ARG:HH22	1.71	0.55
1:N:-43:DT:H2''	1:N:-42:DG:C8	2.41	0.55
3:A:636:ARG:NH1	3:A:878:GLN:OE1	2.40	0.55
10:H:38:LEU:HD13	10:H:124:LEU:HD13	1.89	0.55
2:T:23:DA:H2'	2:T:24:DA:H8	1.72	0.55
3:A:696:TYR:O	3:A:700:HIS:HB2	2.06	0.55
3:A:775:ARG:HH22	3:A:793:PHE:HB3	1.72	0.55
3:A:1097:THR:HG22	3:A:1102:ARG:HB2	1.89	0.55
4:B:480:THR:OG1	4:B:481:TYR:N	2.38	0.55
13:K:29:ASN:ND2	13:K:78:GLU:O	2.40	0.55
16:g:107:THR:HG23	16:g:119:ILE:HD13	1.88	0.55
3:A:243:PRO:O	3:A:248:ARG:NH1	2.37	0.55
3:A:262:ASP:OD2	3:A:321:ARG:NH2	2.40	0.55
3:A:370:SER:H	13:K:2:ASN:HD21	1.54	0.55
4:B:279:ARG:NH1	4:B:316:ILE:O	2.38	0.55
10:H:8:ASP:OD1	10:H:32:THR:OG1	2.25	0.55
14:L:50:CYS:N	14:L:55:HIS:O	2.40	0.55
1:N:-14:DA:C3'	7:E:89:ILE:HG22	2.36	0.55
13:K:55:ASP:OD1	13:K:55:ASP:N	2.40	0.55
3:A:982:ASP:O	3:A:1041:ARG:NH2	2.40	0.55
4:B:807:GLN:N	4:B:1045:THR:HG1	2.04	0.55
7:E:21:MET:HE2	7:E:186:TYR:HA	1.89	0.55
3:A:557:TRP:O	13:K:26:ARG:NH1	2.39	0.55
4:B:833:TYR:HH	13:K:65:HIS:HE2	1.53	0.55
10:H:59:LEU:HD21	10:H:122:MET:HE1	1.88	0.55
3:A:908:SER:OG	3:A:909:ILE:N	2.40	0.55
4:B:570:SER:HB3	4:B:582:ILE:HB	1.89	0.55
4:B:186:CYS:SG	4:B:783:THR:OG1	2.60	0.54
4:B:220:ALA:O	4:B:252:ARG:NH2	2.40	0.54
2:T:-45:DA:H2''	2:T:-44:DA:C8	2.42	0.54
3:A:554:VAL:HG12	3:A:556:SER:H	1.71	0.54
16:g:61:LEU:O	16:g:63:ARG:NH2	2.40	0.54
4:B:58:LEU:HB2	4:B:75:TYR:HB2	1.88	0.54
4:B:825:VAL:N	4:B:1088:GLY:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:h:90:LEU:HB3	17:h:95:ARG:HD2	1.88	0.54
4:B:369:PHE:HB3	4:B:579:TRP:HZ3	1.72	0.54
1:N:24:DC:H1'	1:N:25:DT:O4'	2.07	0.54
3:A:1021:GLN:HB3	3:A:1025:ARG:HH12	1.71	0.54
3:A:1367:ASN:HD21	3:A:1369:ARG:HE	1.52	0.54
4:B:904:ARG:HA	4:B:948:ILE:HG13	1.88	0.54
3:A:755:SER:N	3:A:758:ASN:OD1	2.39	0.54
4:B:71:ILE:HG13	4:B:127:ILE:HG22	1.90	0.54
4:B:72:ASN:ND2	4:B:128:ASP:OD1	2.40	0.54
7:E:54:ARG:HB3	7:E:81:PHE:HB2	1.89	0.54
9:G:1:MET:HG3	9:G:3:PHE:CE2	2.43	0.54
2:T:-8:DC:H2''	2:T:-7:DG:H8	1.72	0.54
3:A:16:GLU:OE2	4:B:1221:SER:N	2.35	0.54
3:A:1072:GLN:NE2	4:B:1137:CYS:SG	2.75	0.54
3:A:1413:PHE:O	3:A:1417:ALA:CB	2.55	0.54
4:B:249:LEU:HA	4:B:261:ILE:HG12	1.89	0.54
4:B:1076:HIS:O	13:K:44:ASN:ND2	2.41	0.54
7:E:12:TRP:NE1	7:E:37:SER:O	2.41	0.54
3:A:706:LYS:HE3	3:A:721:ARG:HH12	1.73	0.54
4:B:794:ASN:HD22	4:B:855:PHE:HA	1.73	0.54
3:A:362:LEU:HA	3:A:472:ASN:HD22	1.72	0.54
3:A:448:GLN:NE2	4:B:1134:GLU:OE2	2.41	0.54
3:A:811:PRO:HG2	4:B:702:MET:HG2	1.89	0.54
5:C:82:SER:HB2	5:C:160:LYS:HB3	1.90	0.54
1:N:5:DT:H2''	1:N:6:DA:O4'	2.07	0.53
4:B:763:GLN:HG2	4:B:765:PRO:HD2	1.90	0.53
3:A:768:GLN:NE2	3:A:769:GLN:O	2.36	0.53
4:B:444:THR:O	4:B:448:SER:CB	2.56	0.53
6:D:141:GLU:OE1	6:D:166:LYS:NZ	2.41	0.53
13:K:40:HIS:O	13:K:43:ALA:N	2.42	0.53
3:A:858:ARG:HG2	3:A:864:ILE:HG12	1.90	0.53
3:A:1199:LEU:HD12	3:A:1211:MET:HE1	1.90	0.53
7:E:177:ILE:N	7:E:212:ILE:O	2.40	0.53
17:h:48:GLY:HA2	17:h:51:TYR:CE2	2.43	0.53
4:B:806:THR:HG1	4:B:809:MET:H	1.55	0.53
16:e:65:LEU:HG	16:e:69:ARG:HH21	1.73	0.53
4:B:354:LEU:HB3	4:B:357:ILE:HD12	1.91	0.53
15:P:3:G:H2'	15:P:4:G:C8	2.43	0.53
17:h:35:ARG:O	17:h:39:ARG:HG2	2.09	0.53
4:B:1155:SER:OG	4:B:1156:ASP:OD1	2.27	0.53
5:C:55:SER:OG	5:C:57:LEU:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:116:PRO:HG2	9:G:119:LEU:HD12	1.90	0.53
1:N:23:DG:H2''	1:N:24:DC:C5	2.43	0.53
3:A:924:VAL:HA	3:A:927:GLN:HB3	1.91	0.53
2:T:30:DA:H2'	2:T:31:DA:C8	2.43	0.53
4:B:1156:ASP:OD1	4:B:1156:ASP:N	2.41	0.53
6:D:93:THR:HG21	6:D:102:VAL:HG21	1.91	0.53
7:E:2:GLU:OE1	7:E:5:ASN:ND2	2.42	0.53
9:G:165:GLU:HB2	9:G:168:LEU:HD12	1.91	0.53
3:A:435:ARG:HH12	3:A:438:MET:H	1.56	0.53
4:B:957:ASN:HD21	4:B:961:LEU:HB2	1.73	0.53
3:A:1153:GLU:OE1	3:A:1196:ARG:NH1	2.37	0.52
8:F:107:VAL:HG12	8:F:109:VAL:H	1.73	0.52
4:B:1165:ILE:O	4:B:1217:TYR:OH	2.24	0.52
16:e:111:ALA:HA	16:e:114:ALA:HB3	1.92	0.52
3:A:569:PRO:HG2	10:H:46:MET:HE3	1.92	0.52
3:A:914:ILE:HA	3:A:981:SER:H	1.74	0.52
4:B:1155:SER:OG	4:B:1156:ASP:N	2.42	0.52
7:E:73:ASP:OD1	7:E:73:ASP:N	2.42	0.52
16:e:108:ASN:O	16:e:112:ILE:N	2.36	0.52
1:N:20:DG:H1'	1:N:21:DG:H5'	1.90	0.52
3:A:252:ALA:O	15:P:1:U:N3	2.42	0.52
5:C:66:LEU:HD23	5:C:69:ILE:HD12	1.92	0.52
17:f:33:ALA:HA	17:f:36:ARG:HE	1.74	0.52
3:A:113:LEU:HG	3:A:115:LEU:H	1.74	0.52
3:A:1416:GLY:HA3	4:B:1212:ILE:HG23	1.91	0.52
3:A:1439:MET:HE1	4:B:1139:ILE:HG12	1.91	0.52
3:A:526:GLN:HB3	4:B:1015:HIS:CG	2.45	0.52
3:A:610:ASP:OD2	3:A:612:LYS:NZ	2.39	0.52
4:B:218:LYS:HE2	4:B:388:GLN:HB3	1.91	0.52
4:B:50:VAL:HG21	4:B:82:ILE:HD11	1.92	0.52
6:D:143:ALA:HB3	9:G:1:MET:HE1	1.90	0.52
6:D:169:VAL:HG12	6:D:170:ASN:H	1.75	0.52
3:A:1190:GLN:OE1	3:A:1243:ARG:NH1	2.43	0.52
3:A:1453:LEU:HD23	3:A:1456:LEU:HD12	1.92	0.52
4:B:641:ASN:HD21	4:B:646:ARG:HA	1.75	0.52
4:B:879:ARG:HA	4:B:885:LEU:HD11	1.91	0.52
5:C:40:VAL:HB	5:C:172:PRO:HG3	1.91	0.52
17:h:26:ILE:HD12	17:h:59:LYS:HB2	1.92	0.52
2:T:7:DC:H2''	2:T:8:DC:C6	2.45	0.51
3:A:352:THR:HG1	3:A:353:VAL:N	2.08	0.51
5:C:104:HIS:ND1	5:C:111:THR:OG1	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:61:TYR:HA	13:K:73:MET:HA	1.92	0.51
3:A:1014:GLN:O	3:A:1018:SER:OG	2.29	0.51
4:B:760:ASP:OD1	4:B:760:ASP:N	2.35	0.51
3:A:512:ILE:HA	3:A:522:MET:HE2	1.92	0.51
3:A:727:ARG:NH1	3:A:766:VAL:O	2.40	0.51
4:B:78:ARG:HB3	4:B:120:GLU:HB3	1.93	0.51
7:E:2:GLU:HG2	7:E:4:ASN:H	1.75	0.51
1:N:-44:DG:H2''	1:N:-43:DT:C6	2.46	0.51
2:T:17:DA:H3'	2:T:18:DC:H6	1.75	0.51
2:T:18:DC:H2'	2:T:19:DC:N1	2.25	0.51
7:E:137:SER:HA	7:E:140:VAL:HG23	1.91	0.51
3:A:454:MET:HB3	3:A:457:MET:HE2	1.92	0.51
4:B:917:PRO:HA	4:B:934:LYS:HA	1.92	0.51
4:B:952:VAL:HG13	4:B:966:VAL:HG22	1.92	0.51
5:C:34:ARG:HE	13:K:41:THR:HG1	1.54	0.51
2:T:-38:DC:H2''	2:T:-37:DG:C8	2.45	0.51
4:B:444:THR:O	4:B:448:SER:OG	2.27	0.51
2:T:8:DC:H2''	2:T:9:DG:C8	2.46	0.51
3:A:9:ALA:HB1	4:B:1192:TYR:HA	1.92	0.51
4:B:609:ILE:HG12	4:B:694:GLU:HB2	1.93	0.51
12:J:9:SER:HB2	12:J:44:CYS:HB2	1.93	0.51
1:N:-21:DG:H2''	1:N:-20:DC:C5	2.45	0.51
2:T:45:DC:H2''	2:T:46:DA:C4	2.46	0.51
3:A:317:GLN:HE21	3:A:323:VAL:HG22	1.76	0.51
3:A:367:VAL:HG21	3:A:461:VAL:HG13	1.92	0.51
4:B:799:PRO:HB2	4:B:818:PRO:HG2	1.92	0.51
7:E:201:SER:HB2	7:E:207:TYR:HB2	1.92	0.51
17:h:33:ALA:O	17:h:37:LEU:HG	2.11	0.51
17:h:55:ARG:O	17:h:59:LYS:N	2.40	0.51
3:A:107:CYS:HB3	3:A:112:LYS:H	1.76	0.51
3:A:395:ASN:ND2	3:A:401:PRO:O	2.36	0.51
3:A:517:SER:OG	3:A:1365:TYR:O	2.28	0.51
17:h:71:THR:O	17:h:75:HIS:N	2.35	0.51
2:T:-51:DC:H4'	16:e:83:ARG:HD2	1.93	0.51
4:B:225:ILE:HD13	4:B:248:LYS:HD3	1.93	0.51
4:B:71:ILE:HG12	4:B:73:LYS:HG3	1.92	0.50
4:B:229:ALA:HB3	4:B:247:ILE:HD12	1.93	0.50
4:B:470:ALA:HB1	15:P:6:U:H4'	1.93	0.50
10:H:102:LYS:HB3	10:H:114:TYR:HB2	1.93	0.50
13:K:36:GLU:OE1	13:K:37:ARG:NH1	2.43	0.50
2:T:-5:DA:H2''	2:T:-4:DC:H5'	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:108:MET:H	3:A:172:GLN:HE22	1.58	0.50
3:A:768:GLN:NE2	3:A:798:LYS:O	2.40	0.50
4:B:303:LEU:HD23	4:B:306:LEU:HD12	1.93	0.50
4:B:950:ASP:OD2	4:B:967:ARG:NH2	2.39	0.50
2:T:-15:DA:H2''	2:T:-14:DA:C8	2.46	0.50
4:B:1114:LEU:HG	4:B:1115:THR:HG23	1.92	0.50
16:g:104:PHE:HA	16:g:107:THR:HG22	1.93	0.50
17:h:31:LYS:HG3	17:h:51:TYR:CZ	2.46	0.50
3:A:669:ASP:OD2	3:A:743:ASN:ND2	2.44	0.50
4:B:572:ARG:HG2	4:B:582:ILE:HG22	1.92	0.50
4:B:595:ASP:HA	4:B:598:ARG:HB2	1.93	0.50
6:D:169:VAL:HG13	6:D:171:LEU:HB3	1.92	0.50
8:F:117:PRO:HA	8:F:120:ILE:HD12	1.94	0.50
2:T:-8:DC:H2''	2:T:-7:DG:C8	2.47	0.50
4:B:82:ILE:HD13	4:B:117:LEU:HD13	1.92	0.50
4:B:252:ARG:HB3	4:B:255:LYS:HB3	1.94	0.50
4:B:320:GLU:HA	4:B:323:LEU:HD12	1.94	0.50
12:J:7:CYS:HB3	12:J:11:GLY:H	1.75	0.50
15:P:1:U:C2'	15:P:2:U:H5'	2.41	0.50
16:g:128:ARG:NH2	17:h:60:VAL:HG11	2.26	0.50
3:A:1285:VAL:HG13	3:A:1311:THR:HG22	1.93	0.50
3:A:1356:LEU:HD13	3:A:1371:MET:HE1	1.94	0.50
4:B:865:ARG:HG3	4:B:871:VAL:HG12	1.93	0.50
2:T:33:DC:OP2	4:B:1122:ARG:N	2.45	0.50
4:B:444:THR:O	4:B:448:SER:HB2	2.12	0.50
4:B:466:MET:N	4:B:466:MET:SD	2.85	0.50
4:B:982:SER:OG	4:B:985:GLY:N	2.44	0.50
16:e:126:LEU:HD22	16:g:113:HIS:CG	2.47	0.50
1:N:6:DA:H2''	1:N:7:DC:H5	1.77	0.50
2:T:9:DG:H2''	2:T:10:DC:C6	2.47	0.50
3:A:250:SER:HB2	3:A:258:GLN:HB2	1.93	0.50
3:A:850:MET:HG3	3:A:1063:GLY:HA2	1.92	0.50
4:B:883:LEU:HG	4:B:935:ARG:HA	1.93	0.50
12:J:22:LEU:HD23	12:J:25:LEU:HD12	1.93	0.50
3:A:337:LEU:HA	3:A:341:LEU:HB2	1.93	0.49
4:B:320:GLU:OE1	4:B:338:ARG:NH1	2.45	0.49
4:B:772:ALA:HB1	15:P:10:U:OP1	2.12	0.49
16:g:67:PHE:HA	16:g:70:LEU:HD23	1.94	0.49
1:N:22:DT:H1'	1:N:23:DG:H5'	1.94	0.49
17:h:70:VAL:O	17:h:73:THR:OG1	2.25	0.49
1:N:-2:DC:C4	1:N:-1:DA:N6	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:344:LYS:NZ	4:B:1156:ASP:OD1	2.46	0.49
3:A:389:LEU:HD23	3:A:392:TYR:HD2	1.77	0.49
3:A:591:ARG:NH1	3:A:622:THR:OG1	2.37	0.49
3:A:858:ARG:NH1	8:F:139:PRO:HB2	2.27	0.49
4:B:563:ASP:OD2	4:B:566:GLN:N	2.44	0.49
7:E:175:PRO:HB2	7:E:211:ARG:HG2	1.93	0.49
15:P:5:G:H2'	15:P:6:U:C6	2.47	0.49
17:h:60:VAL:O	17:h:63:GLU:HG3	2.11	0.49
4:B:91:GLU:OE1	14:L:56:ARG:NH1	2.46	0.49
4:B:1037:ILE:O	12:J:46:ARG:NH2	2.46	0.49
5:C:111:THR:HB	5:C:147:LEU:HB2	1.94	0.49
8:F:149:ASP:OD1	8:F:149:ASP:N	2.45	0.49
13:K:31:ILE:HG13	13:K:75:LEU:HB3	1.94	0.49
3:A:497:GLU:CD	9:G:64:GLY:HA2	2.35	0.49
9:G:106:LEU:HG	9:G:157:ILE:CD1	2.41	0.49
12:J:7:CYS:SG	12:J:9:SER:N	2.86	0.49
3:A:550:MET:HG2	3:A:656:TYR:HD2	1.78	0.49
3:A:942:LYS:NZ	3:A:946:GLU:OE1	2.36	0.49
3:A:1146:LYS:HB2	3:A:1271:LEU:HB3	1.95	0.49
4:B:834:ASN:O	4:B:1013:ASN:ND2	2.45	0.49
1:N:10:DG:H4'	1:N:11:DC:OP1	2.12	0.49
3:A:929:GLU:O	3:A:932:SER:OG	2.31	0.49
4:B:1065:GLN:HE22	4:B:1067:ARG:HB2	1.78	0.49
10:H:115:VAL:HB	10:H:122:MET:HE2	1.95	0.49
16:e:67:PHE:HZ	16:e:92:LEU:HB3	1.78	0.49
3:A:283:ASP:OD1	3:A:283:ASP:N	2.42	0.49
3:A:435:ARG:NH1	3:A:438:MET:H	2.11	0.49
4:B:1112:GLN:HG3	4:B:1119:VAL:HG12	1.93	0.49
16:e:119:ILE:HG23	16:e:123:ASP:HB2	1.94	0.49
3:A:811:PRO:HB2	4:B:702:MET:HE3	1.95	0.49
3:A:819:MET:HG2	4:B:507:LEU:HB3	1.94	0.49
4:B:15:GLU:HA	4:B:18:TRP:HD1	1.77	0.49
4:B:413:LEU:HB3	4:B:446:ILE:HG12	1.94	0.49
4:B:634:GLU:HG2	4:B:641:ASN:HB3	1.94	0.49
7:E:213:CYS:SG	7:E:214:LEU:N	2.85	0.49
1:N:-10:DG:H2''	1:N:-9:DC:H5	1.77	0.48
1:N:32:DG:H1'	1:N:33:DT:C6	2.48	0.48
3:A:22:LEU:HG	4:B:1213:ALA:HB2	1.95	0.48
2:T:13:DT:C6	2:T:14:DT:H72	2.48	0.48
3:A:408:ARG:HD3	3:A:412:ASP:HB2	1.96	0.48
3:A:885:ASP:OD2	3:A:1027:ARG:NE	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:758:PHE:HB3	4:B:761:HIS:HD2	1.78	0.48
5:C:149:ASN:OD1	5:C:150:HIS:ND1	2.46	0.48
8:F:128:ARG:HE	8:F:153:VAL:HG23	1.79	0.48
