



Full wwPDB EM Validation Report ⓘ

Jun 8, 2025 – 01:22 AM JST

PDB ID : 9K3B / pdb_00009k3b
EMDB ID : EMD-62012
Title : Human RNA Polymerase III de novo transcribing complex 10 overall (TC10-overall)
Authors : Wang, Q.; Ren, Y.; Jin, Q.; Chen, X.; Xu, Y.
Deposited on : 2024-10-18
Resolution : 4.80 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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

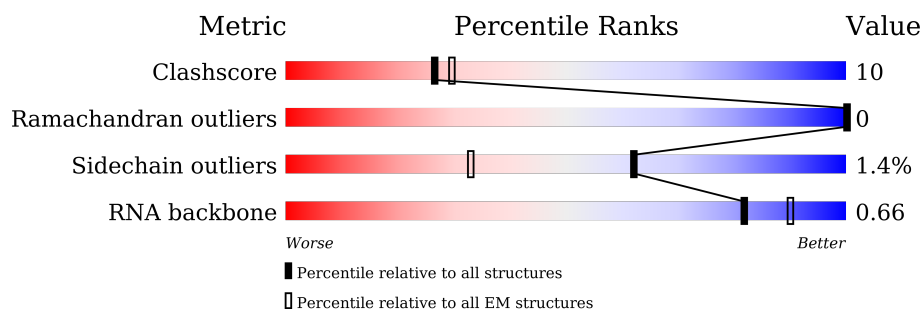
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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.
















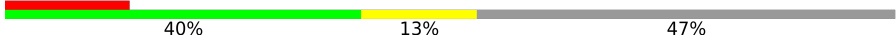

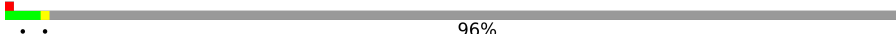
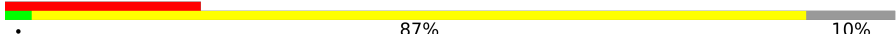
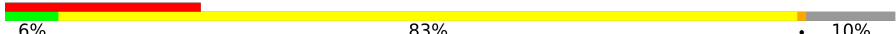
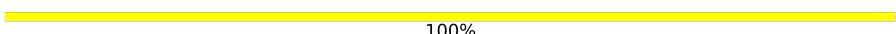
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1	368	<div> <div>40%</div> <div>29% 10% . 60%</div> </div>
2	3	411	<div> <div>91%</div> <div>76% 13% . 9%</div> </div>
3	4	1469	<div> <div>16%</div> <div>14% . 83%</div> </div>
4	A	1390	<div> <div>84% 15% .</div> </div>
5	B	1133	<div> <div>83% 14% .</div> </div>
6	C	346	<div> <div>81% 18% .</div> </div>
7	D	148	<div> <div>67% 16% 18%</div> </div>

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Mol	Chain	Length	Quality of chain
8	E	210	
9	F	127	
10	G	204	
11	H	150	
12	I	108	
13	J	67	
14	K	133	
15	L	58	
16	M	708	
17	N	398	
18	O	534	
19	P	316	
20	Q	223	
21	U	339	
22	V	419	
23	W	2624	
24	X	102	
25	Y	102	
26	Z	9	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	SF4	P	401	-	-	X	-

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 57378 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called snRNA-activating protein complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	146	Total	C	N	O	S	0	0
			1233	804	212	209	8		

- Molecule 2 is a protein called snRNA-activating protein complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	374	Total	C	N	O	S	0	0
			3038	1925	521	571	21		

- Molecule 3 is a protein called snRNA-activating protein complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	247	Total	C	N	O	S	0	0
			2066	1295	378	388	5		

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	1378	Total	C	N	O	S	0	0
			10814	6850	1886	2005	73		

- Molecule 5 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	1105	Total	C	N	O	S	0	0
			8736	5535	1529	1603	69		

- Molecule 6 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	343	Total	C	N	O	S	0	0
			2736	1723	488	514	11		

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	122	Total	C	N	O	S	0	0
			985	614	172	196	3		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	209	Total	C	N	O	S	0	0
			1715	1083	300	324	8		

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	76	Total	C	N	O	S	0	0
			610	392	103	110	5		

- Molecule 10 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	166	Total	C	N	O	S	0	0
			1337	876	211	245	5		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 12 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	54	Total	C	N	O	S	0	0
			426	267	79	74	6		

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	65	Total	C	N	O	S	0	0
			512	331	87	88	6		

- Molecule 14 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	103	Total	C	N	O	S	0	0
			822	513	145	157	7		

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	422	Total	C	N	O	S	0	0
			3382	2138	588	636	20		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	146	Total	C	N	O	S	0	0
			1128	710	191	221	6		

- Molecule 18 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	512	Total	C	N	O	S	0	0
			4075	2565	712	774	24		

- Molecule 19 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	303	Total	C	N	O	S	0	0
			2403	1516	411	460	16		

- Molecule 20 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	87	Total	C	N	O	S	0	0
			754	488	126	134	6		

- Molecule 21 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	178	Total	C	N	O	S	1	0
			1406	912	246	241	7		

- Molecule 22 is a protein called Transcription factor IIIB 50 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	335	Total	C	N	O	S	1	0
			2648	1670	472	483	23		

- Molecule 23 is a protein called Transcription factor TFIIB component B'' homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	111	Total	C	N	O	S	0	0
			943	606	163	170	4		

- Molecule 24 is a DNA chain called DNA (102-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	92	Total	C	N	O	P	0	0
			1887	904	338	553	92		

- Molecule 25 is a DNA chain called DNA (102-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	92	Total	C	N	O	P	0	0
			1885	903	339	551	92		

- Molecule 26 is a RNA chain called RNA (5'-R(P*UP*GP*CP*UP*CP*GP*CP*UP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	9	Total	C	N	O	P	0	0
			186	83	27	67	9		

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
27	A	2	Total	Zn	0
			2	2	
27	B	1	Total	Zn	0
			1	1	
27	I	1	Total	Zn	0
			1	1	

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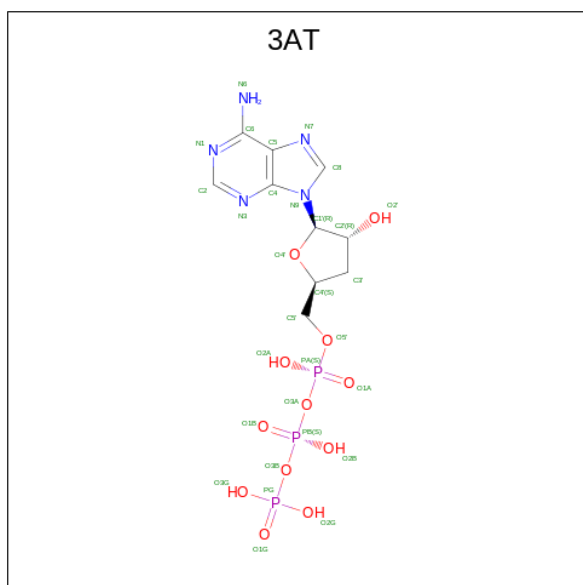
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Mol	Chain	Residues	Atoms		AltConf
27	J	1	Total	Zn	0
			1	1	
27	L	1	Total	Zn	0
			1	1	

- Molecule 28 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

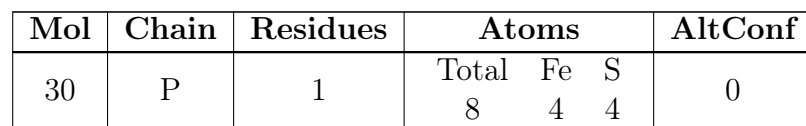
Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total	Mg	0
			1	1	

- Molecule 29 is 3'-DEOXYADENOSINE-5'-TRIPHOSPHATE (CCD ID: 3AT) (formula: C₁₀H₁₆N₅O₁₂P₃).



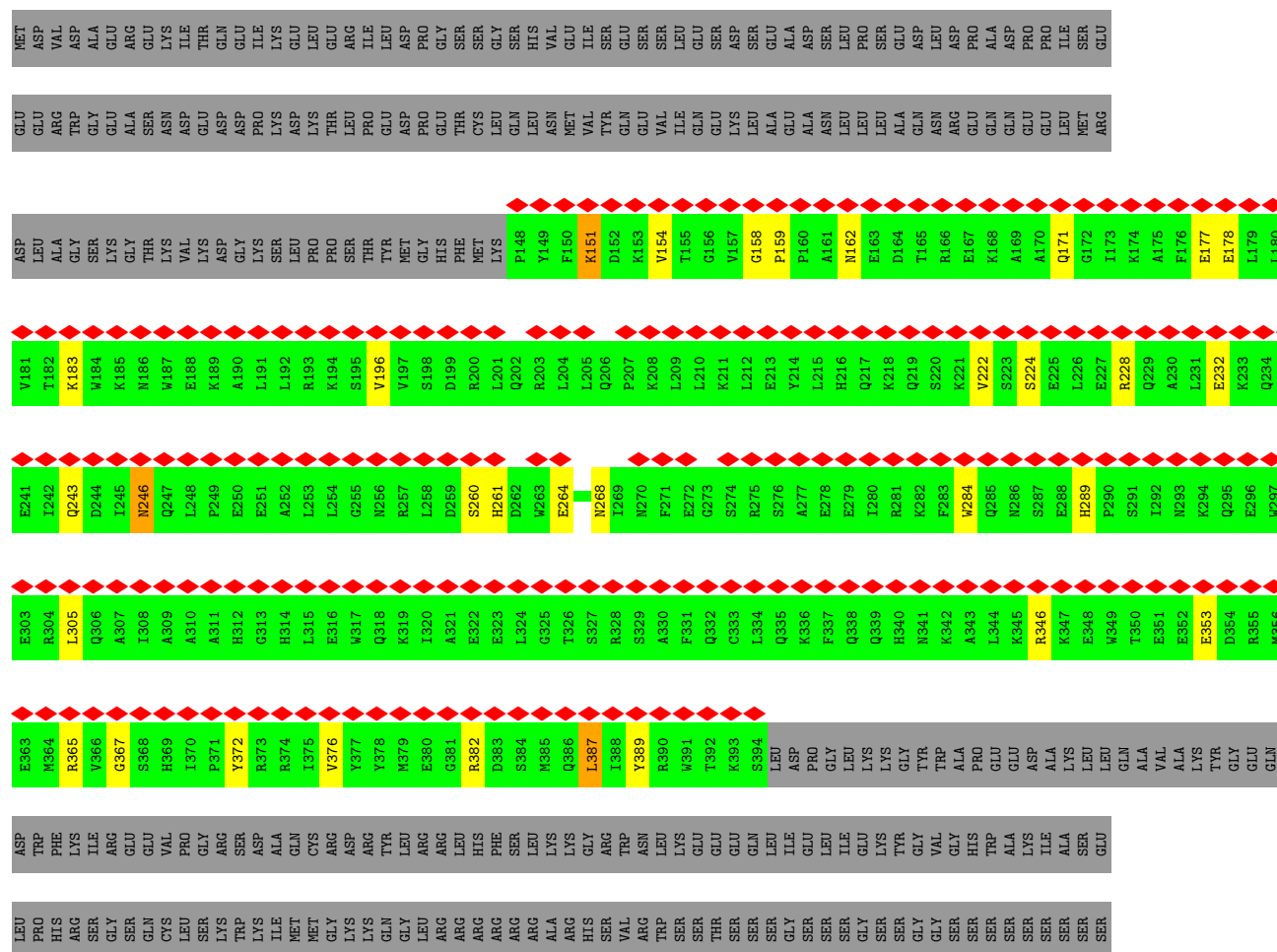
Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	N	O	P	0
			30	10	5	12	3	

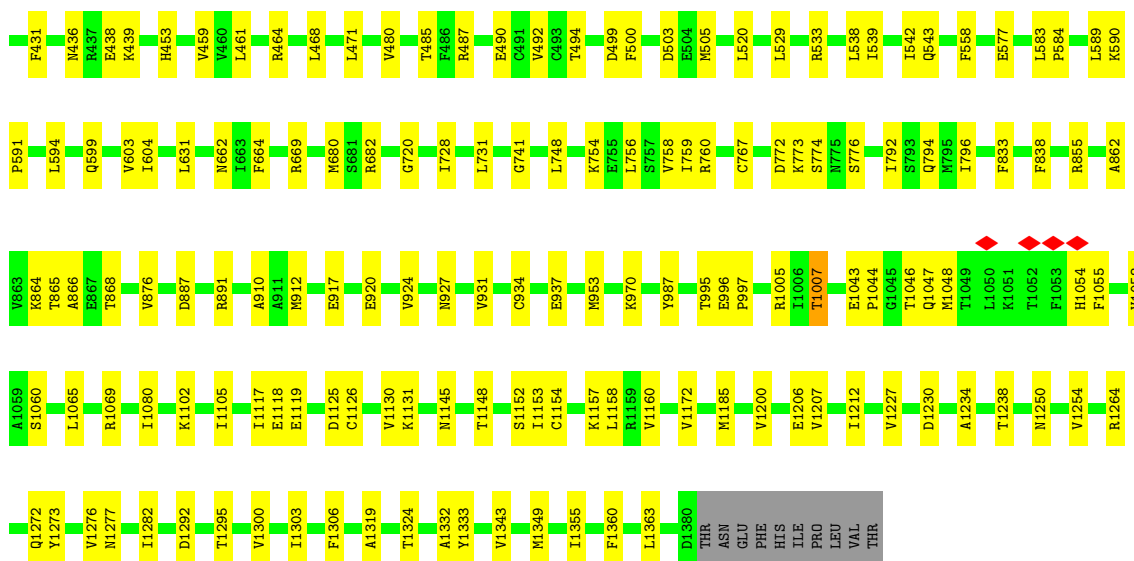
- Molecule 30 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



- # GTP

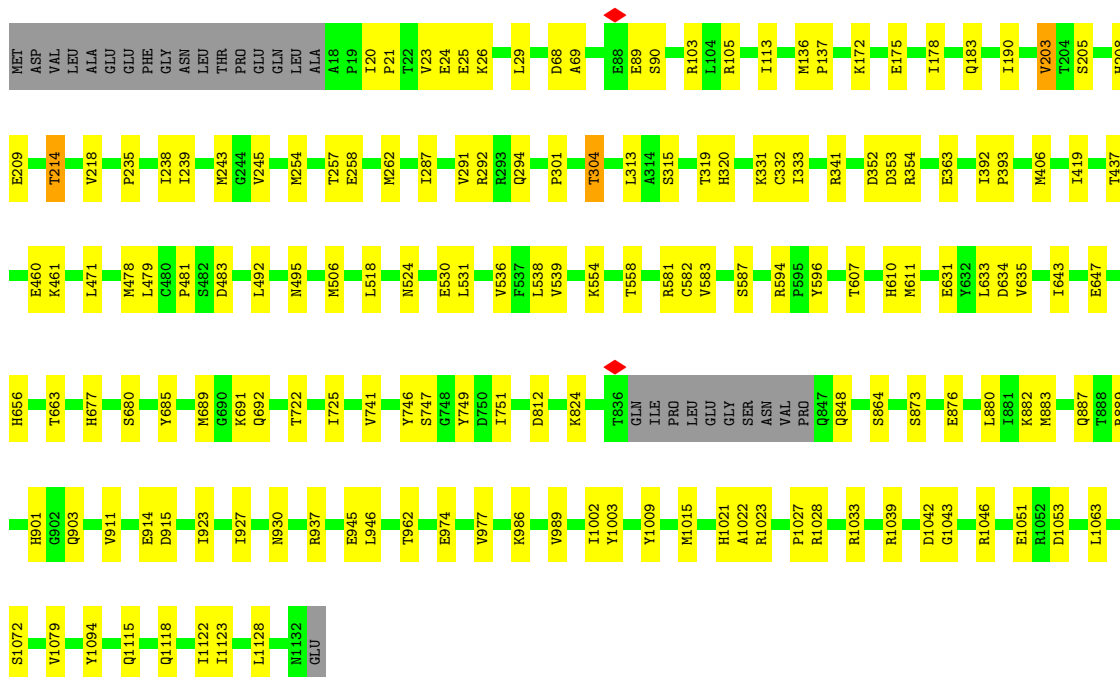
Mol	Chain	Residues	Atoms					AltConf
31	Z	1	Total	C	N	O	P	0
			32	10	5	14	3	





• Molecule 5: DNA-directed RNA polymerase III subunit RPC2

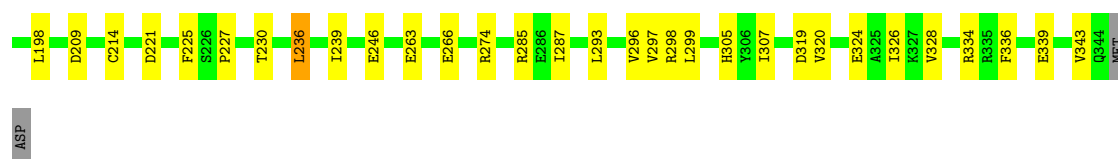
Chain B: 83% 14%



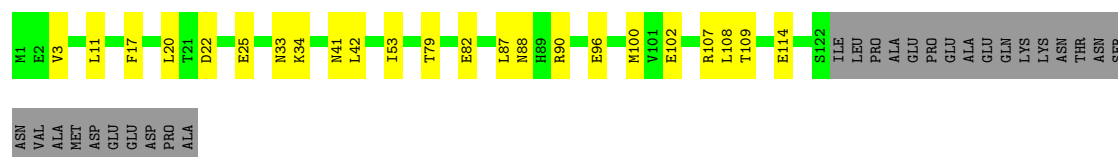
• Molecule 6: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C: 81% 18%

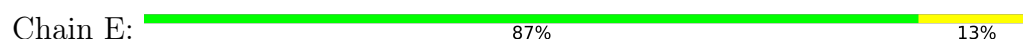




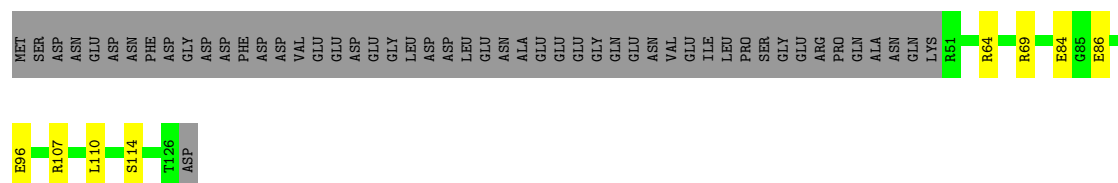
- Molecule 7: DNA-directed RNA polymerase III subunit RPC9



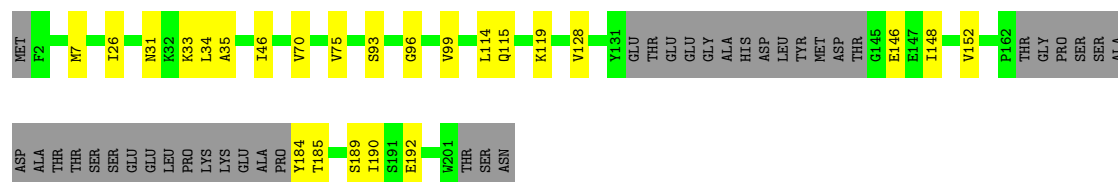
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC1



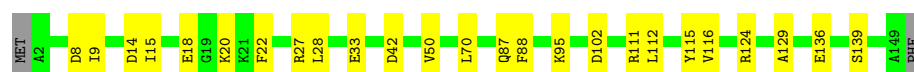
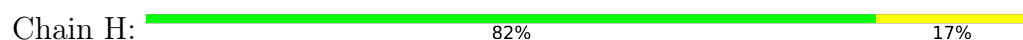
- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC2



- Molecule 10: DNA-directed RNA polymerase III subunit RPC8

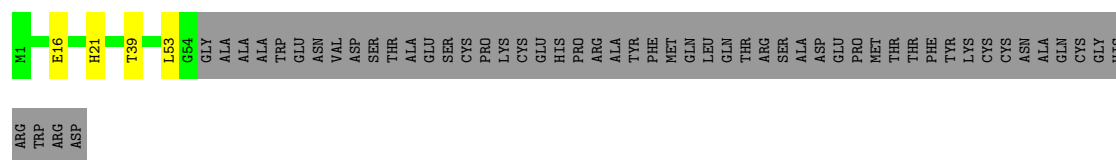


- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3




- Molecule 12: DNA-directed RNA polymerase III subunit RPC10

Chain I:  46% 50%



- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  76% 21%



- Molecule 14: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K:  68% 9% 23%



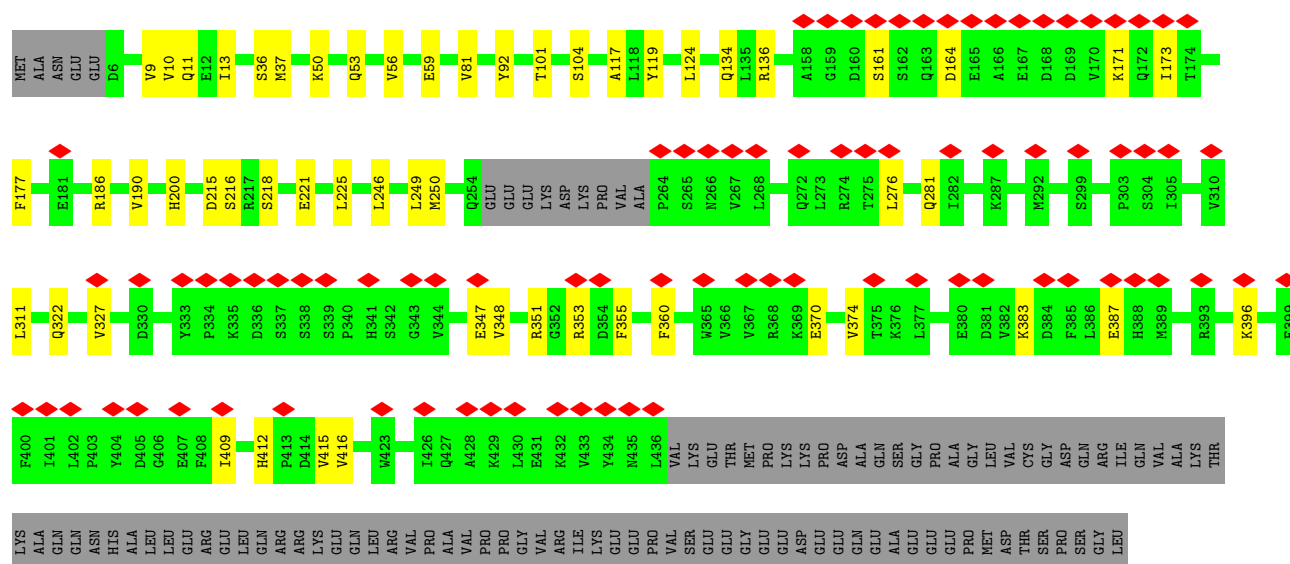
- Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:  66% 14% 21%

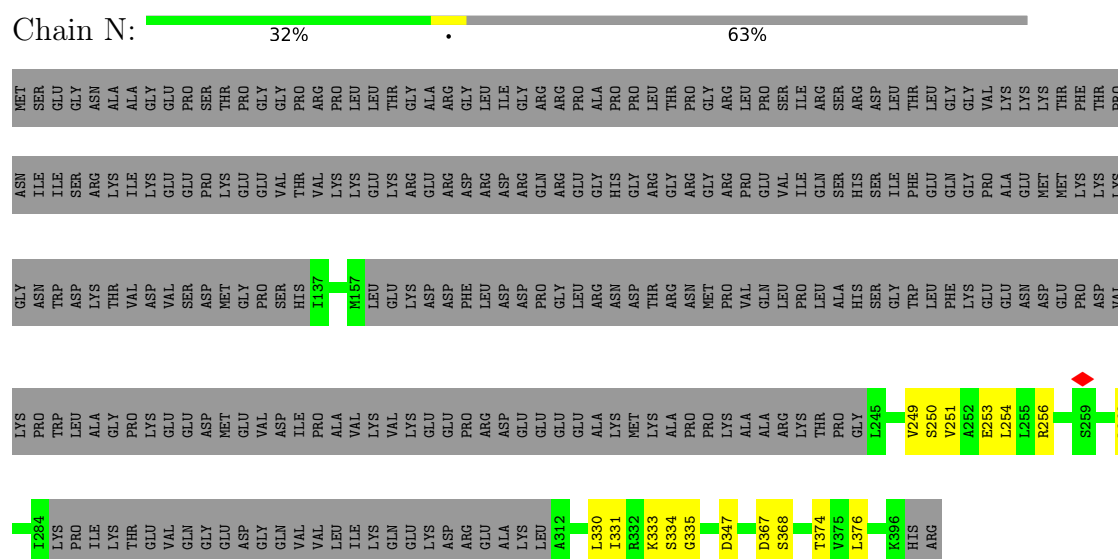


- Molecule 16: DNA-directed RNA polymerase III subunit RPC5

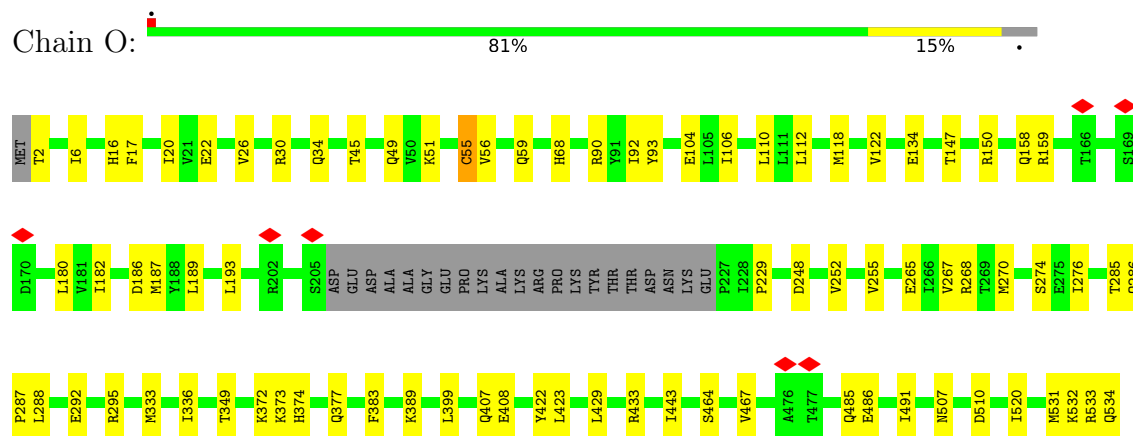
Chain M:  12% 52% 8% 40%



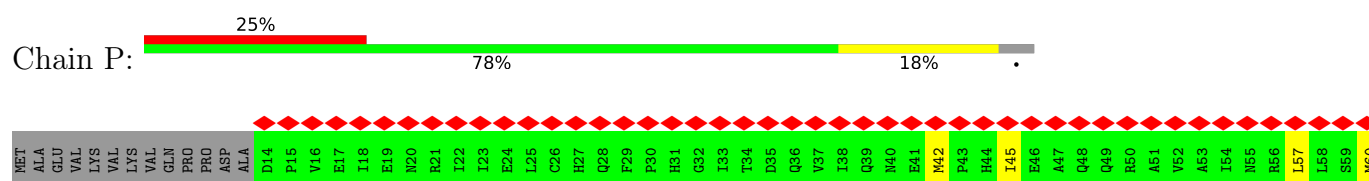
- Molecule 17: DNA-directed RNA polymerase III subunit RPC4

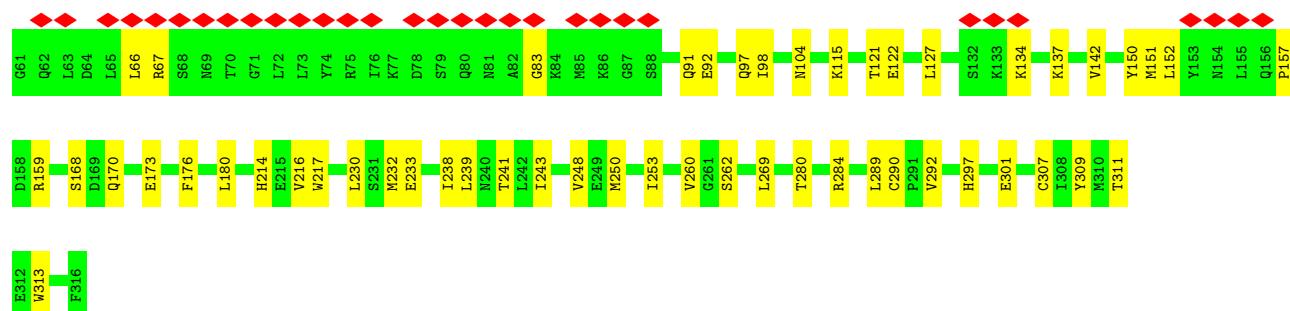


- Molecule 18: DNA-directed RNA polymerase III subunit RPC3

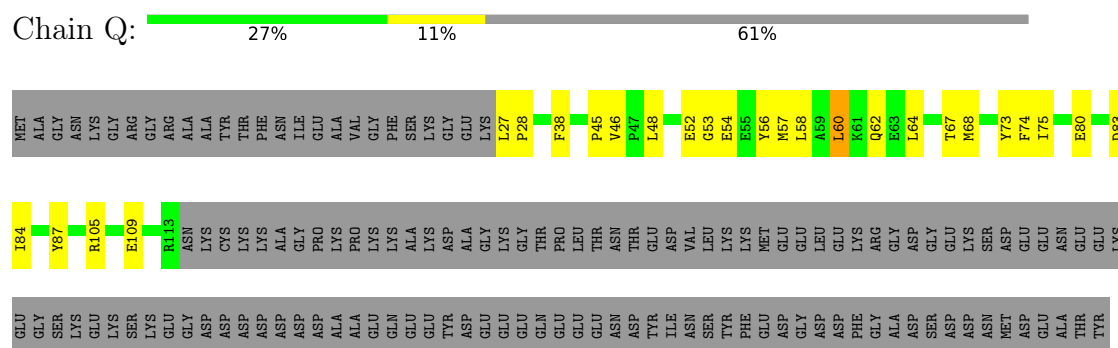


- Molecule 19: DNA-directed RNA polymerase III subunit RPC6

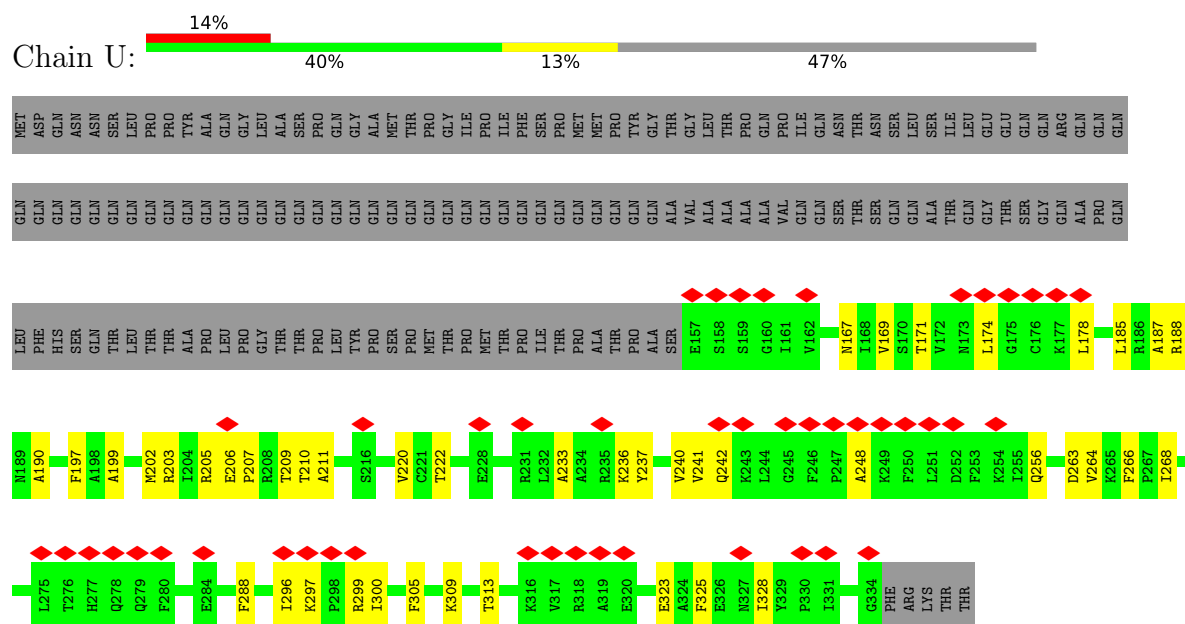




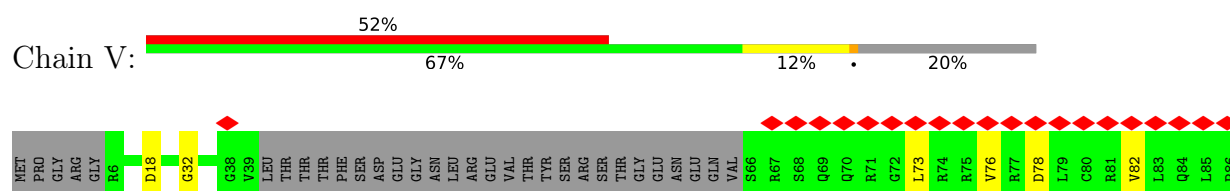
• Molecule 20: DNA-directed RNA polymerase III subunit RPC7