11:I:101:TYR:N	11:I:110:PHE:O	2.33	0.48
17:h:23:ARG:HB3	17:h:27:GLN:HG3	1.95	0.48
3:A:55:ASP:HB3	3:A:58:LEU:HG	1.95	0.48
7:E:84:GLU:OE1	7:E:91:THR:OG1	2.29	0.48
1:N:58:DC:H2''	1:N:59:DA:H8	1.77	0.48
3:A:1148:VAL:HA	3:A:1203:ARG:HD3	1.95	0.48
4:B:892:LYS:HB3	4:B:899:ILE:HD12	1.96	0.48
5:C:100:LEU:HD13	5:C:118:LEU:HD23	1.94	0.48
10:H:63:LEU:HD21	10:H:142:LEU:HD11	1.93	0.48
16:g:98:ALA:O	16:g:102:GLY:N	2.44	0.48
3:A:826:ILE:O	3:A:830:VAL:HB	2.14	0.48
3:A:370:SER:H	13:K:2:ASN:ND2	2.11	0.48
3:A:498:THR:HB	4:B:1146:PHE:HD1	1.78	0.48
2:T:4:DC:C4	2:T:5:DC:N4	2.82	0.48
3:A:697:LYS:O	3:A:702:GLU:N	2.41	0.48
2:T:-20:DC:H2''	2:T:-19:DG:C8	2.49	0.48
2:T:25:DG:P	3:A:310:ALA:HB2	2.54	0.48
3:A:900:VAL:HG22	3:A:1031:ARG:HG3	1.96	0.48
4:B:975:GLN:N	4:B:978:ASP:OD2	2.41	0.48
4:B:1065:GLN:NE2	4:B:1067:ARG:H	2.12	0.48
3:A:516:GLN:NE2	3:A:1076:GLU:OE1	2.46	0.48
3:A:1328:SER:HA	7:E:146:HIS:HA	1.95	0.48
4:B:46:ILE:HG22	4:B:82:ILE:HG13	1.95	0.48
1:N:-37:DG:H1'	4:B:419:ARG:HH12	1.79	0.48
3:A:538:ARG:NE	10:H:119:GLY:O	2.46	0.48
4:B:410:PHE:O	4:B:414:PHE:HB2	2.13	0.48
2:T:-46:DC:C4	2:T:-45:DA:C6	3.02	0.47
3:A:1381:ARG:HH12	3:A:1395:ALA:HA	1.78	0.47
4:B:180:LEU:O	4:B:184:LYS:N	2.48	0.47
1:N:58:DC:H2''	1:N:59:DA:C8	2.48	0.47
4:B:533:SER:N	4:B:536:SER:OG	2.47	0.47
17:f:26:ILE:HG21	17:f:59:LYS:HD2	1.95	0.47
3:A:1152:THR:OG1	11:I:46:HIS:N	2.41	0.47
5:C:32:LEU:HG	5:C:36:MET:HE2	1.95	0.47
2:T:0:DC:H2''	2:T:1:DT:C5	2.49	0.47
3:A:114:LEU:HD11	3:A:172:GLN:HG3	1.95	0.47
3:A:171:THR:HB	3:A:187:LYS:HZ3	1.79	0.47
4:B:394:PHE:H	4:B:510:THR:HG21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:16:DA:N6	2:T:-17:DT:O4	2.48	0.47
2:T:-29:DC:H2'	2:T:-28:DT:H72	1.95	0.47
4:B:477:ASN:O	4:B:484:THR:OG1	2.30	0.47
10:H:107:ASP:HB2	10:H:110:LYS:HB2	1.96	0.47
2:T:20:DG:H4'	2:T:21:DC:OP1	2.14	0.47
3:A:783:ARG:NH2	4:B:696:GLU:O	2.48	0.47
15:P:4:G:OP2	15:P:4:G:H8	1.98	0.47
1:N:33:DT:H1'	1:N:34:DC:C6	2.50	0.47
1:N:47:DA:H4'	1:N:48:DG:OP1	2.14	0.47
2:T:-44:DA:H1'	2:T:-43:DT:C2	2.50	0.47
2:T:-27:DC:H2''	2:T:-26:DT:H71	1.95	0.47
3:A:133:LYS:HA	3:A:136:ASN:HB2	1.97	0.47
3:A:501:GLU:OE1	4:B:1146:PHE:N	2.48	0.47
4:B:802:PRO:HB3	4:B:1091:TYR:CG	2.50	0.47
4:B:1000:PRO:HB2	4:B:1072:MET:HE2	1.96	0.47
4:B:1204:PHE:HE2	4:B:1216:LEU:HD11	1.80	0.47
16:e:124:ILE:HG23	16:e:128:ARG:HH21	1.79	0.47
1:N:-16:DT:H2''	1:N:-15:DA:C8	2.50	0.47
1:N:-10:DG:H2''	1:N:-9:DC:C5	2.50	0.47
1:N:42:DA:H2''	1:N:43:DA:H8	1.79	0.47
3:A:937:LEU:HD21	3:A:1025:ARG:HB3	1.97	0.47
4:B:254:ASP:OD1	4:B:259:ARG:NH2	2.48	0.47
4:B:1165:ILE:HG13	4:B:1190:ASN:HD22	1.80	0.47
6:D:22:GLU:OE1	6:D:22:GLU:N	2.48	0.47
13:K:12:LEU:HD22	13:K:18:LYS:HB2	1.97	0.47
14:L:63:THR:OG1	14:L:64:LYS:N	2.48	0.47
15:P:6:U:H2'	15:P:7:G:C8	2.50	0.47
3:A:841:ARG:NH1	3:A:1108:ASN:OD1	2.48	0.47
3:A:1102:ARG:HH12	3:A:1113:ILE:HD12	1.80	0.47
4:B:483:SER:HA	4:B:775:LYS:HG2	1.96	0.47
5:C:69:ILE:HG12	5:C:142:ILE:HD13	1.96	0.47
3:A:444:LEU:HD21	3:A:456:MET:HE2	1.97	0.47
5:C:54:THR:OG1	5:C:152:GLU:N	2.48	0.47
8:F:100:GLN:NE2	9:G:18:PHE:CE2	2.83	0.47
1:N:-38:DT:H4'	1:N:-37:DG:H5''	1.96	0.46
2:T:31:DA:OP1	4:B:1129:ARG:HD3	2.14	0.46
4:B:957:ASN:OD1	4:B:960:GLY:N	2.48	0.46
5:C:69:ILE:HG12	5:C:142:ILE:HG21	1.97	0.46
5:C:83:ARG:NH2	5:C:166:GLU:OE2	2.47	0.46
7:E:68:LEU:HD12	7:E:68:LEU:HA	1.74	0.46
10:H:100:VAL:HA	10:H:115:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:33:CYS:HB2	14:L:40:PHE:HE1	1.80	0.46
2:T:-5:DA:H8	2:T:-5:DA:P	2.38	0.46
16:e:103:LEU:HA	16:e:106:ASP:HB2	1.96	0.46
1:N:-12:DA:H2''	1:N:-11:DC:OP2	2.14	0.46
3:A:1064:GLU:OE1	8:F:88:TYR:OH	2.33	0.46
2:T:-20:DC:OP1	17:h:47:SER:OG	2.24	0.46
3:A:817:HIS:CD2	4:B:764:SER:H	2.34	0.46
9:G:108:VAL:HG22	9:G:159:ALA:HB3	1.97	0.46
3:A:887:ILE:O	3:A:945:ARG:NH2	2.48	0.46
4:B:365:THR:O	4:B:369:PHE:HB2	2.16	0.46
4:B:985:GLY:O	4:B:987:LYS:N	2.49	0.46
4:B:1092:TYR:HD1	4:B:1092:TYR:HA	1.56	0.46
12:J:7:CYS:HA	12:J:48:MET:HG3	1.97	0.46
17:f:23:ARG:NH2	17:f:25:ASN:HD21	2.14	0.46
16:g:128:ARG:HH22	17:h:60:VAL:CG1	2.27	0.46
1:N:13:DT:H2''	1:N:14:DT:C7	2.45	0.46
3:A:361:GLU:O	3:A:472:ASN:ND2	2.48	0.46
3:A:668:GLY:HA2	3:A:671:ILE:HD12	1.96	0.46
3:A:929:GLU:HB3	3:A:989:ILE:HD13	1.97	0.46
3:A:1400:LEU:HB2	3:A:1429:GLU:HG3	1.98	0.46
4:B:995:ARG:NH2	4:B:997:GLU:OE2	2.49	0.46
4:B:1006:ILE:HD13	12:J:43:TYR:CZ	2.51	0.46
11:I:90:GLN:HE21	11:I:92:ARG:HG3	1.81	0.46
11:I:108:LYS:NZ	11:I:109:THR:O	2.46	0.46
2:T:13:DT:H2''	2:T:14:DT:H5'	1.98	0.46
3:A:930:LEU:HD11	3:A:985:ILE:HG21	1.98	0.46
3:A:1001:VAL:H	3:A:1013:GLN:HE22	1.64	0.46
1:N:-14:DA:H3'	7:E:89:ILE:HG21	1.94	0.46
1:N:10:DG:H8	1:N:10:DG:OP2	1.99	0.46
3:A:254:ASP:OD1	3:A:254:ASP:N	2.48	0.46
3:A:403:ALA:HA	3:A:435:ARG:HA	1.96	0.46
4:B:806:THR:OG1	4:B:808:ALA:N	2.49	0.46
4:B:863:GLU:HG3	4:B:874:PHE:CZ	2.50	0.46
16:g:68:GLN:OE1	16:g:72:ARG:NH2	2.49	0.46
3:A:550:MET:HB3	3:A:550:MET:HE2	1.67	0.46
3:A:970:GLN:HA	3:A:975:LEU:HD12	1.98	0.46
3:A:983:LEU:HD22	3:A:1041:ARG:HA	1.97	0.46
4:B:1169:MET:HB2	4:B:1169:MET:HE3	1.71	0.46
10:H:128:TYR:O	10:H:132:ALA:HB2	2.16	0.46
12:J:43:TYR:HA	12:J:46:ARG:HD3	1.96	0.46
1:N:-4:DG:H2''	1:N:-3:DA:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1107:LEU:HD23	3:A:1107:LEU:HA	1.76	0.46
8:F:140:ASP:OD1	8:F:142:SER:N	2.45	0.46
17:f:38:ALA:HB1	17:f:43:VAL:HB	1.97	0.46
2:T:17:DA:H3'	2:T:18:DC:C6	2.51	0.45
3:A:472:ASN:OD1	3:A:473:LEU:N	2.49	0.45
3:A:632:HIS:HE1	3:A:880:GLU:HG2	1.81	0.45
3:A:846:LEU:O	3:A:848:ASP:N	2.49	0.45
4:B:1077:THR:HA	13:K:44:ASN:ND2	2.30	0.45
16:e:67:PHE:CZ	16:e:92:LEU:HB3	2.51	0.45
17:f:43:VAL:HG12	17:f:46:ILE:HG13	1.97	0.45
1:N:-11:DC:C4	1:N:-10:DG:C6	3.05	0.45
3:A:248:ARG:HB3	3:A:263:LEU:HD12	1.98	0.45
3:A:853:TYR:OH	8:F:89:GLU:OE2	2.27	0.45
3:A:975:LEU:HD23	3:A:975:LEU:HA	1.77	0.45
5:C:241:ASN:N	5:C:241:ASN:OD1	2.47	0.45
9:G:91:VAL:HA	9:G:101:ALA:HA	1.98	0.45
13:K:65:HIS:HB3	13:K:68:PHE:HD2	1.80	0.45
16:g:122:LYS:O	16:g:125:GLN:NE2	2.45	0.45
1:N:35:DT:H2''	1:N:36:DA:C8	2.52	0.45
3:A:868:LEU:HD13	3:A:1002:LEU:HD11	1.99	0.45
3:A:1331:TYR:CZ	3:A:1353:LYS:HD3	2.51	0.45
17:f:63:GLU:O	17:f:67:ARG:HG2	2.16	0.45
2:T:1:DT:H2''	2:T:2:DG:C8	2.51	0.45
4:B:733:SER:HB3	4:B:736:HIS:CE1	2.51	0.45
5:C:116:SER:OG	5:C:139:ASP:O	2.35	0.45
2:T:-14:DA:H2''	2:T:-13:DA:N7	2.31	0.45
3:A:720:SER:O	3:A:724:ASN:ND2	2.50	0.45
4:B:58:LEU:HD21	4:B:426:GLN:HE21	1.81	0.45
4:B:776:GLN:HB2	4:B:1095:LEU:HD22	1.99	0.45
1:N:10:DG:H1'	1:N:11:DC:O5'	2.17	0.45
2:T:44:DC:H2''	2:T:45:DC:C5	2.52	0.45
3:A:1451:LYS:O	3:A:1454:THR:OG1	2.30	0.45
4:B:354:LEU:HD11	4:B:371:LEU:HD11	1.98	0.45
4:B:532:LEU:HD23	4:B:532:LEU:HA	1.78	0.45
7:E:79:VAL:HG13	7:E:110:ILE:HD13	1.98	0.45
4:B:491:THR:OG1	4:B:530:LYS:O	2.25	0.45
4:B:599:SER:OG	4:B:600:GLY:N	2.49	0.45
4:B:1149:GLU:OE2	4:B:1150:ARG:NH2	2.46	0.45
7:E:194:VAL:HG22	7:E:212:ILE:HG13	1.97	0.45
16:e:66:PRO:HA	16:e:69:ARG:HG2	1.98	0.45
1:N:-20:DC:H2''	1:N:-19:DG:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:803:LEU:HD23	4:B:803:LEU:HA	1.76	0.45
1:N:12:DG:C6	2:T:-13:DA:C6	3.05	0.45
2:T:-20:DC:H4'	17:h:47:SER:HA	1.99	0.45
2:T:37:DC:H2''	2:T:38:DA:C8	2.52	0.45
3:A:90:VAL:HG21	3:A:301:VAL:HG11	1.99	0.45
3:A:107:CYS:SG	3:A:108:MET:N	2.90	0.45
3:A:846:LEU:HB3	3:A:849:ILE:HD12	1.98	0.45
4:B:203:LEU:HA	4:B:203:LEU:HD23	1.71	0.45
1:N:-38:DT:H4'	1:N:-37:DG:C5'	2.47	0.44
1:N:-14:DA:H3'	7:E:89:ILE:HG22	1.96	0.44
3:A:544:TYR:OH	13:K:57:THR:O	2.35	0.44
3:A:680:ILE:HD11	3:A:734:ALA:HB2	1.99	0.44
3:A:697:LYS:HB3	3:A:702:GLU:HB2	1.99	0.44
3:A:21:LEU:HD23	3:A:21:LEU:HA	1.75	0.44
3:A:106:ILE:HG22	3:A:113:LEU:HA	1.98	0.44
3:A:355:SER:N	3:A:469:PHE:O	2.44	0.44
3:A:388:ARG:HB3	3:A:392:TYR:CZ	2.52	0.44
3:A:1066:VAL:O	3:A:1070:ALA:HB2	2.17	0.44
4:B:707:LEU:HA	4:B:707:LEU:HD23	1.80	0.44
6:D:53:LEU:HD13	6:D:147:SER:HB3	1.98	0.44
7:E:201:SER:O	7:E:205:GLY:N	2.47	0.44
11:I:57:GLY:H	11:I:89:GLN:HG3	1.82	0.44
12:J:8:PHE:H	12:J:48:MET:HG3	1.81	0.44
2:T:8:DC:H2''	2:T:9:DG:N7	2.32	0.44
3:A:133:LYS:HA	3:A:136:ASN:HD22	1.82	0.44
3:A:240:LEU:HD22	3:A:301:VAL:HG13	1.99	0.44
3:A:526:GLN:HG3	4:B:836:GLU:HG2	1.98	0.44
3:A:1399:ALA:N	3:A:1422:ASP:OD2	2.43	0.44
4:B:794:ASN:ND2	4:B:855:PHE:HA	2.33	0.44
4:B:821:GLN:NE2	4:B:851:PHE:H	2.14	0.44
4:B:1069:PHE:HB3	4:B:1084:GLN:HB3	2.00	0.44
17:h:31:LYS:O	17:h:35:ARG:N	2.44	0.44
3:A:350:ALA:HB2	3:A:375:LEU:HD11	1.99	0.44
3:A:926:LEU:HD11	3:A:986:PRO:HD3	1.98	0.44
7:E:99:ILE:HG23	7:E:104:PHE:HD2	1.82	0.44
16:g:71:VAL:HG22	16:g:84:PHE:CZ	2.52	0.44
3:A:1155:TYR:HD1	11:I:41:PRO:HB2	1.83	0.44
3:A:1367:ASN:ND2	3:A:1369:ARG:HE	2.14	0.44
4:B:262:LYS:HA	4:B:273:PRO:HA	1.99	0.44
7:E:152:HIS:NE2	7:E:183:VAL:HG11	2.33	0.44
17:f:32:PRO:HA	17:f:35:ARG:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:-34:DG:H2"	2:T:-33:DA:C8	2.53	0.44
2:T:45:DC:H2"	2:T:46:DA:C8	2.52	0.44
3:A:5:PRO:HG2	4:B:1159:ARG:HH22	1.83	0.44
3:A:1447:MET:HB2	8:F:133:VAL:HB	1.98	0.44
4:B:803:LEU:HD23	4:B:1041:GLU:HG2	1.99	0.44
16:g:70:LEU:HD11	17:h:26:ILE:HA	2.00	0.44
5:C:37:LEU:HD23	5:C:37:LEU:HA	1.82	0.44
6:D:167:LYS:HA	6:D:167:LYS:HD3	1.73	0.44
16:g:133:GLU:HG2	17:h:61:PHE:CE1	2.53	0.44
3:A:287:GLN:HA	3:A:290:ILE:HD12	2.00	0.44
4:B:369:PHE:HB3	4:B:579:TRP:CZ3	2.52	0.44
4:B:1104:HIS:HE1	4:B:1106:ARG:HB2	1.82	0.44
5:C:34:ARG:CZ	13:K:40:HIS:HB2	2.48	0.44
16:g:106:ASP:HA	16:g:109:LEU:HB3	2.00	0.44
4:B:749:LEU:HB3	4:B:753:ALA:HB3	2.00	0.44
4:B:955:THR:O	4:B:963:PHE:N	2.50	0.44
3:A:90:VAL:O	3:A:237:ILE:N	2.47	0.43
4:B:471:GLY:HA3	15:P:7:G:H5"	1.93	0.43
4:B:773:MET:HE1	4:B:985:GLY:HA2	2.00	0.43
4:B:804:ALA:HB3	4:B:983:ARG:HH22	1.82	0.43
10:H:85:ASP:OD1	10:H:85:ASP:N	2.39	0.43
2:T:0:DC:H2"	2:T:1:DT:C7	2.48	0.43
3:A:868:LEU:N	7:E:207:TYR:OH	2.38	0.43
3:A:958:LEU:HA	3:A:958:LEU:HD23	1.79	0.43
4:B:974:PRO:HG3	4:B:1094:ARG:HH12	1.82	0.43
6:D:169:VAL:CG1	6:D:170:ASN:N	2.78	0.43
15:P:6:U:H2'	15:P:7:G:H8	1.82	0.43
16:e:117:VAL:HG23	16:e:118:THR:HG23	2.01	0.43
16:g:72:ARG:HG2	16:g:84:PHE:HD2	1.82	0.43
2:T:-13:DA:H2"	2:T:-12:DC:C6	2.53	0.43
3:A:340:ASN:ND2	4:B:1117:GLN:OE1	2.48	0.43
4:B:784:ASN:HB3	12:J:62:TYR:OH	2.17	0.43
12:J:22:LEU:HD23	12:J:22:LEU:HA	1.82	0.43
3:A:545:GLU:HA	3:A:548:MET:HE2	2.01	0.43
4:B:202:VAL:O	4:B:473:SER:OG	2.30	0.43
10:H:112:LYS:HG2	10:H:125:GLU:HG2	2.00	0.43
16:e:85:GLN:HG3	16:e:88:ALA:H	1.82	0.43
3:A:212:PHE:HB3	3:A:233:GLU:HB3	2.00	0.43
3:A:237:ILE:HD13	3:A:240:LEU:HD13	2.00	0.43
3:A:266:LYS:HA	3:A:266:LYS:HD3	1.84	0.43
3:A:1439:MET:HA	3:A:1443:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:227:HIS:HB3	4:B:378:LEU:HD11	1.99	0.43
5:C:36:MET:HE3	5:C:36:MET:HB2	1.86	0.43
2:T:-36:DT:H6	2:T:-36:DT:H2'	1.63	0.43
3:A:680:ILE:HG23	3:A:730:ALA:HB1	1.99	0.43
4:B:223:SER:HB3	4:B:252:ARG:HH21	1.84	0.43
7:E:57:MET:HE2	7:E:81:PHE:HE2	1.84	0.43
13:K:38:GLU:HB2	13:K:71:PHE:HE1	1.83	0.43
2:T:-24:DG:H2''	2:T:-23:DC:C5	2.54	0.43
3:A:927:GLN:HE21	3:A:931:ASN:HD21	1.67	0.43
3:A:1116:PRO:HA	3:A:1333:ASN:HD21	1.84	0.43
3:A:1216:ASP:O	3:A:1220:GLU:HG2	2.19	0.43
4:B:546:PRO:HA	4:B:549:ASN:HD22	1.83	0.43
4:B:861:ASP:OD1	4:B:914:LYS:NZ	2.42	0.43
7:E:155:LEU:HD22	7:E:159:GLU:HB3	2.00	0.43
1:N:24:DC:H6	1:N:24:DC:H2'	1.56	0.43
3:A:409:ASP:OD1	3:A:409:ASP:N	2.52	0.43
3:A:914:ILE:HG13	3:A:917:ALA:HB2	1.99	0.43
3:A:1367:ASN:OD1	3:A:1368:TYR:N	2.52	0.43
3:A:1448:ILE:O	9:G:58:LYS:HD3	2.18	0.43
4:B:179:ASP:O	4:B:183:MET:N	2.52	0.43
4:B:371:LEU:HD23	4:B:371:LEU:HA	1.86	0.43
4:B:608:ILE:HG12	4:B:619:ILE:HG12	2.01	0.43
4:B:649:LYS:HD2	4:B:649:LYS:HA	1.88	0.43
4:B:848:ARG:HD3	12:J:7:CYS:O	2.19	0.43
3:A:533:ARG:HD3	3:A:750:ALA:HA	2.01	0.43
4:B:55:ARG:HD3	4:B:78:ARG:HD2	2.01	0.43
4:B:681:LEU:HD22	4:B:686:VAL:HG21	2.00	0.43
4:B:816:GLU:HA	12:J:53:VAL:HG11	2.01	0.43
12:J:8:PHE:HD1	12:J:8:PHE:HA	1.75	0.43
1:N:51:DG:H2''	1:N:52:DC:C5	2.54	0.43
3:A:857:THR:HB	3:A:866:GLN:H	1.84	0.43
3:A:1279:ILE:HD12	3:A:1318:GLU:HB3	2.00	0.43
1:N:13:DT:H6	1:N:13:DT:H2'	1.71	0.42
3:A:80:HIS:H	3:A:244:PRO:HB3	1.83	0.42
3:A:387:HIS:O	3:A:390:THR:OG1	2.31	0.42
3:A:494:GLN:N	4:B:1149:GLU:OE2	2.51	0.42
3:A:1168:ASP:HB3	3:A:1172:VAL:HG13	2.01	0.42
4:B:839:MET:SD	4:B:1010:LEU:HD21	2.59	0.42
5:C:96:VAL:HB	5:C:159:ALA:HB3	2.01	0.42
10:H:89:ALA:HB1	10:H:95:VAL:HG21	2.01	0.42
3:A:897:ARG:HD3	3:A:1032:ARG:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1065:MET:HE3	3:A:1065:MET:HB3	1.77	0.42
3:A:1423:ASP:OD1	3:A:1423:ASP:N	2.49	0.42
4:B:105:ARG:NH2	4:B:165:LEU:HD21	2.34	0.42
4:B:535:LEU:HD23	4:B:535:LEU:HA	1.85	0.42
8:F:123:LYS:O	8:F:126:SER:OG	2.37	0.42
12:J:12:LYS:HB3	12:J:45:CYS:SG	2.58	0.42
13:K:70:ASN:OD1	13:K:70:ASN:N	2.51	0.42
17:f:63:GLU:HA	17:f:66:ILE:HB	2.01	0.42
1:N:10:DG:H2''	1:N:11:DC:H6	1.84	0.42
3:A:392:TYR:CG	3:A:438:MET:HE1	2.54	0.42
3:A:502:LEU:HD23	3:A:502:LEU:HA	1.82	0.42
3:A:92:HIS:CD2	3:A:237:ILE:HD11	2.53	0.42
3:A:765:CYS:SG	3:A:767:GLY:N	2.92	0.42
4:B:107:ARG:HB2	4:B:109:LEU:HG	2.01	0.42
4:B:405:LEU:HD23	4:B:405:LEU:HA	1.80	0.42
4:B:797:TYR:HE1	4:B:854:LEU:HG	1.84	0.42
4:B:1128:LEU:HA	4:B:1128:LEU:HD23	1.80	0.42
7:E:95:PHE:O	7:E:99:ILE:HG12	2.18	0.42
15:P:8:U:C2	15:P:9:U:C5	3.08	0.42
16:g:128:ARG:HD2	17:h:57:VAL:HG22	2.01	0.42
1:N:35:DT:H3'	17:f:35:ARG:HH22	1.84	0.42
4:B:58:LEU:HD12	4:B:425:MET:HE2	2.02	0.42
1:N:42:DA:C6	1:N:43:DA:C6	3.07	0.42
2:T:47:DG:H2''	2:T:48:DG:C8	2.54	0.42
3:A:531:GLY:HA3	3:A:658:LEU:HD22	2.02	0.42
3:A:551:LEU:HD21	3:A:578:LEU:HG	2.01	0.42
6:D:112:PHE:CE1	9:G:88:ASP:HB3	2.53	0.42
11:I:103:CYS:HB3	11:I:107:LYS:H	1.83	0.42
1:N:44:DT:H6	1:N:44:DT:H2'	1.69	0.42
2:T:-6:DT:H2''	2:T:-5:DA:N7	2.35	0.42
3:A:19:PHE:HB3	3:A:1416:GLY:HA2	2.02	0.42
3:A:610:ASP:HA	3:A:971:GLN:HE22	1.85	0.42
3:A:851:VAL:O	3:A:1063:GLY:N	2.48	0.42
3:A:913:VAL:O	3:A:981:SER:N	2.52	0.42
13:K:57:THR:OG1	13:K:76:GLN:O	2.33	0.42
16:g:60:LEU:HD11	16:g:90:MET:SD	2.60	0.42
17:h:34:ILE:HA	17:h:37:LEU:HD12	2.02	0.42
2:T:32:DA:H2''	2:T:33:DC:H5'	2.01	0.42
3:A:1028:LEU:HB3	3:A:1033:ILE:HD11	2.01	0.42
4:B:480:THR:HG21	4:B:777:ALA:HB3	2.02	0.42
4:B:957:ASN:HB3	4:B:963:PHE:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:92:ARG:NH2	9:G:63:PRO:HG3	2.35	0.42
9:G:104:GLY:HA3	9:G:105:PRO:HD3	1.87	0.42
9:G:129:ALA:HB2	9:G:138:THR:HB	2.02	0.42
11:I:19:ASP:HB2	11:I:26:LEU:HD11	2.02	0.42
17:f:32:PRO:O	17:f:36:ARG:N	2.49	0.42
3:A:1162:SER:OG	3:A:1163:THR:N	2.53	0.42
4:B:593:MET:HB3	4:B:608:ILE:HD13	2.01	0.42
5:C:7:VAL:HG11	13:K:105:PHE:HD1	1.84	0.42
7:E:20:GLU:OE1	7:E:142:ASN:ND2	2.45	0.42
7:E:176:ARG:HD3	7:E:214:LEU:HD21	2.01	0.42
17:f:71:THR:O	17:f:74:GLU:HG2	2.19	0.42
1:N:38:DG:H8	1:N:38:DG:P	2.43	0.42
3:A:790:LYS:N	11:I:67:THR:O	2.53	0.42
6:D:169:VAL:HG13	6:D:171:LEU:HB2	2.01	0.42
13:K:12:LEU:HD12	13:K:13:PRO:HD2	2.02	0.42
17:h:31:LYS:HG3	17:h:51:TYR:CE1	2.55	0.42
1:N:-22:DG:O6	2:T:21:DC:N4	2.52	0.41
3:A:115:LEU:HB3	3:A:122:MET:HG2	2.00	0.41
3:A:204:THR:HA	3:A:205:PRO:HD3	1.94	0.41
3:A:551:LEU:HD22	3:A:581:ILE:HG21	2.02	0.41
3:A:1118:LEU:HD23	3:A:1332:SER:HB2	2.02	0.41
4:B:24:PHE:HD1	4:B:678:TRP:CE2	2.38	0.41
4:B:87:PRO:HA	4:B:113:SER:HA	2.01	0.41
4:B:227:HIS:CE1	4:B:382:ALA:HA	2.55	0.41
4:B:951:GLN:OE1	4:B:967:ARG:NH2	2.52	0.41
10:H:111:ILE:HD13	10:H:128:TYR:HD1	1.84	0.41
13:K:39:ASP:HB3	13:K:40:HIS:H	1.70	0.41
16:e:61:LEU:O	17:f:36:ARG:NH2	2.53	0.41
17:f:31:LYS:O	17:f:35:ARG:N	2.35	0.41
1:N:-5:DG:H1'	1:N:-4:DG:H5'	2.02	0.41
2:T:-19:DG:H1'	2:T:-18:DC:O4'	2.20	0.41
2:T:29:DT:H72	4:B:524:GLN:OE1	2.20	0.41
3:A:529:LEU:HD12	3:A:529:LEU:HA	1.81	0.41
3:A:765:CYS:SG	3:A:766:VAL:N	2.92	0.41
3:A:1056:GLN:HB3	8:F:84:TYR:HE2	1.85	0.41
6:D:157:ILE:H	6:D:157:ILE:HG13	1.77	0.41
10:H:36:ILE:HG12	10:H:126:GLY:HA3	2.02	0.41
16:g:131:ARG:NH1	16:g:133:GLU:OE2	2.44	0.41
1:N:-44:DG:H2''	1:N:-43:DT:C5	2.54	0.41
1:N:10:DG:H2''	1:N:11:DC:C6	2.56	0.41
3:A:516:GLN:HE21	3:A:1077:PRO:HG3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:806:THR:OG1	4:B:809:MET:N	2.47	0.41
4:B:1077:THR:C	5:C:30:ASN:HD22	2.29	0.41
4:B:732:THR:OG1	4:B:733:SER:N	2.51	0.41
7:E:45:ILE:HG22	7:E:53:GLN:H	1.86	0.41
9:G:62:ILE:HD11	9:G:69:GLU:HB2	2.01	0.41
12:J:39:LYS:HD3	12:J:39:LYS:HA	1.90	0.41
1:N:-37:DG:C1'	4:B:419:ARG:NH1	2.83	0.41
2:T:-40:DG:OP1	17:f:30:THR:HG21	2.21	0.41
3:A:114:LEU:HD22	3:A:148:CYS:HA	2.02	0.41
3:A:183:TRP:CG	3:A:200:ARG:HH21	2.39	0.41
3:A:408:ARG:HG3	3:A:431:TRP:CZ2	2.56	0.41
4:B:182:LYS:HG3	12:J:63:ASN:HD22	1.85	0.41
4:B:476:LEU:HD12	4:B:476:LEU:HA	1.83	0.41
4:B:622:ASP:OD1	4:B:623:VAL:N	2.54	0.41
4:B:1182:CYS:HB3	4:B:1187:ASN:HB3	2.02	0.41
5:C:171:SER:HB3	12:J:6:ARG:HH12	1.85	0.41
10:H:17:ASN:OD1	10:H:24:SER:OG	2.25	0.41
2:T:-4:DC:H6	2:T:-4:DC:H2'	1.72	0.41
3:A:1209:LEU:HD23	3:A:1277:ARG:HH21	1.86	0.41
4:B:340:LYS:HA	4:B:343:GLN:HB3	2.03	0.41
4:B:544:SER:O	4:B:548:ILE:HG12	2.20	0.41
4:B:1104:HIS:CE1	4:B:1106:ARG:HB2	2.56	0.41
7:E:89:ILE:O	7:E:93:ARG:HB2	2.19	0.41
13:K:31:ILE:HD11	13:K:83:PRO:HB2	2.02	0.41
17:h:67:ARG:O	17:h:71:THR:HG23	2.20	0.41
1:N:3:DC:H2''	1:N:4:DG:H8	1.85	0.41
2:T:-42:DT:C4	2:T:-41:DG:C6	3.08	0.41
2:T:22:DC:H2''	2:T:23:DA:H8	1.86	0.41
4:B:176:ASP:O	4:B:179:ASP:N	2.53	0.41
4:B:797:TYR:O	4:B:799:PRO:HD3	2.20	0.41
11:I:86:PHE:O	11:I:100:PHE:N	2.52	0.41
13:K:46:LEU:HA	13:K:46:LEU:HD23	1.79	0.41
1:N:-26:DC:H2''	1:N:-25:DC:C5'	2.51	0.41
1:N:7:DC:O5'	1:N:7:DC:H6	2.02	0.41
1:N:60:DC:C5	3:A:199:GLU:HG2	2.56	0.41
3:A:962:LEU:HD11	3:A:1024:VAL:HG22	2.03	0.41
3:A:1028:LEU:HA	3:A:1028:LEU:HD23	1.82	0.41
3:A:1389:ARG:O	3:A:1393:ASN:HB2	2.21	0.41
4:B:59:ASP:OD1	4:B:59:ASP:N	2.53	0.41
4:B:746:SER:HB3	4:B:1046:PRO:HG2	2.03	0.41
7:E:20:GLU:OE1	7:E:145:HIS:NE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:99:LEU:O	8:F:102:SER:OG	2.27	0.41
2:T:-56:DC:H2''	2:T:-55:DG:C8	2.56	0.41
2:T:18:DC:H2'	2:T:19:DC:C6	2.56	0.41
3:A:484:ASP:N	3:A:484:ASP:OD1	2.52	0.41
3:A:505:LEU:HD12	4:B:1143:ALA:HB2	2.03	0.41
4:B:86:ARG:NH1	4:B:98:ALA:HB2	2.36	0.41
4:B:112:SER:HB2	4:B:160:LYS:HB3	2.02	0.41
4:B:293:ILE:HG12	4:B:372:GLY:HA2	2.03	0.41
4:B:596:LEU:HA	4:B:596:LEU:HD23	1.79	0.41
4:B:597:ARG:NH1	4:B:608:ILE:H	2.18	0.41
4:B:833:TYR:OH	13:K:65:HIS:NE2	2.50	0.41
5:C:73:SER:HB3	5:C:76:VAL:HB	2.01	0.41
7:E:78:TRP:NE1	7:E:80:GLU:OE1	2.43	0.41
17:f:76:ALA:O	17:f:77:LYS:HG2	2.21	0.41
16:g:59:GLU:HB3	16:g:60:LEU:H	1.71	0.41
1:N:43:DA:H2''	1:N:44:DT:O4	2.21	0.41
3:A:251:ILE:H	3:A:251:ILE:HG13	1.76	0.41
3:A:435:ARG:HH22	3:A:441:ASP:CG	2.29	0.41
3:A:688:LYS:NZ	3:A:802:GLU:OE1	2.53	0.41
4:B:796:LEU:HA	4:B:796:LEU:HD12	1.84	0.41
4:B:882:THR:HG22	4:B:934:LYS:HB2	2.03	0.41
16:e:90:MET:HE2	16:e:90:MET:HA	2.02	0.41
1:N:3:DC:OP1	16:g:86:SER:N	2.36	0.40
1:N:12:DG:H1'	1:N:13:DT:H5'	2.03	0.40
1:N:31:DT:H2''	1:N:32:DG:C8	2.56	0.40
2:T:-26:DT:C4	2:T:-25:DA:C6	3.08	0.40
3:A:900:VAL:HG11	3:A:930:LEU:HD13	2.03	0.40
3:A:1061:HIS:CE1	8:F:87:LYS:HE3	2.56	0.40
3:A:1378:MET:HE2	3:A:1378:MET:HB3	1.83	0.40
3:A:83:HIS:HA	3:A:241:PRO:HA	2.02	0.40
3:A:1441:THR:HB	8:F:92:ARG:HB2	2.03	0.40
4:B:170:CYS:SG	4:B:171:SER:N	2.94	0.40
4:B:1164:GLY:N	4:B:1190:ASN:O	2.37	0.40
1:N:-22:DG:H2''	1:N:-21:DG:C8	2.56	0.40
1:N:1:DC:H1'	1:N:2:DG:C4	2.56	0.40
3:A:453:LYS:HD3	3:A:1069:ILE:HG12	2.03	0.40
3:A:661:ASN:C	3:A:661:ASN:HD22	2.29	0.40
3:A:1348:ARG:NH2	3:A:1368:TYR:OH	2.51	0.40
4:B:406:LEU:HD23	4:B:406:LEU:HA	1.87	0.40
4:B:535:LEU:HB3	4:B:629:PRO:HD2	2.03	0.40
4:B:586:PRO:HG2	4:B:610:ARG:NH2	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:133:VAL:HG11	5:C:236:GLY:HA3	2.04	0.40
16:g:117:VAL:HG21	17:h:44:LYS:HE2	2.02	0.40
3:A:447:ARG:HB2	3:A:488:MET:HE3	2.03	0.40
3:A:676:THR:OG1	3:A:737:ASN:OD1	2.23	0.40
3:A:1204:MET:HE3	3:A:1204:MET:HB3	1.96	0.40
4:B:397:LYS:O	4:B:398:ARG:NH1	2.44	0.40
4:B:804:ALA:HB3	4:B:983:ARG:NH2	2.37	0.40
5:C:147:LEU:HD23	5:C:147:LEU:HA	1.91	0.40
16:e:103:LEU:O	16:e:107:THR:N	2.45	0.40
1:N:11:DC:C4'	1:N:12:DG:H5'	2.51	0.40
3:A:448:GLN:OE1	3:A:489:ASN:ND2	2.54	0.40
4:B:286:ASP:OD2	11:I:12:ASN:ND2	2.35	0.40
4:B:839:MET:HE2	4:B:839:MET:HB3	1.72	0.40
15:P:7:G:C6	15:P:8:U:C4	3.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	1392/1743 (80%)	1248 (90%)	142 (10%)	2 (0%)	48	83
4	B	1151/1227 (94%)	1017 (88%)	132 (12%)	2 (0%)	43	78
5	C	261/304 (86%)	231 (88%)	29 (11%)	1 (0%)	30	67
6	D	148/186 (80%)	136 (92%)	9 (6%)	3 (2%)	6	31
7	E	211/214 (99%)	195 (92%)	16 (8%)	0	100	100
8	F	82/155 (53%)	73 (89%)	9 (11%)	0	100	100
9	G	169/171 (99%)	160 (95%)	7 (4%)	2 (1%)	10	44
10	H	129/145 (89%)	113 (88%)	16 (12%)	0	100	100
11	I	109/115 (95%)	94 (86%)	15 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	J	64/72 (89%)	57 (89%)	7 (11%)	0	100	100
13	K	111/118 (94%)	100 (90%)	11 (10%)	0	100	100
14	L	43/72 (60%)	40 (93%)	3 (7%)	0	100	100
16	e	74/139 (53%)	72 (97%)	2 (3%)	0	100	100
16	g	75/139 (54%)	72 (96%)	3 (4%)	0	100	100
17	f	70/106 (66%)	69 (99%)	1 (1%)	0	100	100
17	h	71/106 (67%)	69 (97%)	2 (3%)	0	100	100
All	All	4160/5012 (83%)	3746 (90%)	404 (10%)	10 (0%)	44	78