• Molecule 21: TATA-box-binding protein



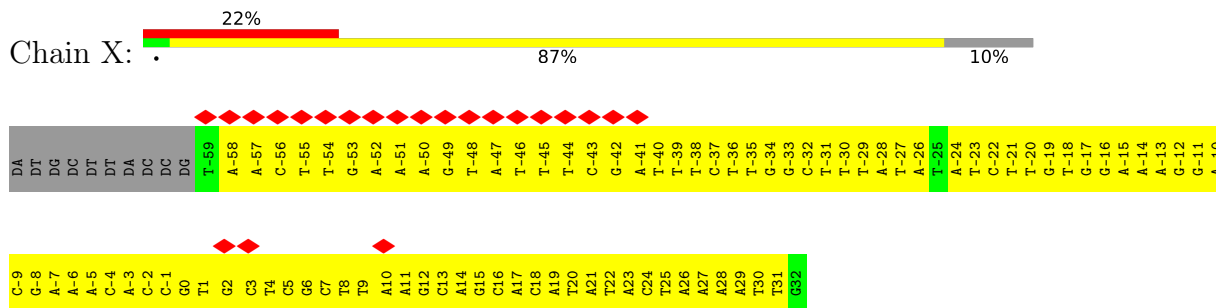
• Molecule 22: Transcription factor IIIB 50 kDa subunit



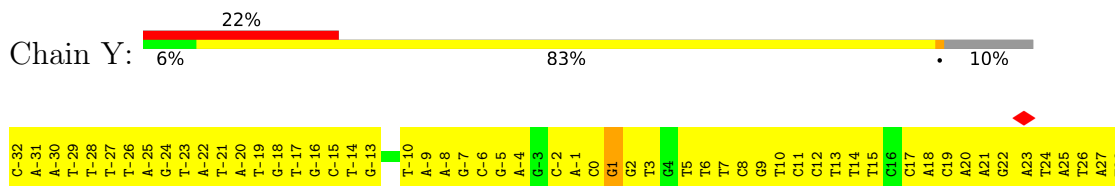


[illegible]

- Molecule 24: DNA (102-MER)

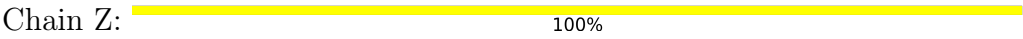


- Molecule 25: DNA (102-MER)





● Molecule 26: RNA (5'-R(P*UP*GP*CP*UP*CP*GP*CP*UP*U)-3')



U2
G3
C4
U5
C6
G7
C8
U9
U10

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	300	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.853	Depositor
Minimum map value	-2.113	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.073	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	426.88, 426.88, 426.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.334, 1.334, 1.334	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 3AT, ZN, MG, GTP

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	1	0.23	0/1266	0.52	2/1708 (0.1%)
2	3	0.21	0/3113	0.48	4/4206 (0.1%)
3	4	0.12	0/2107	0.29	0/2828
4	A	0.11	0/11008	0.24	0/14842
5	B	0.11	0/8905	0.25	0/12011
6	C	0.12	0/2790	0.25	0/3782
7	D	0.13	0/997	0.26	0/1343
8	E	0.12	0/1745	0.23	0/2358
9	F	0.13	0/620	0.23	0/839
10	G	0.13	0/1374	0.27	0/1868
11	H	0.12	0/1207	0.24	0/1628
12	I	0.14	0/434	0.26	0/584
13	J	0.13	0/521	0.24	0/703
14	K	0.13	0/837	0.29	1/1129 (0.1%)
15	L	0.15	0/394	0.28	0/524
16	M	0.11	0/3455	0.24	0/4673
17	N	0.12	0/1137	0.25	0/1530
18	O	0.12	0/4141	0.24	0/5592
19	P	0.12	0/2446	0.23	0/3301
20	Q	0.15	0/777	0.26	0/1050
21	U	0.20	0/1434	0.48	0/1931
22	V	0.13	0/2696	0.29	0/3657
23	W	0.14	0/967	0.30	0/1293
24	X	0.19	0/2116	0.35	0/3264
25	Y	0.28	1/2114 (0.0%)	0.37	0/3260
26	Z	0.07	0/205	0.15	0/316
All	All	0.14	1/58806 (0.0%)	0.29	7/80220 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	1	DG	O3'-P	-8.70	1.48	1.61

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	202	GLN	N-CA-C	10.77	124.24	110.24
2	3	201	TYR	N-CA-C	7.64	120.35	108.96
2	3	200	PRO	N-CA-C	6.25	121.78	113.40
1	1	67	LEU	CA-C-N	-5.81	115.48	119.66
1	1	67	LEU	C-N-CA	-5.81	115.48	119.66
2	3	340	TYR	N-CA-C	-5.44	97.78	109.81
14	K	93	VAL	N-CA-C	-5.07	107.80	111.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1233	0	1231	21	0
2	3	3038	0	2911	38	0
3	4	2066	0	2049	19	0
4	A	10814	0	11059	222	0
5	B	8736	0	8861	109	0
6	C	2736	0	2712	46	0
7	D	985	0	1006	17	0
8	E	1715	0	1733	18	0
9	F	610	0	642	6	0
10	G	1337	0	1306	19	0
11	H	1186	0	1147	18	0
12	I	426	0	428	3	0
13	J	512	0	525	9	0
14	K	822	0	810	12	0
15	L	388	0	393	6	0
16	M	3382	0	3376	63	0
17	N	1128	0	1181	15	0
18	O	4075	0	4149	138	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	P	2403	0	2408	64	0
20	Q	754	0	759	49	0
21	U	1406	0	1496	34	0
22	V	2648	0	2705	38	0
23	W	943	0	924	19	0
24	X	1887	0	1043	193	0
25	Y	1885	0	1042	194	0
26	Z	186	0	96	16	0
27	A	2	0	0	0	0
27	B	1	0	0	0	0
27	I	1	0	0	0	0
27	J	1	0	0	0	0
27	L	1	0	0	0	0
28	A	1	0	0	0	0
29	B	30	0	12	7	0
30	P	8	0	0	3	0
31	Z	32	0	11	1	0
All	All	57378	0	56015	1113	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 10.