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	171	LEU
9	G	134	ASP
6	D	169	VAL
9	G	154	VAL
6	D	164	ALA
4	B	155	LYS
4	B	175	LEU
5	C	90	TYR
3	A	47	ARG
3	A	959	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	1220/1528 (80%)	1216 (100%)	4 (0%)	86	86
4	B	1016/1077 (94%)	1011 (100%)	5 (0%)	81	83
5	C	236/264 (89%)	235 (100%)	1 (0%)	84	84
6	D	133/160 (83%)	130 (98%)	3 (2%)	44	64
7	E	196/197 (100%)	196 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	F	75/137 (55%)	75 (100%)	0	100	100
9	G	148/148 (100%)	147 (99%)	1 (1%)	76	81
10	H	120/130 (92%)	119 (99%)	1 (1%)	73	80
11	I	106/109 (97%)	106 (100%)	0	100	100
12	J	60/66 (91%)	59 (98%)	1 (2%)	53	69
13	K	104/109 (95%)	103 (99%)	1 (1%)	68	78
14	L	38/56 (68%)	38 (100%)	0	100	100
16	e	66/113 (58%)	66 (100%)	0	100	100
16	g	66/113 (58%)	66 (100%)	0	100	100
17	f	60/81 (74%)	60 (100%)	0	100	100
17	h	61/81 (75%)	61 (100%)	0	100	100
All	All	3705/4369 (85%)	3688 (100%)	17 (0%)	78	83