All (1113) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:303:THR:OG1	18:O:377:GLN:NE2	1.62	1.30
16:M:177:PHE:CE2	19:P:98:ILE:HD12	1.76	1.20
25:Y:23:DA:H2''	25:Y:24:DT:H5''	1.34	1.06
4:A:196:SER:HB2	18:O:373:LYS:CB	1.85	1.05
21:U:167:ASN:ND2	25:Y:27:DA:C2	2.25	1.04
24:X:10:DA:H5'	24:X:11:DA:H5''	1.40	1.04
4:A:159:CYS:HB2	18:O:531:MET:HG2	1.39	1.04
25:Y:36:DA:H2''	25:Y:37:DG:H5''	1.40	1.02
4:A:130:LYS:CE	18:O:34:GLN:NE2	2.22	1.02
4:A:130:LYS:HE2	18:O:34:GLN:NE2	1.77	0.99
4:A:203:HIS:NE2	18:O:383:PHE:CZ	2.31	0.98
22:V:76:VAL:HG22	22:V:118:VAL:HG13	1.45	0.98
4:A:230:ILE:O	18:O:2:THR:N	1.99	0.96
25:Y:1:DG:H2''	25:Y:2:DG:H5'	1.47	0.94
16:M:171:LYS:HZ3	19:P:67:ARG:HD2	1.32	0.94
4:A:232:ALA:HB3	18:O:6:ILE:HD11	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:171:LYS:NZ	19:P:67:ARG:HD2	1.83	0.94
16:M:171:LYS:HG3	19:P:67:ARG:HD3	1.47	0.94
24:X:3:DC:H2''	24:X:4:DT:H4'	1.49	0.92
16:M:171:LYS:HZ3	19:P:67:ARG:CD	1.83	0.91
4:A:203:HIS:HE2	18:O:383:PHE:HZ	1.02	0.91
16:M:171:LYS:NZ	19:P:67:ARG:HB2	1.87	0.90
4:A:203:HIS:NE2	18:O:383:PHE:HZ	1.69	0.89
24:X:7:DC:H2''	24:X:8:DT:H5''	1.53	0.89
4:A:196:SER:O	18:O:373:LYS:HB2	1.72	0.89
25:Y:39:DA:H1'	25:Y:40:DA:H5'	1.56	0.88
4:A:231:PRO:HA	18:O:2:THR:OG1	1.74	0.88
4:A:197:PHE:CE2	18:O:374:HIS:CD2	2.60	0.88
22:V:73:LEU:HD11	22:V:94:VAL:HG23	1.54	0.88
4:A:197:PHE:CZ	18:O:374:HIS:NE2	2.42	0.88
24:X:-43:DC:O2	25:Y:43:DG:N2	2.07	0.86
4:A:111:THR:HG23	18:O:429:LEU:CD2	2.06	0.85
4:A:199:THR:OG1	18:O:372:LYS:HD2	1.76	0.85
24:X:-28:DA:C8	24:X:-27:DT:H72	2.12	0.85
4:A:196:SER:HB2	18:O:373:LYS:HB3	1.56	0.84
25:Y:18:DA:H2''	25:Y:19:DC:H5'	1.59	0.84
16:M:177:PHE:HE1	19:P:97:GLN:HB3	1.42	0.84
4:A:196:SER:HB2	18:O:373:LYS:CG	2.07	0.84
25:Y:17:DC:H5''	25:Y:17:DC:H6	1.43	0.83
24:X:-16:DG:H2''	24:X:-15:DA:H5'	1.61	0.82
24:X:-43:DC:N3	25:Y:43:DG:N1	2.27	0.82
4:A:111:THR:HG23	18:O:429:LEU:HD22	1.62	0.82
24:X:7:DC:H2'	24:X:8:DT:H72	1.60	0.81
4:A:196:SER:HB2	18:O:373:LYS:HG3	1.63	0.81
4:A:197:PHE:CZ	18:O:374:HIS:CD2	2.69	0.81
21:U:167:ASN:ND2	25:Y:27:DA:N3	2.28	0.81
21:U:171:THR:HG22	21:U:220:VAL:HG22	1.63	0.80
25:Y:25:DA:H2''	25:Y:26:DT:H5'	1.63	0.80
4:A:130:LYS:CE	18:O:34:GLN:HE21	1.87	0.80
4:A:203:HIS:CE1	18:O:383:PHE:CZ	2.70	0.79
24:X:-28:DA:C8	24:X:-27:DT:C7	2.65	0.79
4:A:130:LYS:HE2	18:O:34:GLN:HE21	1.40	0.79
22:V:267:GLN:NE2	24:X:-38:DT:OP1	2.16	0.79
5:B:172:LYS:NZ	25:Y:-1:DA:OP2	2.16	0.79
24:X:-35:DT:H2'	24:X:-34:DG:C8	2.17	0.79
16:M:171:LYS:HZ3	19:P:67:ARG:CB	1.96	0.78
24:X:-40:DT:H2'	24:X:-39:DT:H71	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:299:TYR:OH	25:Y:36:DA:O4'	2.00	0.78
25:Y:57:DT:H2'	25:Y:58:DT:C7	2.13	0.78
24:X:-28:DA:H8	24:X:-27:DT:H72	1.46	0.78
19:P:284:ARG:HD3	20:Q:48:LEU:HA	1.65	0.78
25:Y:21:DA:H2''	25:Y:22:DG:N7	2.00	0.78
25:Y:49:DC:H2'	25:Y:50:DT:H71	1.64	0.77
4:A:232:ALA:HB3	18:O:6:ILE:CD1	2.14	0.77
25:Y:-1:DA:H2''	25:Y:0:DC:H5''	1.67	0.77
25:Y:10:DT:H2''	25:Y:11:DC:C5	2.19	0.77
21:U:167:ASN:HD22	25:Y:27:DA:H2	1.26	0.77
24:X:-24:DA:H2''	24:X:-23:DT:H71	1.66	0.77
25:Y:-29:DT:H2''	25:Y:-28:DT:H71	1.65	0.77
24:X:16:DC:H2'	24:X:17:DA:C8	2.19	0.76
16:M:177:PHE:CE1	19:P:98:ILE:HG13	2.19	0.76
4:A:159:CYS:HA	18:O:531:MET:SD	2.25	0.76
24:X:-46:DT:H2''	24:X:-45:DT:H71	1.67	0.76
4:A:123:LYS:HD2	18:O:68:HIS:CD2	2.21	0.76
2:3:193:HIS:CE1	24:X:-51:DA:H2''	2.21	0.75
25:Y:11:DC:H2''	25:Y:12:DC:C5	2.21	0.75
24:X:-39:DT:H2'	24:X:-38:DT:H71	1.67	0.75
25:Y:-23:DT:H1'	25:Y:-22:DA:H5'	1.67	0.75
16:M:36:SER:OG	16:M:37:MET:SD	2.43	0.75
4:A:159:CYS:HB2	18:O:531:MET:CG	2.16	0.75
10:G:148:ILE:HG23	10:G:190:ILE:HG23	1.69	0.75
4:A:196:SER:CB	18:O:373:LYS:HG3	2.16	0.75
25:Y:55:DA:H2''	25:Y:56:DG:C8	2.21	0.75
4:A:374:ASN:ND2	5:B:749:TYR:OH	2.20	0.75
8:E:95:GLN:OE1	8:E:125:TYR:OH	2.03	0.75
25:Y:56:DG:C2'	25:Y:57:DT:H71	2.17	0.74
4:A:159:CYS:CB	18:O:531:MET:SD	2.75	0.74
16:M:171:LYS:HZ3	19:P:67:ARG:HB2	1.50	0.74
5:B:1023:ARG:NH1	5:B:1042:ASP:O	2.20	0.74
23:W:379:GLU:OE2	23:W:383:GLN:NE2	2.20	0.74
16:M:177:PHE:CE2	19:P:98:ILE:CD1	2.65	0.74
19:P:137:LYS:NZ	19:P:152:LEU:O	2.20	0.74
22:V:110:ARG:NE	25:Y:22:DG:H5'	2.02	0.74
25:Y:1:DG:H2''	25:Y:2:DG:OP2	1.87	0.74
25:Y:37:DG:H2''	25:Y:38:DA:C8	2.22	0.74
30:P:401:SF4:S3	20:Q:38:PHE:HE2	2.11	0.73
22:V:202:SER:O	22:V:206:GLN:NE2	2.21	0.73
4:A:485:THR:OG1	4:A:487:ARG:NH1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:-49:DG:H2''	24:X:-48:DT:C5	2.24	0.73
4:A:464:ARG:NH1	29:B:1202:3AT:O2'	2.22	0.73
4:A:855:ARG:NH2	5:B:481:PRO:O	2.22	0.73
19:P:290:CYS:SG	30:P:401:SF4:S4	2.87	0.73
5:B:89:GLU:OE2	15:L:42:ARG:NE	2.21	0.73
25:Y:20:DA:H2'	25:Y:21:DA:C8	2.24	0.73
4:A:760:ARG:NH2	4:A:794:GLN:OE1	2.22	0.73
18:O:20:ILE:HD11	20:Q:75:ILE:HG13	1.69	0.73
25:Y:28:DT:OP2	25:Y:28:DT:H3'	1.87	0.73
7:D:96:GLU:HA	7:D:100:MET:HE2	1.70	0.73
24:X:-36:DT:H2'	24:X:-35:DT:C6	2.24	0.73
24:X:6:DG:C1'	24:X:7:DC:H5''	2.18	0.73
25:Y:-25:DA:H2''	25:Y:-24:DG:C8	2.24	0.73
19:P:216:VAL:HG21	19:P:239:LEU:HD11	1.69	0.72
25:Y:47:DT:H2''	25:Y:48:DA:C8	2.24	0.72
4:A:160:GLY:HA3	18:O:532:LYS:HE2	1.71	0.72
4:A:995:THR:HG22	4:A:997:PRO:HD2	1.71	0.72
5:B:301:PRO:O	5:B:304:THR:OG1	2.08	0.72
24:X:-14:DA:H2''	24:X:-13:DA:N7	2.03	0.72
25:Y:50:DT:C2'	25:Y:51:DT:H71	2.19	0.72
24:X:17:DA:H4'	24:X:18:DC:OP1	1.90	0.72
25:Y:57:DT:H2'	25:Y:58:DT:H71	1.70	0.72
25:Y:41:DT:H2''	25:Y:42:DC:C5	2.25	0.72
16:M:177:PHE:CD2	19:P:98:ILE:HD12	2.24	0.71
24:X:26:DA:H2''	24:X:27:DA:C8	2.25	0.71
24:X:27:DA:H2''	24:X:28:DA:C8	2.25	0.71
26:Z:3:G:H2'	26:Z:4:C:C6	2.26	0.71
4:A:282:LYS:NZ	4:A:316:GLN:OE1	2.18	0.71
16:M:177:PHE:CZ	19:P:98:ILE:CG1	2.74	0.71
18:O:104:GLU:OE2	20:Q:56:TYR:OH	2.09	0.71
19:P:232:MET:SD	19:P:262:SER:OG	2.47	0.71
7:D:41:ASN:ND2	10:G:35:ALA:O	2.24	0.71
24:X:-53:DG:C6	25:Y:54:DA:N6	2.59	0.71
25:Y:-22:DA:H2'	25:Y:-21:DT:H71	1.72	0.71
25:Y:50:DT:H2''	25:Y:51:DT:H71	1.70	0.71
4:A:159:CYS:HA	18:O:531:MET:HB3	1.73	0.71
24:X:-29:DT:H2'	24:X:-28:DA:C4	2.26	0.71
24:X:6:DG:H4'	24:X:7:DC:OP1	1.90	0.71
2:3:193:HIS:NE2	24:X:-50:DA:O5'	2.24	0.71
4:A:155:ILE:HD12	18:O:534:GLN:NE2	2.06	0.71
2:3:247:TYR:OH	3:4:171:GLN:NE2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:151:LYS:NZ	3:4:154:VAL:O	2.21	0.70
4:A:130:LYS:HE3	18:O:34:GLN:NE2	2.05	0.70
18:O:112:LEU:HD11	20:Q:64:LEU:HD22	1.72	0.70
25:Y:49:DC:C2'	25:Y:50:DT:H71	2.21	0.70
5:B:313:LEU:O	5:B:331:LYS:NZ	2.21	0.70
16:M:177:PHE:CZ	19:P:98:ILE:HG13	2.26	0.70
26:Z:2:U:OP1	31:Z:101:GTP:O3'	2.07	0.70
4:A:1273:TYR:O	4:A:1277:ASN:ND2	2.25	0.70
24:X:-9:DC:H2''	24:X:-8:DG:C8	2.27	0.70
4:A:159:CYS:CB	18:O:531:MET:HG2	2.20	0.70
7:D:108:LEU:O	7:D:109:THR:OG1	2.08	0.70
24:X:25:DT:H2''	24:X:26:DA:C8	2.27	0.70
5:B:1039:ARG:N	25:Y:-6:DC:OP1	2.25	0.70
18:O:20:ILE:HD11	20:Q:75:ILE:CG1	2.21	0.70
24:X:9:DT:H2''	24:X:10:DA:H4'	1.73	0.69
25:Y:25:DA:H2'	25:Y:26:DT:H71	1.74	0.69
19:P:122:GLU:OE1	19:P:122:GLU:N	2.26	0.69
25:Y:17:DC:H2'	25:Y:18:DA:C8	2.28	0.69
24:X:15:DG:H1	25:Y:-15:DC:H5	1.41	0.69
24:X:30:DT:H2''	24:X:31:DT:C5	2.27	0.69
4:A:217:ASN:OD1	18:O:408:GLU:HB3	1.93	0.69
4:A:232:ALA:CB	18:O:6:ILE:CD1	2.71	0.68
5:B:1023:ARG:NH2	5:B:1027:PRO:O	2.26	0.68
5:B:685:TYR:HE2	29:B:1202:3AT:O1G	1.77	0.68
13:J:3:ILE:HD12	13:J:4:PRO:HD2	1.75	0.68
24:X:3:DC:H2''	24:X:4:DT:C4'	2.21	0.68
4:A:868:THR:HG21	4:A:1046:THR:HG23	1.74	0.68
25:Y:-7:DG:H2'	25:Y:-6:DC:C6	2.28	0.68
18:O:92:ILE:HG21	20:Q:60:LEU:HD11	1.75	0.68
24:X:0:DG:H2''	24:X:1:DT:H5'	1.74	0.68
5:B:903:GLN:OE1	5:B:937:ARG:NH1	2.27	0.68
24:X:5:DC:H2''	24:X:6:DG:H3'	1.76	0.68
21:U:207:PRO:HG2	21:U:233:ALA:HB2	1.75	0.68
24:X:18:DC:H2''	24:X:19:DA:C8	2.29	0.68
3:4:264:GLU:O	3:4:268:ASN:ND2	2.28	0.67
24:X:19:DA:H2''	24:X:20:DT:C6	2.29	0.67
4:A:155:ILE:HB	18:O:534:GLN:HE21	1.60	0.67
5:B:183:GLN:NE2	5:B:363:GLU:OE2	2.27	0.67
5:B:203:VAL:HG13	5:B:214:THR:HG23	1.77	0.67
24:X:-24:DA:H2''	24:X:-23:DT:C7	2.23	0.67
4:A:1157:LYS:O	4:A:1160:VAL:HG23	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:159:ARG:NH1	19:P:233:GLU:OE2	2.28	0.67
25:Y:6:DT:C2'	25:Y:7:DT:H71	2.25	0.67
21:U:188:ARG:NH1	22:V:391:GLN:O	2.27	0.67
23:W:299:TYR:OH	25:Y:36:DA:O5'	2.13	0.67
3:4:151:LYS:NZ	3:4:154:VAL:HG23	2.10	0.66
6:C:149:ASN:ND2	6:C:151:HIS:O	2.28	0.66
6:C:141:ARG:NH1	6:C:209:ASP:OD1	2.28	0.66
21:U:210:THR:HG21	25:Y:26:DT:H4'	1.75	0.66
24:X:-27:DT:H2''	24:X:-26:DA:C5'	2.26	0.66
4:A:720:GLY:HA3	4:A:759:ILE:HD11	1.77	0.66
4:A:464:ARG:HB2	4:A:505:MET:HE3	1.75	0.66
25:Y:-24:DG:H2''	25:Y:-23:DT:C5'	2.26	0.66
21:U:313:THR:HG21	24:X:-28:DA:H1'	1.76	0.66
25:Y:-29:DT:C2'	25:Y:-28:DT:H71	2.25	0.66
4:A:232:ALA:CB	18:O:6:ILE:HD11	2.25	0.66
24:X:-21:DT:C6	24:X:-20:DT:H72	2.31	0.66
2:3:304:LYS:N	2:3:309:TYR:OH	2.29	0.66
24:X:-8:DG:H2''	24:X:-7:DA:C8	2.31	0.66
2:3:195:HIS:CE1	25:Y:47:DT:H72	2.31	0.66
9:F:69:ARG:NE	9:F:96:GLU:OE1	2.29	0.66
24:X:-45:DT:H2''	24:X:-44:DT:C6	2.30	0.65
25:Y:-15:DC:O2	25:Y:-15:DC:H5'	1.96	0.65
4:A:1117:ILE:HG23	4:A:1130:VAL:HG22	1.78	0.65
5:B:692:GLN:NE2	26:Z:8:C:O3'	2.28	0.65
24:X:17:DA:H2''	24:X:18:DC:O5'	1.96	0.65
24:X:5:DC:H4'	24:X:6:DG:OP1	1.95	0.65
25:Y:41:DT:H2''	25:Y:42:DC:H5	1.59	0.65
5:B:190:ILE:HG21	5:B:354:ARG:HE	1.60	0.65
25:Y:8:DC:H2''	25:Y:9:DG:C8	2.31	0.65
25:Y:57:DT:H2''	25:Y:58:DT:O5'	1.96	0.65
2:3:144:ILE:HD13	24:X:-53:DG:OP1	1.97	0.65
25:Y:7:DT:H2''	25:Y:8:DC:C6	2.32	0.65
4:A:414:VAL:HG12	4:A:416:PRO:HD2	1.78	0.65
4:A:773:LYS:O	4:A:774:SER:OG	2.14	0.65
18:O:159:ARG:NH2	18:O:189:LEU:O	2.30	0.65
22:V:273:LEU:HD13	22:V:297:ILE:HG12	1.79	0.65
16:M:171:LYS:HZ1	19:P:67:ARG:HB2	1.61	0.65
25:Y:2:DG:H1'	25:Y:3:DT:C6	2.31	0.65
5:B:254:MET:HE1	5:B:332:CYS:HB3	1.79	0.64
4:A:197:PHE:CE1	18:O:374:HIS:CE1	2.85	0.64
21:U:174:LEU:HD12	21:U:178:LEU:HD11	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1185:MET:SD	4:A:1185:MET:N	2.70	0.64
24:X:-40:DT:C2'	24:X:-39:DT:H71	2.27	0.64
25:Y:-26:DT:H2''	25:Y:-25:DA:C8	2.32	0.64
25:Y:58:DT:H1'	25:Y:59:DA:O4'	1.98	0.64
25:Y:-2:DC:H2''	25:Y:-1:DA:C8	2.33	0.64
5:B:915:ASP:OD1	6:C:78:ARG:NH2	2.31	0.64
22:V:291:ARG:NH1	25:Y:42:DC:H5''	2.13	0.64
24:X:9:DT:O2	24:X:10:DA:H2''	1.97	0.64
25:Y:6:DT:H2'	25:Y:7:DT:H71	1.78	0.64
2:3:334:CYS:HB3	2:3:340:TYR:CD1	2.33	0.64
13:J:36:ASP:OD1	13:J:46:ARG:NH1	2.30	0.64
24:X:22:DT:H1'	24:X:23:DA:C8	2.33	0.64
4:A:159:CYS:CA	18:O:531:MET:SD	2.86	0.64
16:M:171:LYS:HB2	19:P:67:ARG:HB3	1.79	0.64
24:X:6:DG:H1'	24:X:7:DC:H5''	1.79	0.64
16:M:50:LYS:NZ	16:M:200:HIS:O	2.30	0.63
25:Y:56:DG:H2''	25:Y:57:DT:H71	1.80	0.63
5:B:483:ASP:OD2	5:B:495:ASN:ND2	2.31	0.63
24:X:28:DA:H2''	24:X:29:DA:C8	2.33	0.63
5:B:685:TYR:CE2	29:B:1202:3AT:O1G	2.51	0.63
25:Y:37:DG:H2''	25:Y:38:DA:H8	1.61	0.63
5:B:536:VAL:O	5:B:581:ARG:NH1	2.32	0.63
11:H:8:ASP:OD1	11:H:9:ILE:N	2.31	0.63
24:X:-27:DT:OP2	24:X:-27:DT:H3'	1.98	0.63
25:Y:33:DC:H2''	25:Y:34:DC:C6	2.34	0.63
4:A:159:CYS:O	18:O:531:MET:HA	1.99	0.63
24:X:-27:DT:H2''	24:X:-26:DA:O4'	1.97	0.63
7:D:33:ASN:OD1	7:D:34:LYS:N	2.32	0.63
24:X:-41:DA:H2''	24:X:-40:DT:C7	2.29	0.63
24:X:17:DA:H2'	24:X:18:DC:C6	2.32	0.63
4:A:111:THR:CG2	18:O:429:LEU:HD21	2.28	0.63
20:Q:80:GLU:N	20:Q:80:GLU:OE1	2.32	0.63
18:O:270:MET:HE2	18:O:336:ILE:HD11	1.81	0.62
23:W:298:TYR:CE2	24:X:-32:DC:H4'	2.33	0.62
24:X:29:DA:H2'	24:X:30:DT:H72	1.80	0.62
25:Y:58:DT:H1'	25:Y:59:DA:H5'	1.81	0.62
22:V:173:VAL:HG21	22:V:208:VAL:HG21	1.81	0.62
4:A:876:VAL:HG11	5:B:1053:ASP:CG	2.24	0.62
4:A:231:PRO:CA	18:O:2:THR:HG23	2.30	0.62
19:P:121:THR:OG1	19:P:122:GLU:OE1	2.17	0.62
25:Y:2:DG:H2''	25:Y:3:DT:H71	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:21:DA:H1'	24:X:22:DT:H5'	1.80	0.62
25:Y:-31:DA:H2''	25:Y:-30:DA:N7	2.14	0.62
16:M:221:GLU:HB3	17:N:374:THR:HG21	1.81	0.62
24:X:-7:DA:H2''	24:X:-6:DA:C8	2.34	0.62
10:G:115:GLN:NE2	10:G:192:GLU:O	2.33	0.62
11:H:33:GLU:OE1	11:H:33:GLU:N	2.32	0.62
19:P:151:MET:HE1	19:P:157:PRO:HA	1.81	0.62
24:X:21:DA:C1'	24:X:22:DT:H5'	2.29	0.62
25:Y:-5:DG:H2''	25:Y:-4:DA:H5'	1.81	0.62
4:A:1234:ALA:O	4:A:1238:THR:HG23	2.00	0.61
7:D:3:VAL:HG12	10:G:7:MET:HG2	1.81	0.61
4:A:159:CYS:HB3	18:O:531:MET:SD	2.40	0.61
23:W:299:TYR:CE2	25:Y:35:DA:H1'	2.35	0.61
24:X:7:DC:OP1	24:X:7:DC:H4'	2.00	0.61
10:G:152:VAL:HG22	10:G:189:SER:OG	1.99	0.61
19:P:83:GLY:N	19:P:92:GLU:OE2	2.32	0.61
24:X:-41:DA:H2''	24:X:-40:DT:H72	1.82	0.61
5:B:633:LEU:HD11	5:B:656:HIS:CD2	2.34	0.61
21:U:309:LYS:HD3	25:Y:30:DA:H5''	1.82	0.61
24:X:9:DT:C2'	24:X:10:DA:H4'	2.30	0.61
25:Y:1:DG:H2''	25:Y:2:DG:C5'	2.28	0.61
4:A:1152:SER:OG	4:A:1200:VAL:O	2.17	0.61
24:X:-31:DT:H2'	24:X:-30:DT:C6	2.36	0.61
4:A:5:GLN:HB2	10:G:185:THR:HG21	1.82	0.61
23:W:294:PHE:CE1	24:X:-31:DT:H4'	2.34	0.61
25:Y:-28:DT:H2'	25:Y:-27:DT:H72	1.83	0.61
25:Y:27:DA:H2''	25:Y:28:DT:C2'	2.31	0.61
16:M:177:PHE:CZ	19:P:98:ILE:HD12	2.32	0.61
24:X:6:DG:C4'	24:X:7:DC:H5''	2.30	0.61
25:Y:23:DA:C2'	25:Y:24:DT:H5''	2.21	0.61
9:F:84:GLU:N	9:F:86:GLU:OE1	2.34	0.60
14:K:64:GLU:OE1	14:K:64:GLU:N	2.34	0.60
25:Y:1:DG:C2'	25:Y:2:DG:H5'	2.24	0.60
25:Y:2:DG:H2''	25:Y:3:DT:C7	2.31	0.60
5:B:287:ILE:O	5:B:291:VAL:HG23	2.01	0.60
17:N:333:LYS:O	17:N:334:SER:OG	2.17	0.60
5:B:461:LYS:HB2	5:B:492:LEU:HD12	1.83	0.60
22:V:76:VAL:CG2	22:V:118:VAL:HG13	2.27	0.60
24:X:-39:DT:C2'	24:X:-38:DT:H71	2.32	0.60
22:V:146:LEU:HD13	22:V:146:LEU:O	2.02	0.60
4:A:361:VAL:HG12	5:B:1072:SER:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:17:PHE:C	20:Q:74:PHE:CD1	2.79	0.60
18:O:374:HIS:HB3	18:O:423:LEU:HD23	1.82	0.60
25:Y:51:DT:H2''	25:Y:52:DT:H71	1.82	0.60
25:Y:58:DT:H1'	25:Y:59:DA:C5'	2.32	0.60
30:P:401:SF4:S3	20:Q:38:PHE:CE2	2.94	0.60
4:A:155:ILE:HB	18:O:534:GLN:NE2	2.16	0.60
26:Z:4:C:H2'	26:Z:5:U:C6	2.36	0.60
4:A:111:THR:HG23	18:O:429:LEU:HD21	1.82	0.59
4:A:1054:HIS:HD2	4:A:1065:LEU:HD12	1.65	0.59
7:D:17:PHE:HB2	7:D:53:ILE:HG21	1.84	0.59
18:O:274:SER:OG	18:O:285:THR:OG1	2.19	0.59
2:3:55:LEU:HD13	2:3:57:GLY:H	1.66	0.59
4:A:231:PRO:HA	18:O:2:THR:CB	2.33	0.59
18:O:147:THR:HG22	18:O:150:ARG:HH22	1.67	0.59
24:X:-37:DC:C2'	24:X:-36:DT:H71	2.32	0.59
24:X:20:DT:H4'	24:X:21:DA:OP1	2.02	0.59
18:O:45:THR:OG1	18:O:49:GLN:OE1	2.20	0.59
10:G:93:SER:OG	10:G:96:GLY:O	2.16	0.59
4:A:471:LEU:HD22	4:A:538:LEU:HD12	1.82	0.59
24:X:-7:DA:H2''	24:X:-6:DA:H8	1.67	0.59
6:C:336:PHE:HE1	14:K:44:LEU:HD22	1.68	0.59
24:X:-16:DG:H2''	24:X:-15:DA:C5'	2.31	0.59
25:Y:-20:DA:C2'	25:Y:-19:DT:H72	2.33	0.59
4:A:1230:ASP:OD1	4:A:1250:ASN:ND2	2.36	0.59
21:U:169:VAL:HG22	21:U:222:THR:HG22	1.84	0.59
24:X:-52:DA:H2''	24:X:-51:DA:N7	2.17	0.59
24:X:-46:DT:C2'	24:X:-45:DT:H71	2.32	0.59
24:X:-23:DT:H2''	24:X:-22:DC:C5	2.38	0.59
4:A:159:CYS:HA	18:O:531:MET:CG	2.33	0.59
18:O:158:GLN:HB2	18:O:187:MET:HE3	1.85	0.59
18:O:248:ASP:O	18:O:252:VAL:HG23	2.02	0.58
24:X:21:DA:C4'	24:X:22:DT:H5'	2.33	0.58
23:W:297:ASN:OD1	23:W:298:TYR:N	2.36	0.58
24:X:-6:DA:H2''	24:X:-5:DA:C8	2.37	0.58
16:M:53:GLN:OE1	16:M:200:HIS:ND1	2.36	0.58
4:A:1043:GLU:OE2	4:A:1047:GLN:NE2	2.37	0.58
5:B:647:GLU:N	5:B:647:GLU:OE1	2.36	0.58
4:A:461:LEU:HD21	5:B:1063:LEU:HD21	1.85	0.58
6:C:109:ARG:NH2	6:C:198:LEU:O	2.36	0.58
25:Y:-32:DC:H2''	25:Y:-31:DA:C8	2.38	0.58
3:4:260:SER:O	3:4:261:HIS:ND1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:104:ILE:HD11	4:A:1333:TYR:HE1	1.68	0.58
4:A:159:CYS:CB	18:O:531:MET:CG	2.81	0.58
23:W:299:TYR:HE2	25:Y:35:DA:H1'	1.66	0.58
4:A:97:TYR:O	4:A:101:VAL:HG23	2.04	0.58
22:V:274:LEU:HD21	22:V:289:ASP:C	2.29	0.58
18:O:92:ILE:HG21	20:Q:60:LEU:CD1	2.34	0.57
4:A:937:GLU:OE1	4:A:1007:THR:OG1	2.22	0.57
5:B:258:GLU:OE1	5:B:258:GLU:N	2.37	0.57
25:Y:42:DC:H2''	25:Y:43:DG:C8	2.39	0.57
25:Y:57:DT:H2'	25:Y:58:DT:C5	2.38	0.57
5:B:315:SER:O	5:B:319:THR:HG22	2.04	0.57
4:A:772:ASP:OD1	4:A:773:LYS:N	2.37	0.57
8:E:5:GLU:N	8:E:5:GLU:OE1	2.38	0.57
16:M:412:HIS:O	16:M:416:VAL:HG23	2.03	0.57
19:P:214:HIS:HB3	19:P:260:VAL:HG22	1.87	0.57
24:X:12:DG:H2''	24:X:13:DC:O5'	2.05	0.57
25:Y:-7:DG:H2''	25:Y:-6:DC:H5'	1.87	0.57
17:N:254:LEU:HD12	17:N:331:ILE:HD11	1.87	0.57
21:U:202:MET:HE2	21:U:202:MET:HA	1.86	0.57
4:A:1054:HIS:CD2	4:A:1065:LEU:HD12	2.39	0.57
5:B:530:GLU:OE1	5:B:530:GLU:N	2.36	0.57
24:X:-43:DC:H2''	24:X:-42:DG:N7	2.19	0.57
25:Y:-15:DC:C2'	25:Y:-14:DT:H71	2.35	0.57
19:P:127:LEU:HD13	19:P:150:TYR:CZ	2.40	0.57
4:A:26:GLU:HG2	19:P:297:HIS:HB2	1.87	0.57
4:A:590:LYS:NZ	11:H:88:PHE:O	2.38	0.56
4:A:1102:LYS:HB2	4:A:1212:ILE:HD11	1.86	0.56
5:B:746:TYR:O	5:B:747:SER:OG	2.21	0.56
25:Y:28:DT:H3'	25:Y:28:DT:P	2.45	0.56
4:A:1055:PHE:O	4:A:1058:VAL:HG22	2.05	0.56
4:A:1295:THR:HG22	4:A:1300:VAL:HG22	1.87	0.56
21:U:203:ARG:NH1	25:Y:27:DA:OP1	2.36	0.56
24:X:-8:DG:H2''	24:X:-7:DA:H8	1.68	0.56
4:A:123:LYS:CD	18:O:68:HIS:CD2	2.88	0.56
4:A:130:LYS:HE3	18:O:34:GLN:HE22	1.70	0.56
4:A:231:PRO:HA	18:O:2:THR:HG23	1.87	0.56
5:B:23:VAL:HG23	5:B:26:LYS:HB2	1.87	0.56
8:E:39:GLU:OE2	8:E:43:GLN:NE2	2.38	0.56
11:H:20:LYS:NZ	11:H:22:PHE:O	2.38	0.56
13:J:28:GLU:OE2	16:M:396:LYS:N	2.38	0.56
18:O:180:LEU:HD23	20:Q:105:ARG:NH2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:0:DG:H2'	24:X:1:DT:H3'	1.87	0.56
24:X:3:DC:H2''	24:X:4:DT:C5'	2.35	0.56
24:X:14:DA:H2''	24:X:15:DG:C8	2.41	0.56
4:A:1206:GLU:OE1	4:A:1206:GLU:N	2.37	0.56
6:C:266:GLU:N	6:C:266:GLU:OE1	2.39	0.56
25:Y:27:DA:H2''	25:Y:28:DT:H2'	1.86	0.56
4:A:111:THR:CG2	18:O:429:LEU:CD2	2.81	0.56
4:A:295:LYS:HB2	20:Q:28:PRO:HB3	1.88	0.56
24:X:7:DC:H2'	24:X:8:DT:C7	2.34	0.56
16:M:218:SER:HA	17:N:374:THR:HG23	1.88	0.56
25:Y:12:DC:H2''	25:Y:13:DT:H73	1.87	0.56
25:Y:39:DA:H1'	25:Y:40:DA:C5'	2.33	0.56
4:A:231:PRO:HA	18:O:2:THR:CG2	2.36	0.56
4:A:1319:ALA:O	4:A:1324:THR:HG22	2.06	0.56
10:G:184:TYR:O	10:G:185:THR:OG1	2.18	0.56
23:W:343:ARG:NH2	24:X:-34:DG:H3'	2.20	0.56
8:E:121:MET:HE2	8:E:121:MET:HA	1.87	0.56
16:M:311:LEU:HD21	16:M:415:VAL:HG21	1.88	0.56
24:X:6:DG:H4'	24:X:7:DC:H5''	1.87	0.56
7:D:88:ASN:O	7:D:90:ARG:NH2	2.38	0.56
25:Y:2:DG:H4'	25:Y:3:DT:OP1	2.05	0.56
25:Y:36:DA:C2'	25:Y:37:DG:H5''	2.24	0.56
4:A:303:THR:HG1	18:O:377:GLN:HE21	1.51	0.56
6:C:86:THR:HG21	6:C:227:PRO:HB3	1.88	0.56
11:H:70:LEU:HD23	11:H:70:LEU:H	1.71	0.56
21:U:288:PHE:CE1	24:X:-30:DT:H1'	2.41	0.56
25:Y:18:DA:H2'	25:Y:19:DC:C6	2.41	0.56
4:A:503:ASP:OD1	26:Z:10:U:H5'	2.06	0.55
20:Q:27:LEU:HD23	24:X:-2:DC:P	2.46	0.55
4:A:295:LYS:HD2	20:Q:27:LEU:C	2.30	0.55
14:K:28:GLU:N	14:K:28:GLU:OE1	2.39	0.55
21:U:206:GLU:HB3	21:U:207:PRO:HD3	1.88	0.55
4:A:197:PHE:CZ	18:O:374:HIS:CE1	2.95	0.55
4:A:438:GLU:N	4:A:438:GLU:OE1	2.39	0.55
5:B:539:VAL:HG12	5:B:583:VAL:HB	1.89	0.55
5:B:751:ILE:O	5:B:930:ASN:ND2	2.40	0.55
16:M:9:VAL:HG23	16:M:10:VAL:HG22	1.87	0.55
24:X:-47:DA:H2''	24:X:-46:DT:C5	2.41	0.55
24:X:-22:DC:C2'	24:X:-21:DT:H72	2.36	0.55
4:A:1360:PHE:O	9:F:64:ARG:NH1	2.39	0.55
5:B:254:MET:HE3	5:B:333:ILE:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1046:ARG:HD3	25:Y:-8:DA:H5'	1.87	0.55
6:C:263:GLU:OE2	6:C:274:ARG:NH1	2.40	0.55
24:X:-41:DA:H2''	24:X:-40:DT:C5	2.42	0.55
10:G:115:GLN:O	10:G:119:LYS:NZ	2.32	0.55
24:X:-44:DT:H2''	24:X:-43:DC:C6	2.42	0.55
1:1:63:TRP:HE3	1:1:82:LEU:HD13	1.72	0.55
6:C:319:ASP:OD1	6:C:320:VAL:N	2.39	0.55
16:M:347:GLU:OE2	16:M:351:ARG:NH2	2.40	0.55
22:V:145:ASP:OD1	22:V:146:LEU:N	2.40	0.55
24:X:-4:DC:H2''	24:X:-3:DA:O5'	2.07	0.55
24:X:3:DC:H2'	24:X:3:DC:OP2	2.07	0.55
25:Y:47:DT:H2''	25:Y:48:DA:H8	1.66	0.55
2:3:193:HIS:NE2	24:X:-50:DA:H2'	2.22	0.55
5:B:876:GLU:N	5:B:876:GLU:OE1	2.40	0.55
7:D:79:THR:HG23	7:D:82:GLU:H	1.72	0.55
22:V:232:LEU:HD12	22:V:269:LEU:HD23	1.89	0.55
25:Y:-10:DT:H2'	25:Y:-9:DA:C8	2.41	0.55
4:A:464:ARG:HH21	26:Z:10:U:H3'	1.72	0.54
4:A:529:LEU:HA	4:A:539:ILE:HD13	1.88	0.54
25:Y:-7:DG:H2'	25:Y:-6:DC:H6	1.73	0.54
5:B:741:VAL:HG22	5:B:927:ILE:HB	1.89	0.54
21:U:305:PHE:CZ	25:Y:30:DA:H1'	2.42	0.54
2:3:202:GLN:HB3	2:3:343:LEU:HD11	1.88	0.54
19:P:57:LEU:HD23	19:P:60:MET:HE2	1.88	0.54
4:A:159:CYS:HA	18:O:531:MET:CB	2.37	0.54
6:C:50:ARG:NH1	6:C:52:ASP:OD2	2.40	0.54
18:O:17:PHE:O	20:Q:74:PHE:CD1	2.61	0.54
2:3:174:MET:HE1	2:3:335:LEU:HD13	1.89	0.54
16:M:171:LYS:HG3	19:P:67:ARG:CD	2.29	0.54