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	236	ILE
3	A	661	ASN
3	A	805	TYR
3	A	1128	LEU
4	B	196	ILE
4	B	825	VAL
4	B	948	ILE
4	B	1010	LEU
4	B	1099	VAL
5	C	188	HIS
6	D	72	ASN
6	D	171	LEU
6	D	185	TYR
9	G	106	LEU
10	H	42	ILE
12	J	8	PHE
13	K	19	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	136	ASN
3	A	278	GLN
3	A	287	GLN
3	A	291	ASN
3	A	298	GLN
3	A	317	GLN
3	A	446	ASN
3	A	516	GLN
3	A	590	GLN
3	A	632	HIS
3	A	651	GLN
3	A	661	ASN
3	A	724	ASN
3	A	742	ASN
3	A	743	ASN
3	A	787	HIS
3	A	927	GLN
3	A	968	ASN
3	A	1013	GLN
3	A	1072	GLN
3	A	1213	GLN
3	A	1261	GLN
4	B	227	HIS
4	B	388	GLN
4	B	426	GLN
4	B	549	ASN
4	B	567	HIS
4	B	735	HIS
4	B	761	HIS
4	B	767	ASN
4	B	776	GLN
4	B	794	ASN
4	B	807	GLN
4	B	887	HIS
4	B	996	HIS
4	B	1025	HIS
4	B	1093	GLN
4	B	1112	GLN
4	B	1187	ASN
5	C	8	ASN
7	E	4	ASN
7	E	36	GLN
7	E	53	GLN