18:O:93:TYR:CE1	20:Q:53:GLY:HA2	2.43	0.54
24:X:-53:DG:C5	25:Y:54:DA:N6	2.76	0.54
5:B:607:THR:HG1	5:B:610:HIS:HD1	1.55	0.54
6:C:49:PHE:CZ	14:K:110:VAL:HG23	2.43	0.54
25:Y:-24:DG:OP2	25:Y:-24:DG:H3'	2.08	0.54
4:A:300:GLY:HA3	18:O:389:LYS:HA	1.90	0.54
17:N:251:VAL:HG23	17:N:331:ILE:HG21	1.90	0.54
24:X:0:DG:C2'	24:X:1:DT:H3'	2.38	0.54
24:X:26:DA:H2''	24:X:27:DA:H8	1.70	0.54
4:A:159:CYS:O	18:O:531:MET:CA	2.55	0.54
4:A:631:LEU:HD11	11:H:115:TYR:HE2	1.73	0.54
5:B:24:GLU:OE1	5:B:24:GLU:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:741:VAL:HG21	5:B:1009:TYR:CE1	2.43	0.54
22:V:147:ASP:OD1	22:V:148:VAL:N	2.41	0.54
4:A:1125:ASP:OD1	4:A:1126:CYS:N	2.38	0.54
13:J:40:LEU:HD11	13:J:49:LEU:HD12	1.90	0.54
19:P:313:TRP:HZ2	20:Q:48:LEU:HD21	1.73	0.54
24:X:-32:DC:C6	24:X:-31:DT:H72	2.43	0.54
24:X:22:DT:P	24:X:22:DT:H3'	2.48	0.54
5:B:901:HIS:NE2	5:B:945:GLU:OE1	2.40	0.54
19:P:284:ARG:HB3	20:Q:48:LEU:HD13	1.90	0.54
25:Y:14:DT:H2'	25:Y:15:DT:H72	1.90	0.54
25:Y:51:DT:H1'	25:Y:52:DT:H5'	1.90	0.54
1:1:35:ASN:OD1	1:1:36:MET:N	2.42	0.53
24:X:-41:DA:H2''	24:X:-40:DT:C6	2.43	0.53
4:A:197:PHE:CE2	18:O:374:HIS:CG	2.97	0.53
24:X:-10:DA:H2''	24:X:-9:DC:C6	2.43	0.53
25:Y:52:DT:H2''	25:Y:53:DC:C6	2.43	0.53
2:3:193:HIS:CE1	24:X:-50:DA:H8	2.26	0.53
11:H:112:LEU:HD13	11:H:129:ALA:HB2	1.89	0.53
16:M:134:GLN:OE1	16:M:136:ARG:NH2	2.39	0.53
16:M:215:ASP:OD1	16:M:216:SER:N	2.42	0.53
25:Y:11:DC:H1'	25:Y:12:DC:C2	2.44	0.53
4:A:558:PHE:HB3	4:A:594:LEU:HD13	1.91	0.53
18:O:180:LEU:HD21	20:Q:105:ARG:CZ	2.38	0.53
4:A:499:ASP:OD1	4:A:499:ASP:N	2.40	0.53
4:A:1044:PRO:HG2	4:A:1282:ILE:HD11	1.91	0.53
16:M:177:PHE:CZ	19:P:98:ILE:CD1	2.91	0.53
4:A:1343:VAL:HG21	4:A:1355:ILE:HD13	1.91	0.53
18:O:485:GLN:N	18:O:485:GLN:OE1	2.42	0.53
16:M:171:LYS:HZ3	19:P:67:ARG:CG	2.21	0.53
8:E:75:PHE:HZ	8:E:94:MET:HE3	1.74	0.53
25:Y:5:DT:C6	25:Y:6:DT:H72	2.43	0.53
4:A:230:ILE:C	18:O:2:THR:N	2.66	0.53
26:Z:7:G:H2'	26:Z:8:C:O4'	2.09	0.53
1:1:7:LEU:HD23	1:1:58:ALA:HB2	1.91	0.52
4:A:927:ASN:O	4:A:931:VAL:HG23	2.08	0.52
8:E:115:LYS:O	8:E:119:VAL:HG23	2.09	0.52
18:O:486:GLU:N	18:O:486:GLU:OE1	2.43	0.52
24:X:-33:DG:H4'	24:X:-32:DC:OP1	2.09	0.52
24:X:16:DC:H2'	24:X:17:DA:H8	1.73	0.52
24:X:22:DT:H4'	24:X:23:DA:O5'	2.09	0.52
4:A:428:MET:HA	4:A:428:MET:HE2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:85:LYS:O	8:E:89:VAL:HG23	2.09	0.52
15:L:26:ASN:ND2	15:L:36:CYS:SG	2.82	0.52
22:V:78:ASP:O	22:V:82:VAL:HG23	2.09	0.52
24:X:5:DC:C2'	24:X:6:DG:H3'	2.38	0.52
20:Q:27:LEU:HD23	24:X:-2:DC:OP2	2.10	0.52
25:Y:1:DG:OP2	25:Y:1:DG:H3'	2.09	0.52
4:A:533:ARG:NH1	4:A:1043:GLU:OE1	2.42	0.52
5:B:946:LEU:HD22	5:B:1003:TYR:CZ	2.45	0.52
6:C:296:VAL:HG23	6:C:297:VAL:HG13	1.92	0.52
11:H:95:LYS:C	11:H:116:VAL:HG13	2.35	0.52
25:Y:-17:DT:H2''	25:Y:-16:DG:N7	2.25	0.52
25:Y:-1:DA:C2'	25:Y:0:DC:H5''	2.38	0.52
4:A:741:GLY:HA3	12:I:53:LEU:HD21	1.91	0.52
4:A:912:MET:HE3	4:A:917:GLU:C	2.33	0.52
18:O:507:ASN:OD1	20:Q:62:GLN:NE2	2.41	0.52
19:P:168:SER:OG	19:P:173:GLU:OE2	2.27	0.52
24:X:-43:DC:H2''	24:X:-42:DG:C8	2.45	0.52
24:X:5:DC:H2''	24:X:6:DG:O5'	2.10	0.52
1:I:99:VAL:N	1:I:136:HIS:O	2.39	0.52
16:M:409:ILE:HG23	16:M:416:VAL:HG21	1.92	0.52
24:X:30:DT:C2'	24:X:31:DT:H72	2.40	0.52
3:4:382:ARG:HB3	3:4:387:LEU:HD13	1.91	0.52
5:B:209:GLU:N	5:B:209:GLU:OE1	2.42	0.52
6:C:115:ILE:HG22	6:C:117:ALA:H	1.75	0.52
18:O:349:THR:HG23	19:P:280:THR:HG21	1.90	0.52
24:X:-19:DG:H2''	24:X:-18:DT:OP2	2.10	0.52
3:4:365:ARG:NH1	3:4:367:GLY:O	2.42	0.52
11:H:27:ARG:NE	11:H:42:ASP:OD1	2.40	0.52
4:A:436:ASN:OD1	4:A:439:LYS:N	2.39	0.52
5:B:20:ILE:HD12	5:B:21:PRO:HD2	1.92	0.52
6:C:9:GLU:OE2	6:C:298:ARG:NH1	2.43	0.52
18:O:510:ASP:HB2	20:Q:58:LEU:CD1	2.40	0.52
4:A:589:LEU:HD12	4:A:590:LYS:N	2.24	0.52
5:B:1118:GLN:HA	5:B:1123:ILE:HD13	1.91	0.52
13:J:8:PHE:CD2	13:J:48:MET:HE1	2.45	0.52
19:P:42:MET:HG2	19:P:45:ILE:HD12	1.91	0.52
2:3:340:TYR:HB3	2:3:341:PRO:HD3	1.92	0.51
4:A:415:HIS:CE1	4:A:480:VAL:HG11	2.45	0.51
5:B:137:PRO:HG2	5:B:419:ILE:HD12	1.91	0.51
5:B:235:PRO:HD2	5:B:238:ILE:HD12	1.92	0.51
6:C:326:ILE:HG21	14:K:111:LEU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:94:MET:HE2	8:E:94:MET:HA	1.91	0.51
1:1:7:LEU:HD11	1:1:54:PHE:CE2	2.45	0.51
2:3:266:GLU:OE2	2:3:266:GLU:N	2.43	0.51
4:A:1105:ILE:HG22	4:A:1238:THR:HG21	1.92	0.51
8:E:65:ASN:OD1	8:E:66:ASP:N	2.43	0.51
10:G:99:VAL:HG11	10:G:148:ILE:HD11	1.92	0.51
22:V:176:TYR:CD1	22:V:223:LEU:HD11	2.45	0.51
2:3:193:HIS:HE2	24:X:-50:DA:H2'	1.74	0.51
19:P:98:ILE:HD13	19:P:115:LYS:HD3	1.91	0.51
25:Y:-24:DG:H2''	25:Y:-23:DT:H5'	1.91	0.51
1:1:72:PHE:O	1:1:76:VAL:HG23	2.10	0.51
4:A:233:GLU:HA	18:O:30:ARG:O	2.10	0.51
16:M:246:LEU:HD12	16:M:249:LEU:HD11	1.92	0.51
1:1:99:VAL:HG12	1:1:100:ALA:N	2.25	0.51
2:3:305:LEU:HD21	2:3:326:ILE:HG13	1.92	0.51
5:B:105:ARG:NH2	5:B:873:SER:O	2.43	0.51
5:B:1021:HIS:NE2	5:B:1043:GLY:O	2.40	0.51
16:M:161:SER:OG	16:M:164:ASP:OD1	2.27	0.51
24:X:-41:DA:C2'	24:X:-40:DT:H72	2.40	0.51
1:1:121:ASP:OD1	1:1:122:ALA:N	2.43	0.51
5:B:824:LYS:NZ	22:V:18:ASP:OD1	2.43	0.51
6:C:130:GLU:N	6:C:130:GLU:OE1	2.41	0.51
16:M:56:VAL:N	16:M:104:SER:OG	2.43	0.51
24:X:-53:DG:H2''	24:X:-52:DA:C8	2.46	0.51
25:Y:17:DC:H5''	25:Y:17:DC:C6	2.35	0.51
4:A:920:GLU:O	4:A:924:VAL:HG23	2.11	0.51
5:B:68:ASP:OD1	5:B:69:ALA:N	2.44	0.51
6:C:133:THR:O	6:C:137:THR:HG22	2.10	0.51
8:E:29:THR:HG23	8:E:32:GLU:H	1.76	0.51
22:V:238:GLN:NE2	22:V:241:ASP:OD2	2.43	0.51
25:Y:28:DT:H1'	25:Y:29:DA:C5	2.46	0.51
26:Z:3:G:H2'	26:Z:4:C:H6	1.76	0.51
5:B:524:ASN:O	16:M:134:GLN:NE2	2.43	0.51
5:B:1051:GLU:N	5:B:1051:GLU:OE1	2.40	0.51
6:C:133:THR:OG1	6:C:136:ASP:OD1	2.27	0.51
16:M:177:PHE:HE1	19:P:97:GLN:CB	2.18	0.51
21:U:188:ARG:NE	22:V:393:LEU:O	2.44	0.51
24:X:-11:DG:H2''	24:X:-10:DA:C8	2.46	0.51
2:3:193:HIS:HE1	24:X:-51:DA:H2''	1.75	0.51
3:4:232:GLU:OE1	3:4:236:ARG:NH1	2.43	0.51
5:B:178:ILE:HG12	5:B:437:THR:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:6:DG:C2'	24:X:7:DC:H5''	2.41	0.51
25:Y:5:DT:C2'	25:Y:6:DT:H72	2.40	0.51
7:D:107:ARG:NH2	20:Q:87:TYR:HB2	2.26	0.51
7:D:114:GLU:OE1	7:D:114:GLU:N	2.41	0.51
11:H:111:ARG:C	11:H:112:LEU:HD12	2.36	0.51
24:X:-28:DA:N7	24:X:-27:DT:O4	2.44	0.51
24:X:5:DC:H2''	24:X:6:DG:C3'	2.40	0.51
25:Y:-15:DC:O2	25:Y:-15:DC:H2'	2.12	0.51
6:C:89:VAL:HG22	6:C:214:CYS:SG	2.51	0.50
7:D:102:GLU:OE1	7:D:102:GLU:N	2.43	0.50
16:M:177:PHE:CZ	19:P:98:ILE:HB	2.46	0.50
16:M:225:LEU:HD11	17:N:376:LEU:HD13	1.93	0.50
4:A:77:ALA:O	5:B:1033:ARG:NH1	2.41	0.50
16:M:383:LYS:NZ	16:M:387:GLU:OE2	2.35	0.50
24:X:-18:DT:H2''	24:X:-17:DG:OP2	2.11	0.50
25:Y:58:DT:OP2	25:Y:58:DT:H2'	2.11	0.50
19:P:289:LEU:CD1	20:Q:45:PRO:HA	2.41	0.50
24:X:10:DA:H2'	24:X:10:DA:N3	2.26	0.50
25:Y:18:DA:H8	25:Y:18:DA:OP2	1.94	0.50
25:Y:23:DA:H2''	25:Y:24:DT:C5'	2.23	0.50
18:O:90:ARG:HA	20:Q:57:MET:HE3	1.92	0.50
24:X:29:DA:H2''	24:X:30:DT:C6	2.46	0.50
4:A:539:ILE:HG22	4:A:680:MET:HE1	1.93	0.50
5:B:294:GLN:N	5:B:294:GLN:OE1	2.45	0.50
22:V:232:LEU:HD21	22:V:266:LEU:HD11	1.94	0.50
24:X:-28:DA:H8	24:X:-27:DT:C7	2.13	0.50
6:C:188:GLY:O	6:C:191:ARG:NH1	2.41	0.50
16:M:11:GLN:CB	17:N:331:ILE:HD12	2.41	0.50
16:M:81:VAL:HG11	16:M:92:TYR:HE2	1.76	0.50
25:Y:-28:DT:H2''	25:Y:-27:DT:C6	2.45	0.50
2:3:260:ASN:ND2	2:3:269:ASP:OD1	2.45	0.50
4:A:159:CYS:CA	18:O:531:MET:CG	2.90	0.50
4:A:728:ILE:HD13	4:A:748:LEU:HD21	1.93	0.50
11:H:28:LEU:HD21	11:H:50:VAL:HG21	1.94	0.50
19:P:91:GLN:OE1	19:P:91:GLN:N	2.45	0.50
19:P:238:ILE:O	19:P:241:THR:OG1	2.28	0.50
20:Q:54:GLU:OE1	20:Q:54:GLU:N	2.43	0.50
22:V:243:LEU:HD13	22:V:243:LEU:O	2.11	0.50
4:A:203:HIS:NE2	18:O:383:PHE:CE2	2.77	0.50
4:A:415:HIS:NE2	4:A:480:VAL:HG11	2.26	0.50
18:O:134:GLU:N	18:O:134:GLU:OE1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:116:VAL:HG11	22:V:152:THR:HB	1.93	0.50
4:A:268:SER:OG	4:A:273:GLY:O	2.30	0.50
22:V:147:ASP:OD1	22:V:148:VAL:HG13	2.12	0.50
22:V:238:GLN:OE1	22:V:242:ARG:NH2	2.45	0.50
25:Y:8:DC:H2''	25:Y:9:DG:H8	1.76	0.50
4:A:731:LEU:HD23	4:A:748:LEU:HD22	1.94	0.49
5:B:923:ILE:HD11	13:J:42:ARG:HB2	1.92	0.49
24:X:-28:DA:C8	24:X:-27:DT:H71	2.47	0.49
25:Y:1:DG:C2'	25:Y:2:DG:OP2	2.59	0.49
4:A:155:ILE:HD12	18:O:534:GLN:CD	2.37	0.49
5:B:103:ARG:NE	5:B:175:GLU:OE2	2.44	0.49
5:B:746:TYR:HE2	5:B:911:VAL:HG11	1.76	0.49
10:G:189:SER:C	10:G:190:ILE:HD12	2.37	0.49
18:O:20:ILE:HD11	20:Q:75:ILE:HG12	1.94	0.49
4:A:887:ASP:OD2	4:A:891:ARG:NH2	2.45	0.49
25:Y:-6:DC:H2'	25:Y:-5:DG:C8	2.47	0.49
26:Z:5:U:O2'	26:Z:6:C:H5'	2.12	0.49
4:A:1303:ILE:O	4:A:1303:ILE:HG22	2.13	0.49
5:B:483:ASP:OD1	5:B:691:LYS:NZ	2.38	0.49
17:N:367:ASP:OD1	17:N:368:SER:N	2.44	0.49
18:O:16:HIS:CG	20:Q:68:MET:CE	2.95	0.49
22:V:186:SER:OG	22:V:189:VAL:HG12	2.12	0.49
25:Y:-28:DT:C2'	25:Y:-27:DT:H72	2.42	0.49
5:B:914:GLU:O	6:C:78:ARG:NH1	2.45	0.49
29:B:1202:3AT:N6	25:Y:-10:DT:O4	2.32	0.49
24:X:-27:DT:H2''	24:X:-26:DA:O5'	2.13	0.49
25:Y:-15:DC:H2'	25:Y:-14:DT:H71	1.92	0.49
5:B:1079:VAL:HB	5:B:1128:LEU:HD11	1.94	0.49
11:H:87:GLN:N	11:H:87:GLN:OE1	2.45	0.49
25:Y:-21:DT:H2''	25:Y:-20:DA:C8	2.47	0.49
11:H:14:ASP:OD1	11:H:15:ILE:N	2.46	0.49
16:M:171:LYS:HZ2	19:P:67:ARG:HD2	1.70	0.49
24:X:-58:DA:H2''	24:X:-57:DA:C8	2.47	0.49
25:Y:9:DG:H2''	25:Y:10:DT:H71	1.95	0.49
4:A:282:LYS:HZ1	4:A:319:LEU:HB2	1.77	0.49
24:X:-9:DC:H2''	24:X:-8:DG:H8	1.76	0.49
25:Y:7:DT:H2''	25:Y:8:DC:C5	2.48	0.49
25:Y:42:DC:H2''	25:Y:43:DG:H8	1.77	0.49
5:B:634:ASP:OD1	5:B:635:VAL:N	2.42	0.49
24:X:-36:DT:H3'	24:X:-35:DT:C7	2.43	0.49
24:X:-15:DA:H2''	24:X:-14:DA:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:295:LYS:HD2	20:Q:28:PRO:N	2.28	0.48
14:K:63:PRO:O	14:K:87:ARG:NE	2.39	0.48
23:W:295:ARG:HG2	25:Y:34:DC:H5'	1.95	0.48
24:X:-37:DC:H2'	24:X:-36:DT:H71	1.94	0.48
1:1:29:PHE:CZ	1:1:76:VAL:HG12	2.48	0.48
2:3:96:ALA:O	2:3:100:LEU:HD23	2.12	0.48
3:4:183:LYS:HD2	24:X:-48:DT:H5'	1.95	0.48
4:A:34:ILE:HD11	4:A:60:MET:HG3	1.94	0.48
6:C:86:THR:OG1	6:C:225:PHE:O	2.29	0.48
24:X:-57:DA:H2''	24:X:-56:DC:C5	2.47	0.48
24:X:15:DG:H2''	24:X:16:DC:O5'	2.13	0.48
6:C:28:ASP:O	14:K:61:LYS:NZ	2.47	0.48
5:B:29:LEU:HG	5:B:611:MET:HE1	1.96	0.48
6:C:339:GLU:O	6:C:343:VAL:HG23	2.13	0.48
4:A:1306:PHE:CE2	24:X:15:DG:H4'	2.49	0.48
5:B:946:LEU:HD22	5:B:1003:TYR:CE2	2.48	0.48
24:X:-47:DA:H2''	24:X:-46:DT:C6	2.49	0.48
25:Y:45:DA:H2''	25:Y:46:DA:C8	2.48	0.48
4:A:464:ARG:NH2	26:Z:10:U:H3'	2.28	0.48
4:A:1117:ILE:HG12	4:A:1130:VAL:HG13	1.94	0.48
29:B:1202:3AT:H2'1	29:B:1202:3AT:N3	2.27	0.48
23:W:353:ASP:O	23:W:357:GLN:NE2	2.47	0.48
24:X:24:DC:C2'	24:X:25:DT:H71	2.44	0.48
4:A:838:PHE:O	5:B:677:HIS:ND1	2.41	0.48
5:B:531:LEU:HD22	5:B:538:LEU:HD21	1.94	0.48
18:O:265:GLU:OE1	18:O:268:ARG:NH1	2.47	0.48
1:1:63:TRP:NE1	1:1:103:ASP:OD2	2.47	0.48
2:3:181:ILE:HD13	2:3:340:TYR:CZ	2.49	0.48
2:3:195:HIS:HE1	25:Y:47:DT:H72	1.74	0.48
5:B:946:LEU:HD23	5:B:946:LEU:C	2.39	0.48
16:M:327:VAL:O	16:M:353:ARG:NH1	2.43	0.48
25:Y:-20:DA:C8	25:Y:-19:DT:H72	2.48	0.48
7:D:87:LEU:O	7:D:90:ARG:NH1	2.47	0.48
22:V:110:ARG:CZ	25:Y:22:DG:H5'	2.43	0.48
25:Y:-15:DC:H2''	25:Y:-14:DT:H71	1.95	0.48
2:3:270:LEU:HD13	3:4:162:ASN:ND2	2.29	0.47
4:A:864:LYS:NZ	4:A:1048:MET:O	2.45	0.47
5:B:471:LEU:HD21	5:B:481:PRO:HB3	1.96	0.47
16:M:117:ALA:HB1	16:M:124:LEU:HD11	1.96	0.47
24:X:20:DT:H2''	24:X:21:DA:H8	1.78	0.47
4:A:30:GLN:NE2	5:B:1094:TYR:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:130:LYS:NZ	18:O:34:GLN:HE21	2.12	0.47
20:Q:83:ASP:OD1	20:Q:84:ILE:N	2.45	0.47
24:X:-55:DT:H2''	24:X:-54:DT:C6	2.48	0.47
4:A:258:PRO:HB2	4:A:262:ILE:HD12	1.95	0.47
5:B:889:ARG:NH1	5:B:1015:MET:SD	2.81	0.47
21:U:207:PRO:HB2	21:U:209:THR:HG23	1.96	0.47
4:A:288:PHE:O	4:A:292:VAL:HG23	2.15	0.47
4:A:754:LYS:O	4:A:758:VAL:HG23	2.14	0.47
24:X:-28:DA:H3'	24:X:-27:DT:H72	1.97	0.47
5:B:205:SER:OG	5:B:320:HIS:N	2.45	0.47
5:B:341:ARG:NH2	5:B:582:CYS:SG	2.86	0.47
16:M:249:LEU:HD12	16:M:250:MET:HG2	1.95	0.47
24:X:-57:DA:H2''	24:X:-56:DC:C6	2.50	0.47
25:Y:40:DA:H2''	25:Y:41:DT:C6	2.49	0.47
2:3:289:GLN:N	2:3:289:GLN:OE1	2.48	0.47
4:A:15:ILE:HD13	4:A:1349:MET:HE2	1.96	0.47
4:A:415:HIS:O	4:A:453:HIS:ND1	2.48	0.47
5:B:518:LEU:HD21	5:B:558:THR:HG21	1.96	0.47
6:C:324:GLU:O	6:C:328:VAL:HG23	2.15	0.47
9:F:84:GLU:N	9:F:84:GLU:OE1	2.48	0.47
16:M:177:PHE:CZ	19:P:98:ILE:CB	2.98	0.47
24:X:-36:DT:C6	24:X:-35:DT:H72	2.50	0.47
24:X:-36:DT:H2''	24:X:-35:DT:O5'	2.14	0.47
25:Y:-27:DT:H2''	25:Y:-26:DT:C6	2.50	0.47
25:Y:17:DC:H6	25:Y:17:DC:C5'	2.20	0.47
4:A:304:GLN:N	4:A:304:GLN:OE1	2.43	0.47
5:B:25:GLU:O	5:B:611:MET:HE2	2.14	0.47
5:B:722:THR:HG23	5:B:962:THR:HA	1.95	0.47
18:O:287:PRO:HB2	18:O:333:MET:HE3	1.96	0.47
21:U:197:PHE:CE2	21:U:199:ALA:HB3	2.50	0.47
24:X:9:DT:H2''	24:X:10:DA:C4'	2.42	0.47
25:Y:30:DA:H2'	25:Y:31:DA:C8	2.50	0.47
25:Y:51:DT:H1'	25:Y:52:DT:C5'	2.44	0.47
4:A:590:LYS:HB3	4:A:591:PRO:HD3	1.97	0.47
16:M:276:LEU:O	16:M:281:GLN:NE2	2.46	0.47
21:U:313:THR:CG2	24:X:-28:DA:H1'	2.44	0.47
24:X:-29:DT:H2'	24:X:-28:DA:N9	2.29	0.47
25:Y:28:DT:H2''	25:Y:29:DA:N7	2.30	0.47
25:Y:51:DT:H2''	25:Y:52:DT:C7	2.45	0.47
2:3:325:ASP:OD1	2:3:326:ILE:N	2.48	0.47
4:A:111:THR:HG22	18:O:429:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:196:SER:HB2	18:O:373:LYS:HB2	1.88	0.47
4:A:214:ALA:HB1	18:O:407:GLN:HE21	1.79	0.47
4:A:756:LEU:HD22	4:A:833:PHE:CD1	2.50	0.47
25:Y:45:DA:H2''	25:Y:46:DA:N7	2.30	0.47
4:A:206:GLU:OE1	4:A:206:GLU:N	2.46	0.47
4:A:604:ILE:HG23	4:A:682:ARG:HB2	1.96	0.47
8:E:75:PHE:CZ	8:E:94:MET:HE3	2.51	0.47
16:M:186:ARG:O	16:M:190:VAL:HG23	2.15	0.47
18:O:159:ARG:NH1	18:O:186:ASP:OD2	2.48	0.47
26:Z:4:C:O2'	26:Z:5:U:H5'	2.15	0.47
24:X:-45:DT:OP2	24:X:-45:DT:H2'	2.15	0.46
25:Y:-6:DC:H2'	25:Y:-5:DG:H8	1.78	0.46
4:A:26:GLU:OE1	4:A:26:GLU:N	2.43	0.46
4:A:669:ARG:NH2	4:A:910:ALA:O	2.48	0.46
24:X:-23:DT:H2''	24:X:-22:DC:H5	1.78	0.46
5:B:864:SER:OG	5:B:887:GLN:NE2	2.46	0.46
25:Y:28:DT:H1'	25:Y:29:DA:C4	2.50	0.46
5:B:883:MET:SD	5:B:883:MET:N	2.88	0.46
10:G:26:ILE:HG21	10:G:70:VAL:HG21	1.98	0.46
2:3:375:ASP:HB3	2:3:376:PRO:HD3	1.97	0.46
6:C:287:ILE:HD11	6:C:293:LEU:HB3	1.98	0.46
23:W:338:LYS:NZ	25:Y:26:DT:OP2	2.49	0.46
25:Y:11:DC:H2''	25:Y:12:DC:C6	2.50	0.46
4:A:29:ARG:NH1	19:P:301:GLU:OE1	2.49	0.46
4:A:123:LYS:HD2	18:O:68:HIS:HD2	1.78	0.46
5:B:848:GLN:OE1	5:B:848:GLN:N	2.47	0.46
6:C:236:LEU:HD13	6:C:305:HIS:CE1	2.51	0.46
21:U:325:PHE:HA	21:U:328:ILE:HG22	1.98	0.46
23:W:295:ARG:CG	25:Y:34:DC:H5'	2.45	0.46
1:1:76:VAL:HG13	1:1:80:TYR:CE2	2.51	0.46
4:A:56:LEU:HA	4:A:260:LEU:HD21	1.98	0.46
4:A:1332:ALA:HB2	5:B:1122:ILE:HG23	1.96	0.46
5:B:257:THR:O	5:B:262:MET:HE1	2.15	0.46
5:B:689:MET:HE1	26:Z:9:U:H5''	1.97	0.46
24:X:-28:DA:C5	24:X:-27:DT:O4	2.69	0.46
6:C:134:GLU:O	6:C:181:GLN:NE2	2.47	0.46
18:O:180:LEU:CD2	20:Q:105:ARG:NH2	2.79	0.46
19:P:307:CYS:O	19:P:311:THR:OG1	2.24	0.46
21:U:211:ALA:HB2	21:U:237:TYR:CE2	2.50	0.46
24:X:-45:DT:H2''	24:X:-44:DT:H71	1.98	0.46
25:Y:-24:DG:H2''	25:Y:-23:DT:O5'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:6:DT:H2''	25:Y:7:DT:H71	1.94	0.46
25:Y:19:DC:H2''	25:Y:20:DA:O4'	2.16	0.46
2:3:394:ASN:OD1	2:3:395:LYS:N	2.49	0.46
4:A:464:ARG:HH12	29:B:1202:3AT:HO2'	1.55	0.46
18:O:92:ILE:HG13	20:Q:60:LEU:HD21	1.97	0.46
24:X:22:DT:H3'	24:X:22:DT:OP2	2.16	0.46
25:Y:26:DT:OP2	25:Y:26:DT:H3'	2.16	0.46
1:1:99:VAL:HG12	1:1:100:ALA:H	1.80	0.46
4:A:1272:GLN:O	4:A:1276:VAL:HG23	2.16	0.46
6:C:49:PHE:HZ	14:K:110:VAL:HG23	1.80	0.46
6:C:57:ASP:N	6:C:57:ASP:OD1	2.49	0.46
6:C:334:ARG:NH2	14:K:104:MET:SD	2.88	0.46
17:N:269:LEU:HD12	17:N:269:LEU:O	2.16	0.46
22:V:110:ARG:CD	25:Y:22:DG:H5'	2.46	0.46
24:X:-19:DG:C8	24:X:-18:DT:H72	2.51	0.46
24:X:6:DG:H4'	24:X:7:DC:C5'	2.45	0.46
4:A:1153:ILE:HG22	4:A:1154:CYS:N	2.31	0.45
18:O:16:HIS:CG	20:Q:68:MET:HE1	2.51	0.45
24:X:-17:DG:H2''	24:X:-16:DG:H8	1.81	0.45
5:B:722:THR:H	5:B:725:ILE:HD12	1.80	0.45
16:M:13:ILE:HD13	16:M:119:TYR:HE1	1.81	0.45
18:O:443:ILE:HD12	18:O:520:ILE:CD1	2.46	0.45
18:O:510:ASP:HB2	20:Q:58:LEU:HD13	1.97	0.45
4:A:459:VAL:HG21	4:A:520:LEU:HB2	1.98	0.45
4:A:1207:VAL:HG13	4:A:1227:VAL:HG13	1.98	0.45
6:C:144:VAL:HG21	6:C:168:VAL:HG13	1.97	0.45
21:U:169:VAL:HG13	21:U:222:THR:HG22	1.97	0.45
25:Y:-21:DT:H2''	25:Y:-20:DA:H8	1.81	0.45
2:3:34:LEU:HD12	2:3:38:ASN:HD21	1.81	0.45
5:B:352:ASP:OD1	5:B:353:ASP:N	2.50	0.45
5:B:594:ARG:NH2	5:B:663:THR:OG1	2.41	0.45
24:X:-19:DG:C2'	24:X:-18:DT:H72	2.47	0.45
12:I:16:GLU:OE1	12:I:21:HIS:ND1	2.49	0.45
19:P:243:ILE:HD11	19:P:250:MET:HB2	1.99	0.45
24:X:-19:DG:H2'	24:X:-18:DT:H72	1.98	0.45
25:Y:1:DG:H1'	25:Y:2:DG:C5'	2.46	0.45
4:A:1131:LYS:HE2	4:A:1172:VAL:HG22	1.98	0.45
5:B:1028:ARG:NH1	5:B:1072:SER:O	2.50	0.45
10:G:152:VAL:HG22	10:G:189:SER:HG	1.82	0.45
16:M:59:GLU:OE1	16:M:101:THR:HG22	2.16	0.45
24:X:-48:DT:H2''	24:X:-47:DA:H5'	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:30:DT:H2''	24:X:31:DT:H72	1.98	0.45
25:Y:-5:DG:C2'	25:Y:-4:DA:H5'	2.47	0.45
4:A:1119:GLU:N	4:A:1119:GLU:OE1	2.48	0.45
25:Y:-23:DT:H2''	25:Y:-22:DA:C8	2.52	0.45
4:A:112:CYS:HA	18:O:433:ARG:CZ	2.47	0.45
4:A:987:TYR:OH	11:H:102:ASP:N	2.49	0.45
18:O:59:GLN:HG2	20:Q:73:TYR:CE1	2.52	0.45
22:V:384:ILE:HD12	22:V:385:SER:H	1.82	0.45
23:W:311:PHE:HE1	23:W:337:ILE:HG23	1.80	0.45
2:3:149:ALA:CB	24:X:-53:DG:H4'	2.47	0.45
4:A:221:LEU:HD13	18:O:399:LEU:O	2.17	0.45
4:A:862:ALA:O	4:A:865:THR:OG1	2.34	0.45
4:A:1158:LEU:HD12	4:A:1158:LEU:O	2.17	0.44
4:A:1264:ARG:NE	4:A:1292:ASP:OD1	2.48	0.44
21:U:288:PHE:CD1	24:X:-30:DT:H1'	2.52	0.44
24:X:-30:DT:O5'	24:X:-30:DT:H6	1.99	0.44
25:Y:51:DT:H2''	25:Y:52:DT:OP2	2.17	0.44
4:A:1145:ASN:N	4:A:1148:THR:OG1	2.45	0.44
19:P:292:VAL:O	19:P:292:VAL:HG22	2.17	0.44
20:Q:27:LEU:C	20:Q:27:LEU:HD12	2.42	0.44
24:X:-22:DC:H2''	24:X:-21:DT:C7	2.47	0.44
1:1:7:LEU:N	1:1:7:LEU:HD12	2.32	0.44
6:C:102:GLN:HE22	13:J:1:MET:HE1	1.82	0.44
19:P:104:ASN:HA	19:P:151:MET:HE3	2.00	0.44
25:Y:-15:DC:H2''	25:Y:-14:DT:C6	2.52	0.44
25:Y:36:DA:H2''	25:Y:37:DG:H8	1.82	0.44
25:Y:54:DA:H1'	25:Y:55:DA:H5'	1.99	0.44
2:3:148:ARG:O	2:3:149:ALA:HB3	2.17	0.44
3:4:389:TYR:OH	25:Y:59:DA:N6	2.45	0.44
4:A:631:LEU:HD11	11:H:124:ARG:HD3	1.98	0.44
4:A:1363:LEU:HD11	9:F:107:ARG:HH11	1.83	0.44
5:B:506:MET:HE2	5:B:587:SER:O	2.18	0.44
5:B:596:TYR:CD2	5:B:633:LEU:HD12	2.53	0.44
6:C:236:LEU:HD12	6:C:307:ILE:HD11	1.99	0.44
19:P:142:VAL:HG23	19:P:170:GLN:HA	1.98	0.44
19:P:289:LEU:HD12	20:Q:45:PRO:HA	1.99	0.44
2:3:181:ILE:HD13	2:3:340:TYR:OH	2.18	0.44
3:4:158:GLY:N	3:4:159:PRO:CD	2.81	0.44
10:G:146:GLU:N	10:G:146:GLU:OE1	2.50	0.44
21:U:169:VAL:HG22	21:U:222:THR:CG2	2.48	0.44
21:U:309:LYS:CD	25:Y:30:DA:H5''	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:-25:DA:H2''	25:Y:-24:DG:H8	1.80	0.44
26:Z:3:G:O2'	26:Z:4:C:H5'	2.17	0.44
2:3:205:LEU:HB3	2:3:340:TYR:HE2	1.83	0.44
4:A:262:ILE:HD11	5:B:1115:GLN:HB3	2.00	0.44
4:A:350:GLY:O	4:A:354:GLY:N	2.47	0.44
4:A:953:MET:HE3	4:A:970:LYS:HE3	1.99	0.44
5:B:239:ILE:HG22	5:B:243:MET:HE2	2.00	0.44
16:M:370:GLU:O	16:M:374:VAL:HG23	2.17	0.44
24:X:-22:DC:H2''	24:X:-21:DT:H72	1.98	0.44
25:Y:5:DT:H2'	25:Y:6:DT:H72	2.00	0.44
1:1:148:MET:SD	1:1:148:MET:N	2.87	0.44
5:B:392:ILE:N	5:B:393:PRO:CD	2.81	0.44
18:O:464:SER:HA	18:O:467:VAL:HG22	1.98	0.44
24:X:-31:DT:H3'	24:X:-30:DT:H72	2.00	0.44
22:V:221:HIS:CD2	25:Y:33:DC:H5''	2.53	0.44
22:V:381:ASP:OD1	22:V:381:ASP:N	2.49	0.44
26:Z:4:C:H2'	26:Z:5:U:H6	1.78	0.44
4:A:76:LEU:O	5:B:1033:ARG:NH2	2.51	0.44
4:A:158:HIS:O	18:O:533:ARG:HG3	2.18	0.44
4:A:583:LEU:HD12	4:A:584:PRO:HD2	2.00	0.44
16:M:355:PHE:CZ	16:M:374:VAL:HG11	2.53	0.44
23:W:288:THR:HG23	23:W:289:THR:H	1.83	0.44
6:C:93:LEU:N	6:C:93:LEU:HD12	2.33	0.43
10:G:33:LYS:C	10:G:34:LEU:HD22	2.42	0.43
10:G:46:ILE:HB	10:G:75:VAL:HG23	1.99	0.43
24:X:29:DA:C2'	24:X:30:DT:H72	2.47	0.43
5:B:631:GLU:OE2	5:B:656:HIS:NE2	2.43	0.43
21:U:237:TYR:O	21:U:241:VAL:HG23	2.18	0.43
4:A:369:ILE:HD12	4:A:500:PHE:CE1	2.53	0.43
11:H:18:GLU:N	11:H:18:GLU:OE1	2.51	0.43
3:4:305:LEU:C	3:4:305:LEU:HD23	2.44	0.43
4:A:934:CYS:O	4:A:1005:ARG:NH2	2.46	0.43
8:E:102:ALA:C	8:E:103:LEU:HD12	2.43	0.43
10:G:114:LEU:HD23	10:G:114:LEU:H	1.83	0.43