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Mol	Chain	Res	Type
7	E	112	GLN
7	E	120	ASN
8	F	100	GLN
9	G	118	ASN
9	G	125	ASN
10	H	44	ASN
11	I	90	GLN
11	I	105	ASN
12	J	63	ASN
13	K	2	ASN
13	K	29	ASN
13	K	44	ASN
13	K	110	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	10/11 (90%)	5 (50%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	1	U
15	P	2	U
15	P	4	G
15	P	8	U
15	P	9	U

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [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.

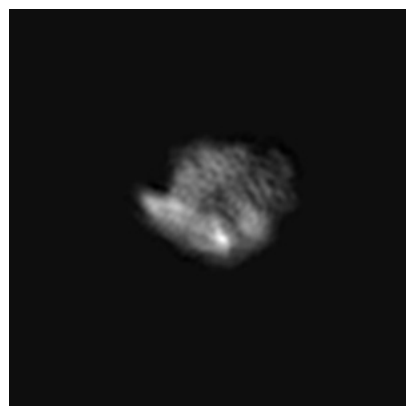
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64226. These allow visual inspection of the internal detail of the map and identification of artifacts.

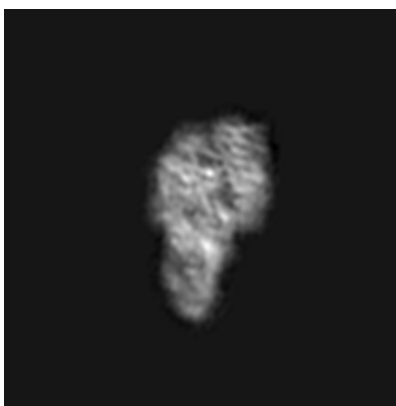
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

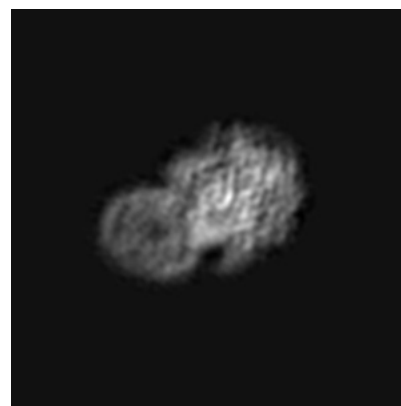
6.1.1 Primary map



X

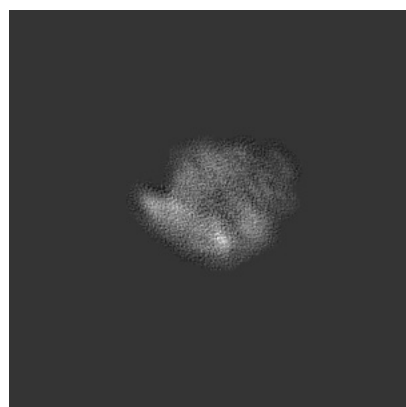


Y



Z

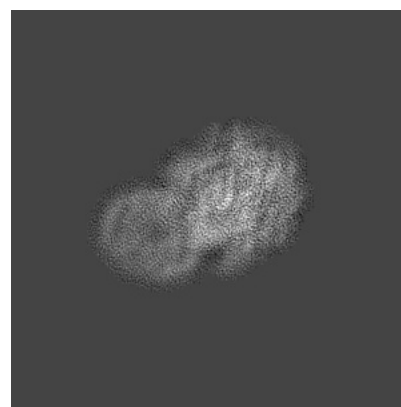
6.1.2 Raw map



X



Y

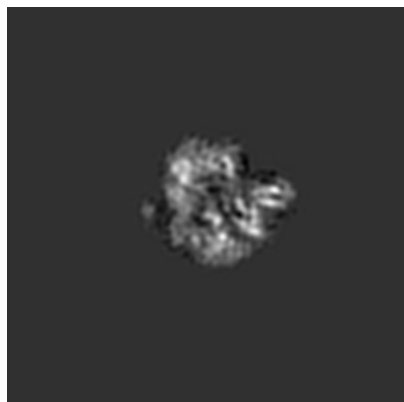


Z

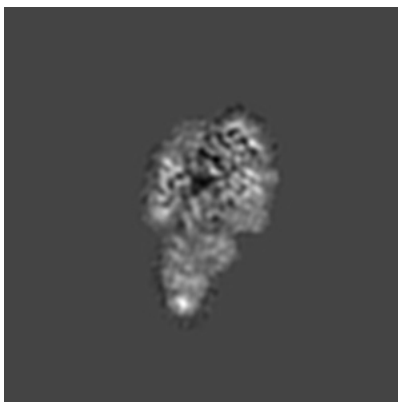
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

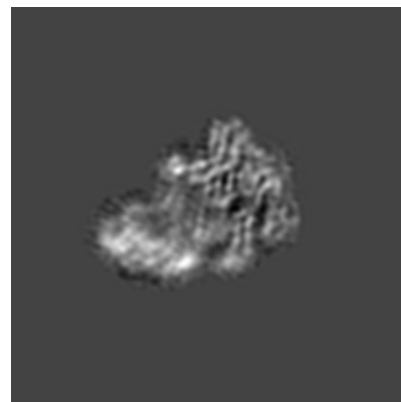
6.2.1 Primary map



X Index: 180

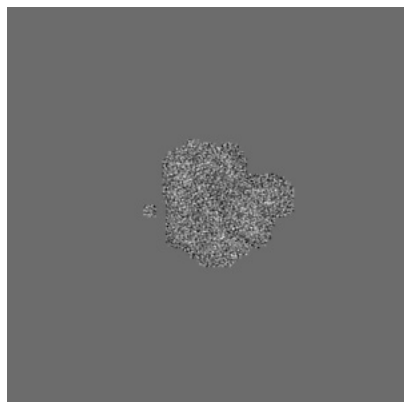


Y Index: 180



Z Index: 180

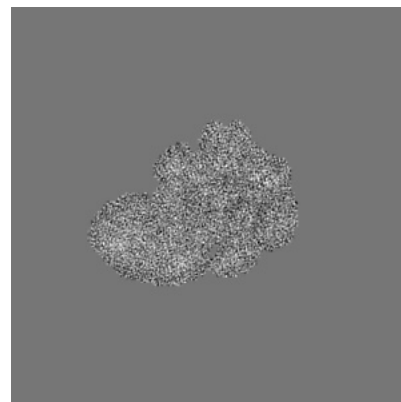
6.2.2 Raw map



X Index: 180



Y Index: 180

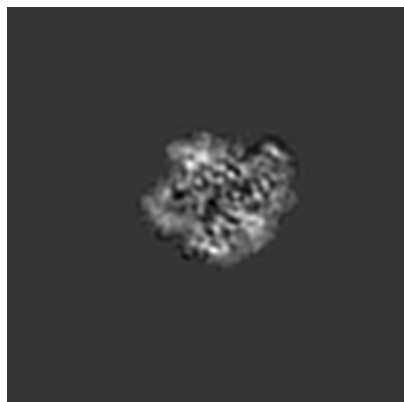


Z Index: 180

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

6.3 Largest variance slices [i](#)

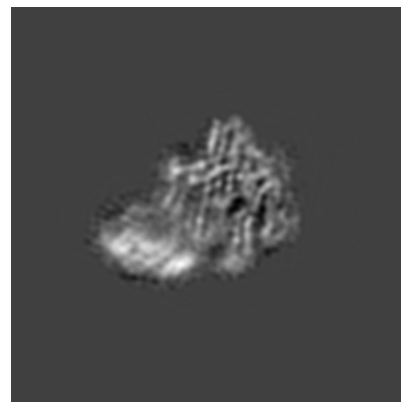
6.3.1 Primary map



X Index: 208

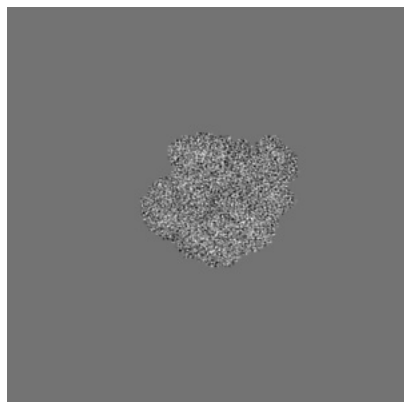


Y Index: 190

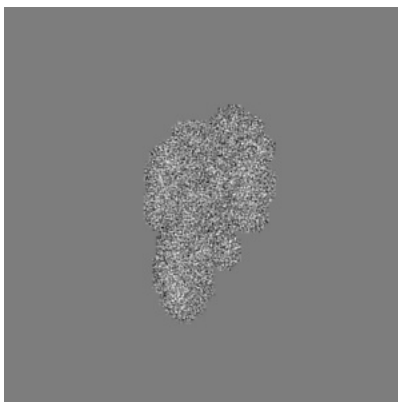


Z Index: 182

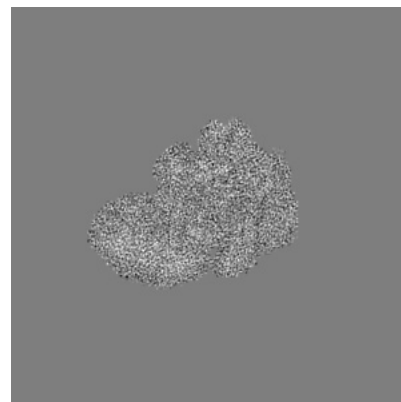
6.3.2 Raw map



X Index: 207



Y Index: 185

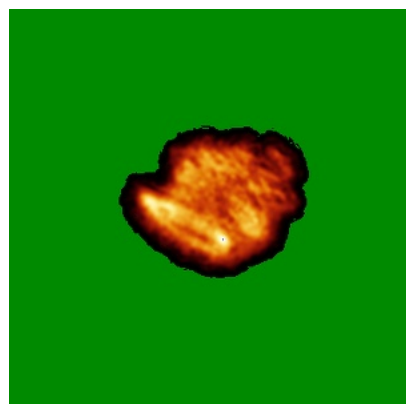


Z Index: 181

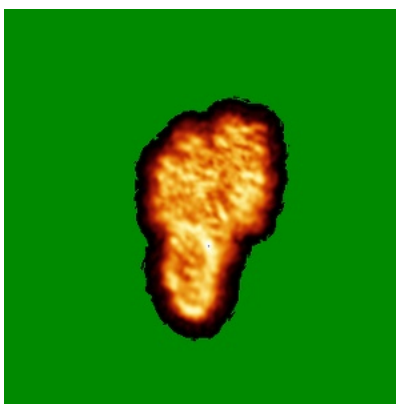
The images above show the largest variance slices of the map in three orthogonal directions.

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

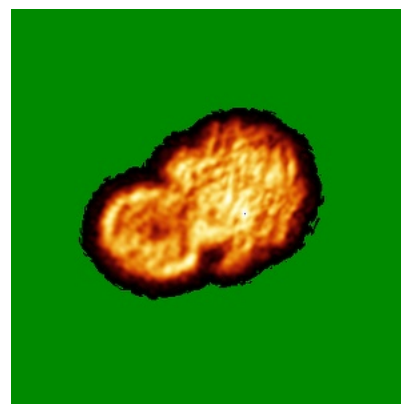
6.4.1 Primary map



X

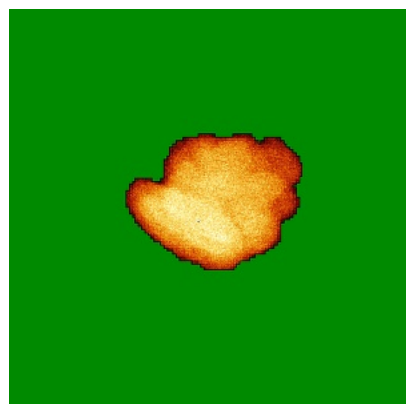


Y

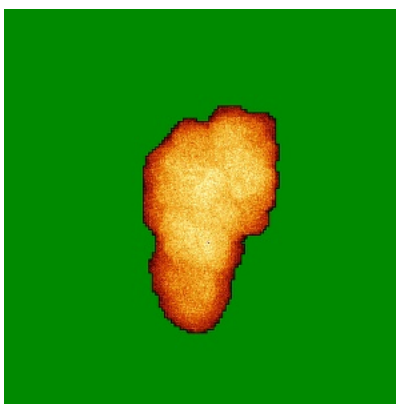


Z

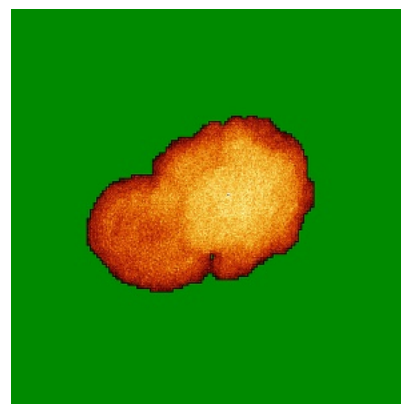
6.4.2 Raw map



X



Y

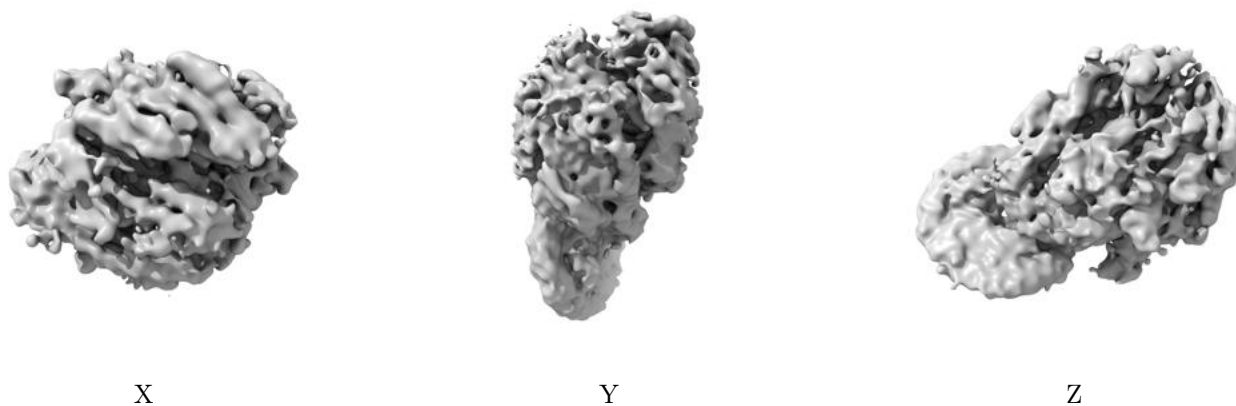


Z

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

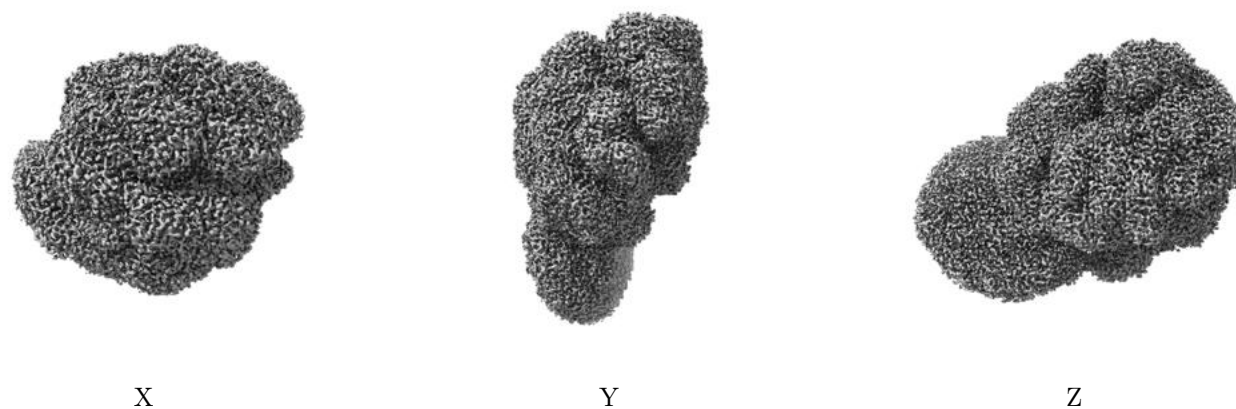
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

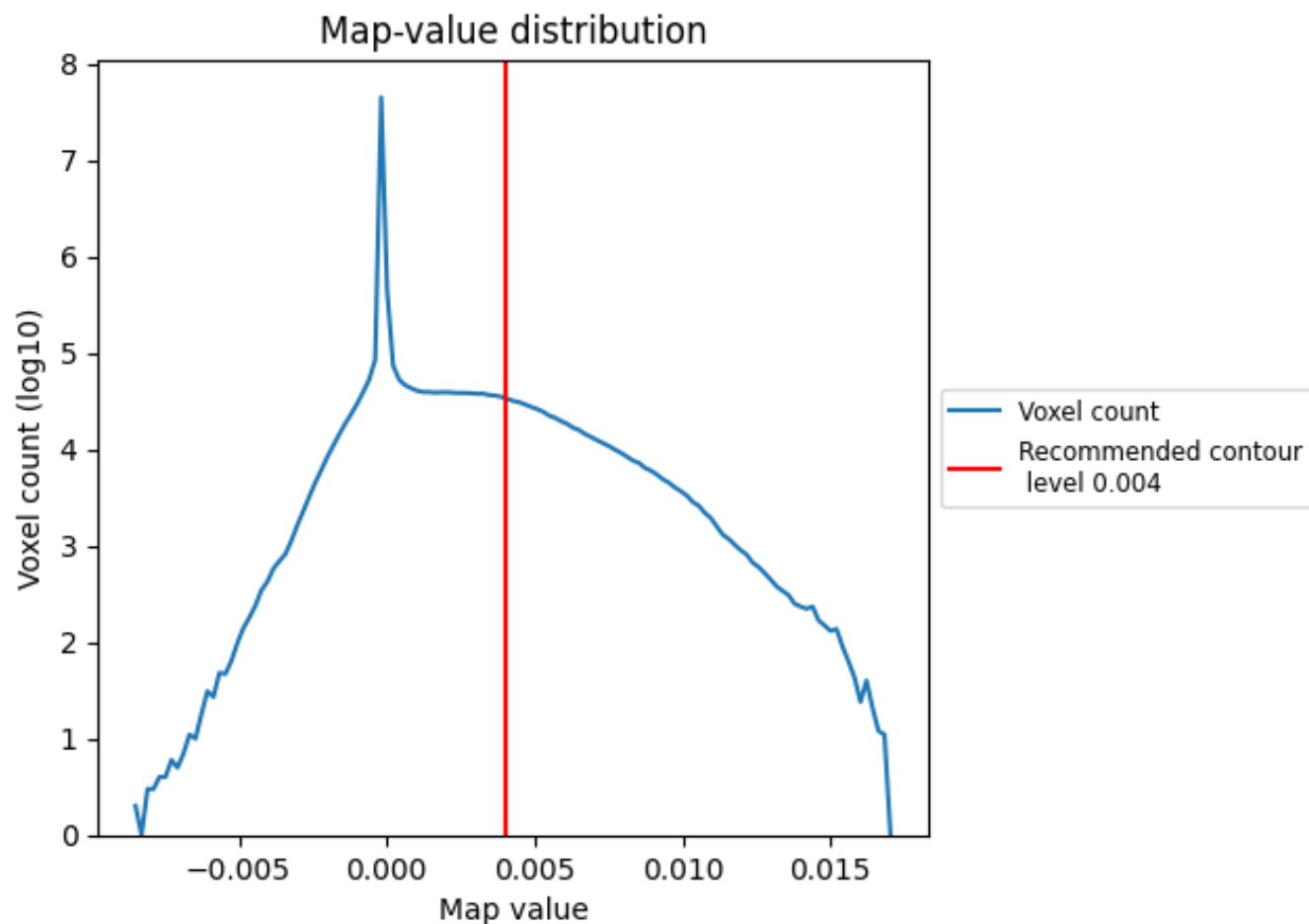
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

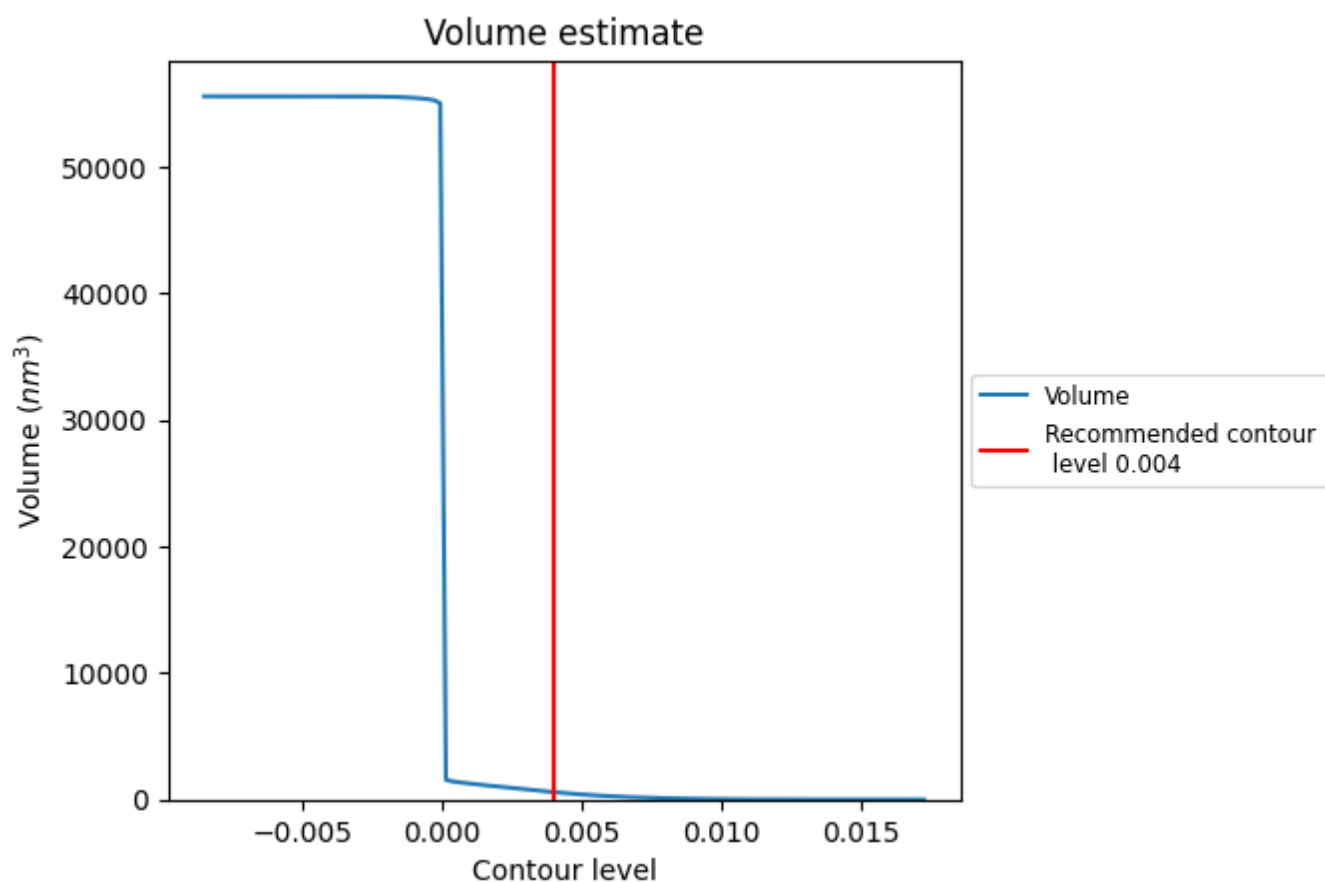
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

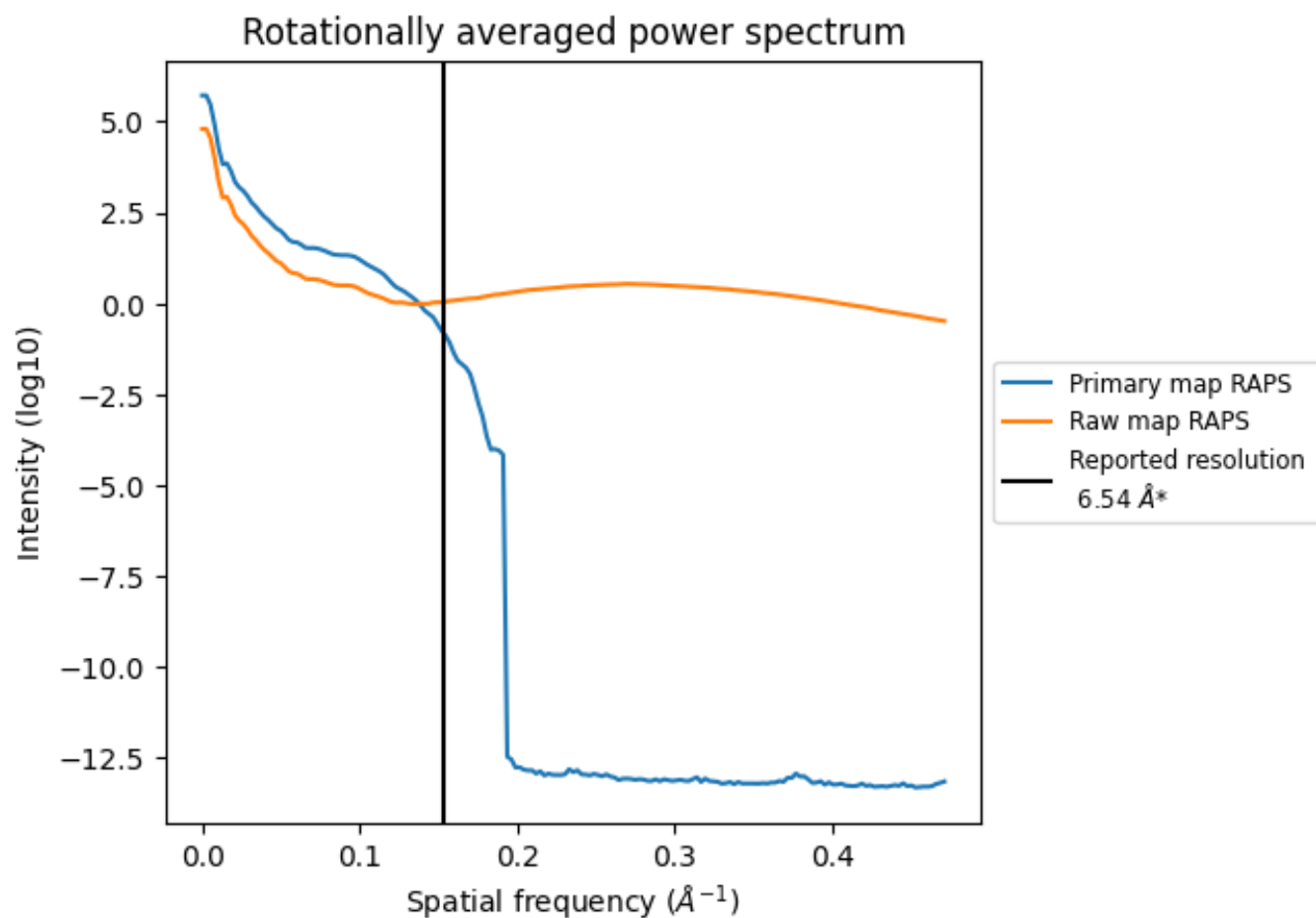
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 589 nm³; this corresponds to an approximate mass of 532 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 ⓘ

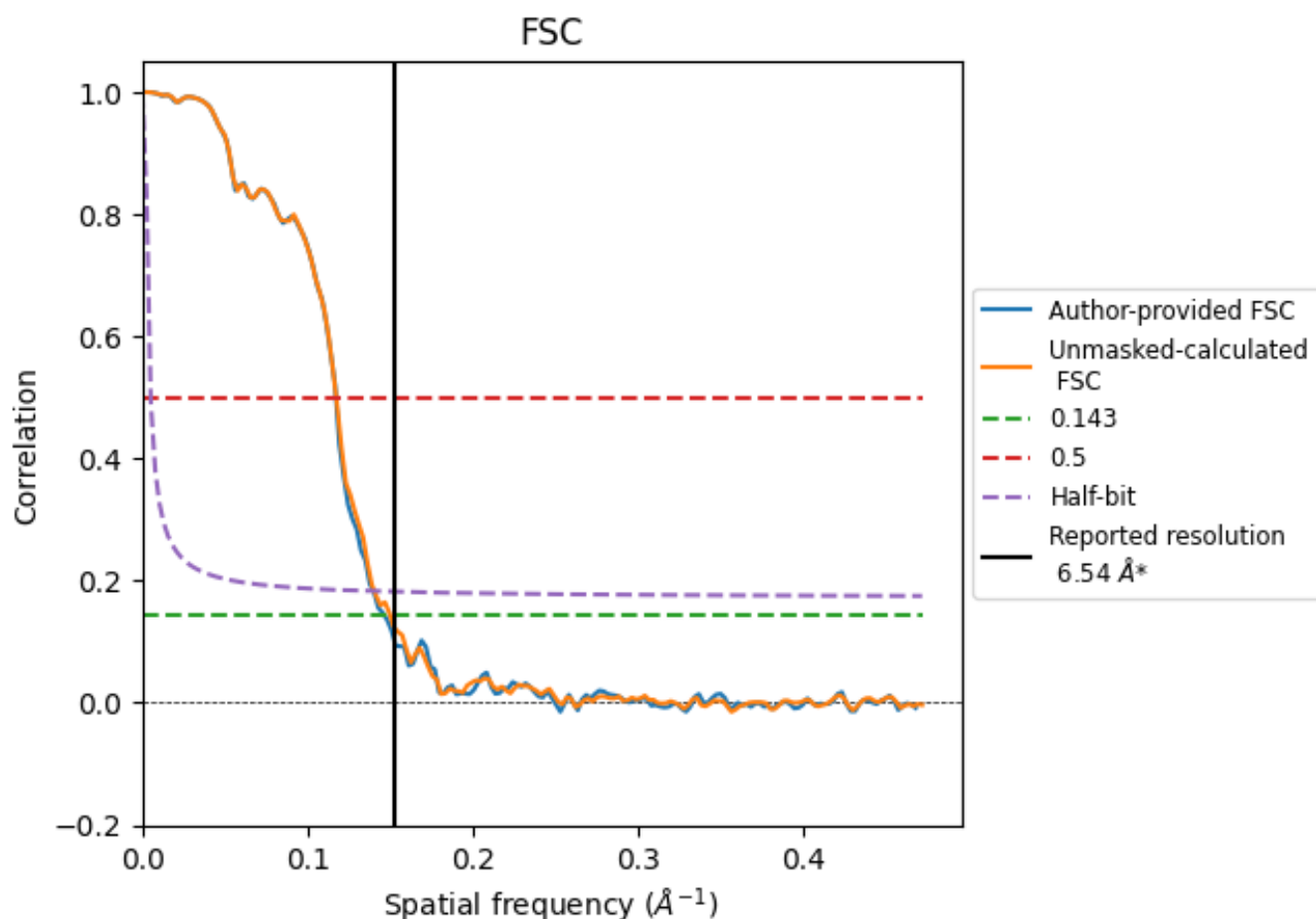


*Reported resolution corresponds to spatial frequency of 0.153 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.153 \AA^{-1}

8.2 Resolution estimates [i](#)

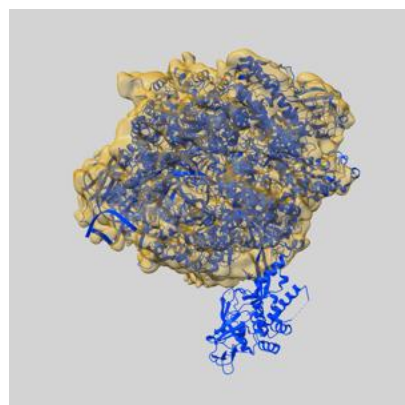
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.54	-	-
Author-provided FSC curve	6.83	8.53	7.15
Unmasked-calculated*	6.67	8.52	7.12

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

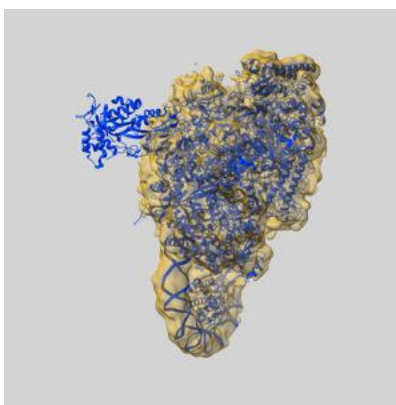
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64226 and PDB model 9UJT. Per-residue inclusion information can be found in section [3](#) on page [8](#).

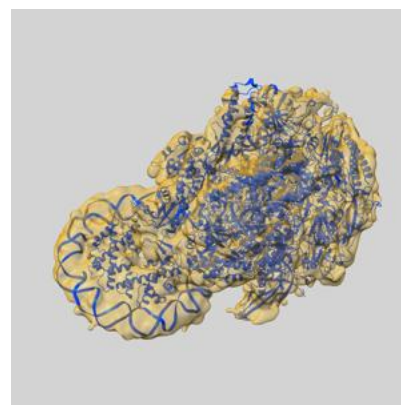
9.1 Map-model overlay [i](#)



X



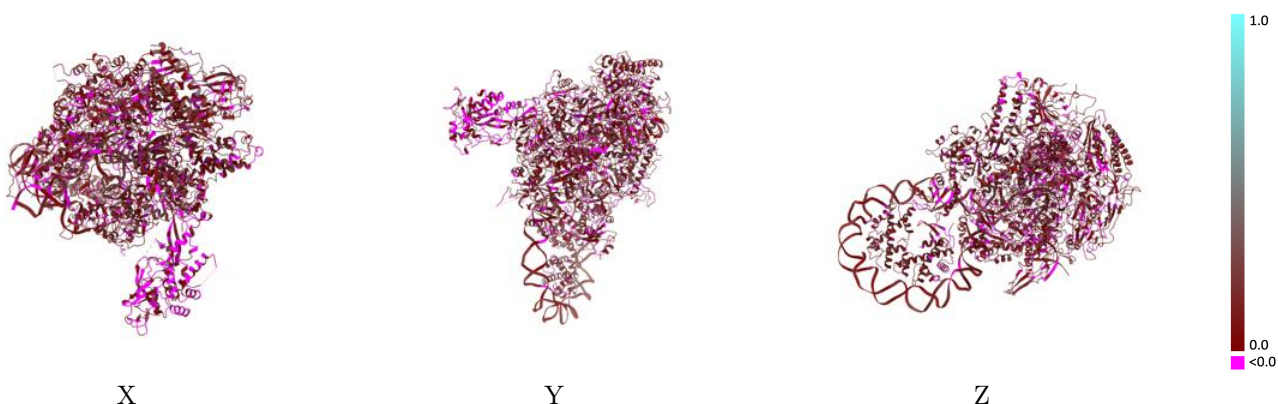
Y



Z

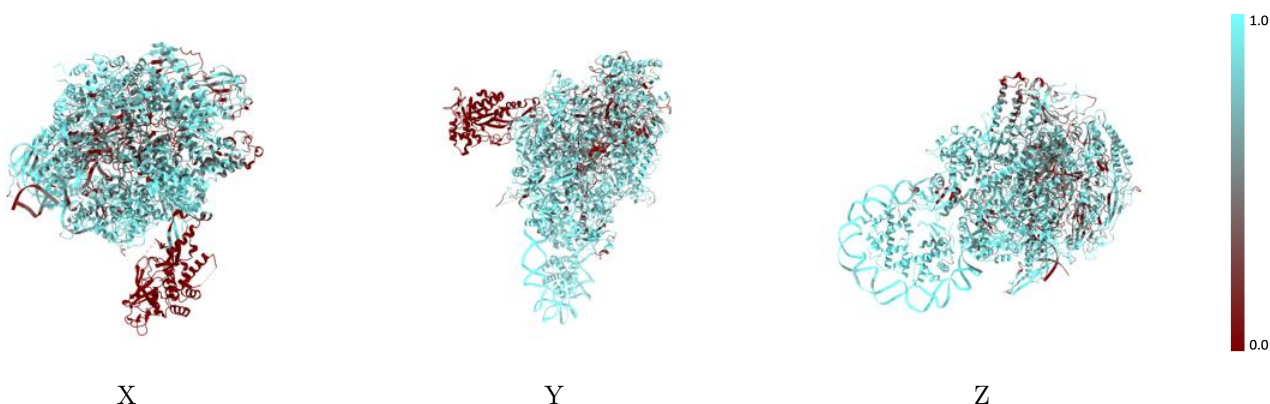
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



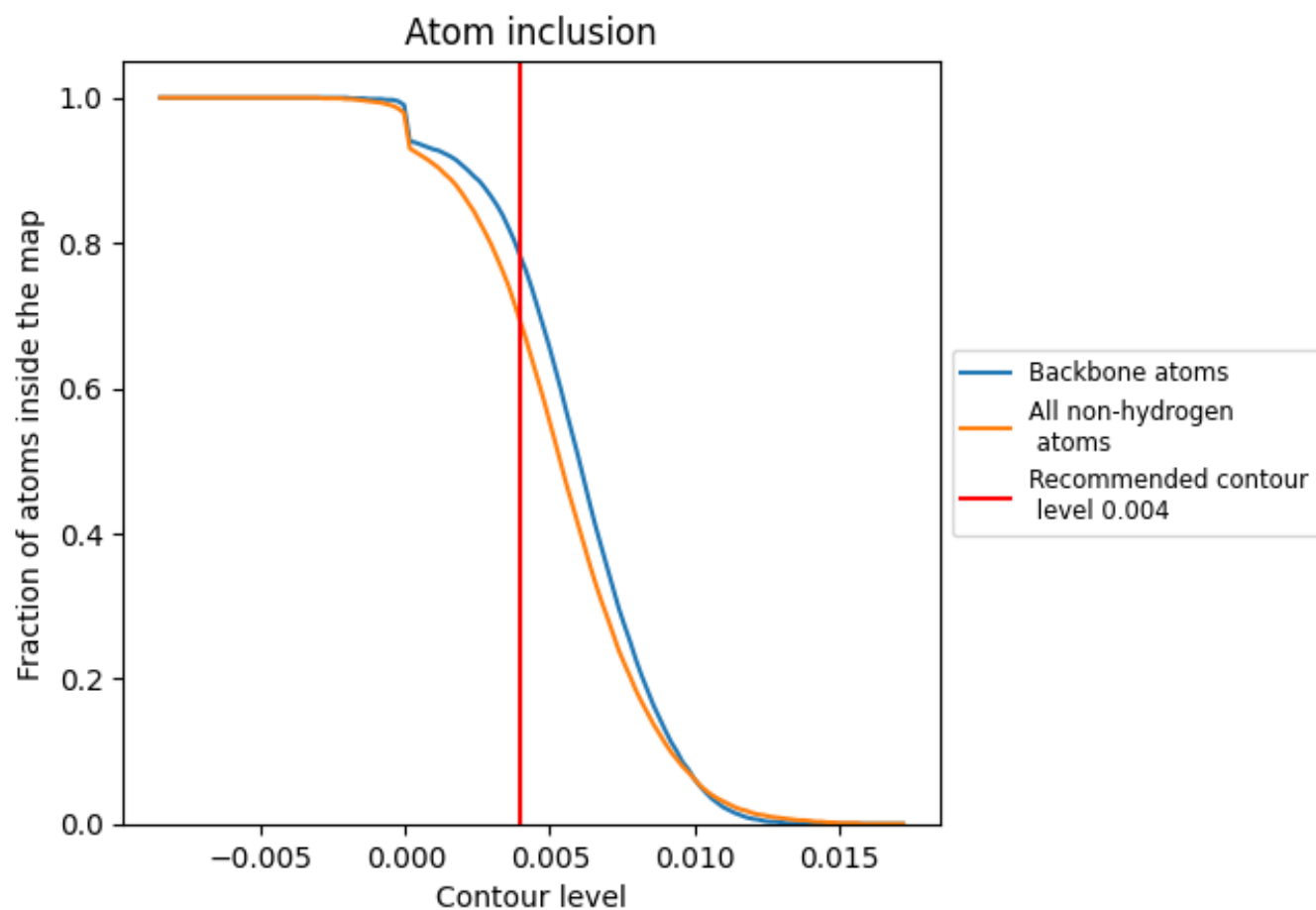
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).









































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 69% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6890	 0.1170
A	 0.6960	 0.1260
B	 0.6920	 0.1160
C	 0.6730	 0.1350
D	 0.0020	 -0.0040
E	 0.8660	 0.1470
F	 0.8920	 0.0950
G	 0.0850	 0.0050
H	 0.5560	 0.1340
I	 0.7370	 0.0740
J	 0.7180	 0.1160
K	 0.6460	 0.1170
L	 0.6740	 0.1360
N	 0.8640	 0.1210
P	 0.5560	 0.1900
T	 0.8360	 0.1450
e	 0.9430	 0.1420
f	 0.8910	 0.1330
g	 0.9440	 0.1370
h	 0.9470	 0.1390