19:P:217:TRP:NE1	19:P:230:LEU:O	2.45	0.43
24:X:-27:DT:H2'	24:X:-26:DA:C8	2.53	0.43
25:Y:52:DT:H6	25:Y:52:DT:H2'	1.72	0.43
5:B:478:MET:C	5:B:479:LEU:HD12	2.44	0.43
14:K:73:THR:OG1	14:K:77:GLU:OE2	2.36	0.43
16:M:173:ILE:HG12	19:P:66:LEU:CD2	2.49	0.43
18:O:112:LEU:HD11	20:Q:64:LEU:CD2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:276:VAL:HG23	23:W:276:VAL:O	2.19	0.43
24:X:27:DA:H2''	24:X:28:DA:H8	1.76	0.43
4:A:868:THR:CG2	4:A:1046:THR:HG23	2.44	0.43
6:C:108:HIS:CE1	6:C:112:LEU:HD11	2.53	0.43
24:X:20:DT:H2''	24:X:21:DA:C8	2.53	0.43
4:A:1058:VAL:HG23	4:A:1060:SER:H	1.84	0.43
6:C:336:PHE:CE1	14:K:44:LEU:HD22	2.52	0.43
7:D:42:LEU:HD11	10:G:31:ASN:HB3	2.00	0.43
24:X:18:DC:H2''	24:X:19:DA:H8	1.82	0.43
25:Y:8:DC:C2	25:Y:9:DG:C5	3.07	0.43
2:3:251:PHE:HE2	2:3:270:LEU:HD12	1.84	0.43
4:A:160:GLY:CA	18:O:532:LYS:HE2	2.43	0.43
5:B:974:GLU:HA	5:B:977:VAL:HG12	2.00	0.43
16:M:177:PHE:CD2	19:P:98:ILE:CD1	2.97	0.43
17:N:253:GLU:OE2	17:N:256:ARG:NH2	2.51	0.43
18:O:16:HIS:HA	20:Q:68:MET:HE3	2.00	0.43
20:Q:64:LEU:HA	20:Q:67:THR:HG22	2.01	0.43
21:U:266:PHE:HE1	21:U:268[A]:ILE:HD11	1.84	0.43
25:Y:58:DT:H2''	25:Y:58:DT:H6	1.68	0.43
8:E:50:GLU:OE2	8:E:56:THR:OG1	2.37	0.43
3:4:353:GLU:O	3:4:357:LEU:HD13	2.19	0.43
6:C:239:ILE:HD12	6:C:239:ILE:N	2.34	0.43
18:O:193:LEU:HD22	18:O:229:PRO:HG2	2.01	0.43
18:O:429:LEU:HD21	18:O:433:ARG:HE	1.84	0.43
24:X:23:DA:H2''	24:X:24:DC:OP2	2.18	0.43
25:Y:-16:DG:H2''	25:Y:-15:DC:OP2	2.19	0.43
2:3:369:ASP:OD2	2:3:388:HIS:NE2	2.52	0.42
4:A:996:GLU:HB3	4:A:997:PRO:HD3	2.01	0.42
4:A:1250:ASN:O	4:A:1254:VAL:HG23	2.19	0.42
5:B:880:LEU:HD21	5:B:882:LYS:HE3	2.00	0.42
8:E:36:THR:HG23	8:E:39:GLU:H	1.84	0.42
23:W:288:THR:O	23:W:289:THR:HG23	2.19	0.42
24:X:-49:DG:H2''	24:X:-48:DT:C6	2.54	0.42
24:X:-37:DC:H2''	24:X:-36:DT:H71	1.99	0.42
24:X:14:DA:C2	25:Y:-13:DG:C2	3.07	0.42
25:Y:-20:DA:H2''	25:Y:-19:DT:C7	2.48	0.42
2:3:148:ARG:HE	2:3:148:ARG:HA	1.84	0.42
3:4:222:VAL:HG12	3:4:224:SER:H	1.84	0.42
4:A:232:ALA:HB2	18:O:6:ILE:CD1	2.49	0.42
4:A:468:LEU:HD22	4:A:1046:THR:HG21	2.01	0.42
5:B:89:GLU:OE1	5:B:90:SER:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:155:ASP:HB3	16:M:348:VAL:HG21	2.01	0.42
7:D:108:LEU:C	7:D:109:THR:HG1	2.16	0.42
15:L:16:ILE:HD11	15:L:25:GLU:HB3	2.00	0.42
25:Y:-21:DT:C2	25:Y:-20:DA:C5	3.06	0.42
25:Y:6:DT:H2''	25:Y:7:DT:C6	2.54	0.42
25:Y:11:DC:H2''	25:Y:12:DC:C4	2.54	0.42
4:A:360:ARG:NH2	25:Y:-7:DG:OP2	2.44	0.42
16:M:173:ILE:HG12	19:P:66:LEU:HD22	2.01	0.42
25:Y:32:DG:H2''	25:Y:33:DC:C6	2.54	0.42
1:1:26:PHE:O	1:1:30:THR:HG23	2.20	0.42
4:A:386:VAL:HG13	5:B:1022:ALA:HB2	2.01	0.42
4:A:1069:ARG:HH12	4:A:1080:ILE:HD12	1.84	0.42
5:B:989:VAL:HG21	5:B:1002:ILE:HB	2.01	0.42
11:H:9:ILE:N	11:H:9:ILE:HD12	2.35	0.42
19:P:309:TYR:HE2	20:Q:38:PHE:HD2	1.67	0.42
24:X:1:DT:H4'	24:X:2:DG:OP2	2.18	0.42
25:Y:-24:DG:H3'	25:Y:-24:DG:P	2.59	0.42
4:A:360:ARG:NH1	25:Y:-7:DG:OP1	2.50	0.42
16:M:322:GLN:NE2	16:M:360:PHE:O	2.52	0.42
3:4:196:VAL:HG11	3:4:284:TRP:CZ2	2.55	0.42
17:N:251:VAL:HG11	17:N:335:GLY:HA2	2.00	0.42
18:O:255:VAL:HG21	18:O:267:VAL:HG11	2.02	0.42
24:X:-36:DT:H3'	24:X:-35:DT:H72	2.01	0.42
24:X:14:DA:H1'	24:X:15:DG:C8	2.55	0.42
1:1:89:GLN:C	1:1:91:CYS:H	2.26	0.42
16:M:37:MET:SD	16:M:37:MET:N	2.93	0.42
16:M:177:PHE:CE1	19:P:97:GLN:HB3	2.34	0.42
18:O:118:MET:O	18:O:122:VAL:HG13	2.20	0.42
19:P:284:ARG:HA	20:Q:46:VAL:O	2.20	0.42
25:Y:49:DC:H6	25:Y:49:DC:H5'	1.85	0.42
3:4:243:GLN:O	3:4:246:ASN:ND2	2.52	0.42
6:C:221:ASP:OD2	15:L:58:ARG:NH2	2.52	0.42
8:E:154:GLU:OE1	8:E:154:GLU:N	2.46	0.42
24:X:-3:DA:H2'	24:X:-2:DC:C4	2.55	0.42
24:X:7:DC:C2'	24:X:8:DT:H5''	2.36	0.42
24:X:12:DG:H2''	24:X:13:DC:C6	2.55	0.42
2:3:261:ASP:OD1	2:3:263:ARG:NE	2.51	0.42
4:A:866:ALA:HB2	25:Y:-10:DT:H72	2.01	0.42
5:B:113:ILE:HD11	5:B:136:MET:HG2	2.01	0.42
18:O:55:CYS:SG	18:O:56:VAL:N	2.91	0.42
22:V:179:SER:HG	23:W:288:THR:CB	2.25	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:50:DT:H2'	25:Y:51:DT:H71	1.98	0.42
25:Y:58:DT:H2''	25:Y:59:DA:O5'	2.19	0.42
6:C:230:THR:HG21	13:J:42:ARG:CZ	2.50	0.42
18:O:51:LYS:HE2	20:Q:109:GLU:O	2.20	0.42
21:U:171:THR:HG23	21:U:256:GLN:HG3	2.01	0.42
22:V:106:ILE:HG23	22:V:117:LEU:HD22	2.02	0.42
24:X:-17:DG:H2''	24:X:-16:DG:C8	2.55	0.42
24:X:-13:DA:H2''	24:X:-12:DG:C8	2.54	0.42
24:X:9:DT:O3'	24:X:10:DA:H4'	2.20	0.42
25:Y:20:DA:H2''	25:Y:21:DA:C5'	2.49	0.42
2:3:373:PRO:HD2	2:3:377:CYS:SG	2.59	0.41
4:A:159:CYS:O	18:O:532:LYS:N	2.48	0.41
5:B:596:TYR:CE1	5:B:643:ILE:HD13	2.55	0.41
5:B:986:LYS:O	6:C:285:ARG:NH2	2.53	0.41
22:V:270:LEU:HD23	22:V:273:LEU:HD12	2.01	0.41
24:X:-53:DG:C2	25:Y:54:DA:C5	3.07	0.41
24:X:-32:DC:H2'	24:X:-31:DT:H72	2.01	0.41
4:A:303:THR:OG1	18:O:377:GLN:CD	2.51	0.41
4:A:372:ASP:N	4:A:490:GLU:OE2	2.53	0.41
4:A:396:VAL:HG22	4:A:404:LEU:CD1	2.51	0.41
4:A:731:LEU:CD2	4:A:748:LEU:HD22	2.50	0.41
29:B:1202:3AT:H1'	26:Z:10:U:H2'	2.02	0.41
16:M:81:VAL:HG11	16:M:92:TYR:CE2	2.53	0.41
18:O:276:ILE:HD12	18:O:276:ILE:N	2.35	0.41
20:Q:52:GLU:OE1	20:Q:52:GLU:N	2.45	0.41
3:4:346:ARG:NH1	3:4:353:GLU:OE2	2.53	0.41
4:A:577:GLU:HB3	14:K:29:MET:HE1	2.02	0.41
5:B:245:VAL:HG13	5:B:245:VAL:O	2.20	0.41
18:O:286:GLN:O	18:O:288:LEU:HD22	2.20	0.41
2:3:190:VAL:HG12	2:3:190:VAL:O	2.20	0.41
4:A:66:ASP:OD1	4:A:67:ARG:N	2.54	0.41
4:A:232:ALA:HB2	18:O:6:ILE:HD12	2.02	0.41
4:A:599:GLN:O	4:A:603:VAL:HG23	2.19	0.41
5:B:554:LYS:NZ	17:N:347:ASP:OD2	2.26	0.41
6:C:93:LEU:HD23	15:L:52:LEU:HD11	2.02	0.41
17:N:330:LEU:HD12	17:N:330:LEU:N	2.36	0.41
24:X:-52:DA:H2''	24:X:-51:DA:C8	2.56	0.41
3:4:372:TYR:O	3:4:376:VAL:HG23	2.21	0.41
4:A:350:GLY:O	4:A:354:GLY:CA	2.68	0.41
4:A:792:ILE:HG23	4:A:796:ILE:HD12	2.03	0.41
4:A:1118:GLU:OE1	12:I:39:THR:OG1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:218:VAL:HG22	5:B:218:VAL:O	2.20	0.41
7:D:11:LEU:HD23	7:D:11:LEU:H	1.84	0.41
11:H:136:GLU:O	11:H:139:SER:OG	2.32	0.41
19:P:176:PHE:CE2	19:P:180:LEU:HD11	2.56	0.41
24:X:-30:DT:N3	24:X:-29:DT:O4	2.53	0.41
25:Y:-7:DG:C2	26:Z:9:U:N3	2.89	0.41
4:A:542:ILE:HG13	4:A:543:GLN:H	1.86	0.41
5:B:812:ASP:OD2	15:L:46:LYS:NZ	2.54	0.41
18:O:106:ILE:O	18:O:110:LEU:HD23	2.21	0.41
19:P:253:ILE:HD13	19:P:269:LEU:HD11	2.02	0.41
21:U:185:LEU:HD11	22:V:399:VAL:HG13	2.02	0.41
21:U:236:LYS:O	21:U:240:VAL:HG23	2.21	0.41
25:Y:-20:DA:H2'	25:Y:-19:DT:H72	2.02	0.41
25:Y:-9:DA:H2'	25:Y:-8:DA:O4'	2.20	0.41
8:E:59:THR:OG1	8:E:71:GLN:OE1	2.36	0.41
13:J:10:CYS:SG	13:J:11:GLY:N	2.94	0.41
18:O:56:VAL:HG23	20:Q:73:TYR:HD1	1.85	0.41
18:O:182:ILE:HD11	18:O:187:MET:SD	2.61	0.41
18:O:292:GLU:HA	18:O:295:ARG:HG2	2.02	0.41
18:O:422:TYR:C	18:O:423:LEU:HD12	2.45	0.41
18:O:491:ILE:HG22	18:O:491:ILE:O	2.20	0.41
24:X:-45:DT:H2''	24:X:-44:DT:C5	2.55	0.41
25:Y:27:DA:H2''	25:Y:28:DT:C1'	2.49	0.41
1:1:63:TRP:HA	1:1:82:LEU:HD11	2.03	0.41
4:A:349:GLN:OE1	4:A:349:GLN:N	2.53	0.41
9:F:110:LEU:HD12	9:F:114:SER:HB3	2.02	0.41
25:Y:2:DG:P	25:Y:2:DG:H3'	2.61	0.41
25:Y:53:DC:OP1	25:Y:53:DC:H4'	2.20	0.41
25:Y:58:DT:C4	25:Y:59:DA:C5	3.09	0.41
4:A:295:LYS:HE2	20:Q:27:LEU:N	2.36	0.41
5:B:1046:ARG:NE	25:Y:-8:DA:OP1	2.52	0.41
6:C:144:VAL:HG11	6:C:168:VAL:HG22	2.03	0.41
7:D:22:ASP:O	7:D:25:GLU:HG3	2.21	0.41
18:O:16:HIS:CG	20:Q:68:MET:HE3	2.56	0.41
22:V:201:LEU:HD13	22:V:201:LEU:C	2.46	0.41
24:X:21:DA:H4'	24:X:22:DT:OP1	2.20	0.41
4:A:159:CYS:O	18:O:531:MET:CB	2.68	0.41
4:A:396:VAL:HG22	4:A:404:LEU:HD13	2.02	0.41
5:B:208:HIS:O	5:B:208:HIS:ND1	2.54	0.41
7:D:20:LEU:HD12	7:D:53:ILE:HD12	2.03	0.41
8:E:19:GLN:OE1	8:E:138:ASN:ND2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:35:GLN:NE2	8:E:39:GLU:OE1	2.53	0.41
21:U:242:GLN:NE2	21:U:248:ALA:O	2.48	0.41
23:W:343:ARG:HH22	24:X:-34:DG:H3'	1.84	0.41
2:3:192:PHE:CE2	2:3:200:PRO:HB3	2.57	0.40
4:A:219:ASN:OD1	4:A:222:VAL:HG23	2.21	0.40
18:O:22:GLU:O	18:O:26:VAL:HG23	2.20	0.40
18:O:180:LEU:CD2	20:Q:105:ARG:CZ	2.99	0.40
19:P:243:ILE:CG1	19:P:248:VAL:HG23	2.51	0.40
24:X:24:DC:H2'	24:X:25:DT:H71	2.03	0.40
25:Y:-7:DG:H2''	25:Y:-6:DC:C5'	2.51	0.40
1:1:64:ARG:HA	1:1:67:LEU:HD12	2.03	0.40
1:1:76:VAL:HG13	1:1:80:TYR:CD2	2.56	0.40
1:1:94:LYS:H	1:1:94:LYS:HG3	1.50	0.40
4:A:431:PHE:N	22:V:32:GLY:O	2.44	0.40
4:A:604:ILE:HG23	4:A:682:ARG:CB	2.51	0.40
6:C:299:LEU:HD12	6:C:299:LEU:N	2.37	0.40
24:X:30:DT:H2''	24:X:31:DT:C7	2.51	0.40
25:Y:-19:DT:H2''	25:Y:-18:DG:C8	2.56	0.40
6:C:246:GLU:OE1	6:C:246:GLU:N	2.53	0.40
10:G:190:ILE:HD12	10:G:190:ILE:N	2.36	0.40
17:N:249:VAL:HG22	17:N:250:SER:N	2.37	0.40
25:Y:-17:DT:H2''	25:Y:-16:DG:C8	2.56	0.40
1:1:62:ALA:HB3	1:1:82:LEU:HD21	2.04	0.40
16:M:11:GLN:HB3	17:N:331:ILE:HD12	2.01	0.40
21:U:263:ASP:OD1	21:U:264:VAL:N	2.54	0.40
22:V:378:VAL:O	22:V:378:VAL:HG23	2.22	0.40
24:X:-1:DC:H1'	24:X:0:DG:H4'	2.02	0.40
25:Y:55:DA:H2''	25:Y:56:DG:N7	2.35	0.40
4:A:217:ASN:OD1	18:O:407:GLN:O	2.38	0.40
4:A:662:ASN:OD1	4:A:664:PHE:N	2.52	0.40
21:U:187:ALA:HB3	21:U:190:ALA:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	144/368 (39%)	133 (92%)	11 (8%)	0	100	100
2	3	368/411 (90%)	347 (94%)	21 (6%)	0	100	100
3	4	245/1469 (17%)	238 (97%)	7 (3%)	0	100	100
4	A	1376/1390 (99%)	1346 (98%)	30 (2%)	0	100	100
5	B	1101/1133 (97%)	1069 (97%)	32 (3%)	0	100	100
6	C	341/346 (99%)	337 (99%)	4 (1%)	0	100	100
7	D	120/148 (81%)	118 (98%)	2 (2%)	0	100	100
8	E	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
9	F	74/127 (58%)	71 (96%)	3 (4%)	0	100	100
10	G	160/204 (78%)	148 (92%)	12 (8%)	0	100	100
11	H	146/150 (97%)	145 (99%)	1 (1%)	0	100	100
12	I	52/108 (48%)	52 (100%)	0	0	100	100
13	J	63/67 (94%)	60 (95%)	3 (5%)	0	100	100
14	K	101/133 (76%)	99 (98%)	2 (2%)	0	100	100
15	L	44/58 (76%)	41 (93%)	3 (7%)	0	100	100
16	M	418/708 (59%)	403 (96%)	15 (4%)	0	100	100
17	N	140/398 (35%)	140 (100%)	0	0	100	100
18	O	508/534 (95%)	499 (98%)	9 (2%)	0	100	100
19	P	301/316 (95%)	296 (98%)	5 (2%)	0	100	100
20	Q	85/223 (38%)	84 (99%)	1 (1%)	0	100	100
21	U	177/339 (52%)	169 (96%)	8 (4%)	0	100	100
22	V	330/419 (79%)	316 (96%)	14 (4%)	0	100	100
23	W	109/2624 (4%)	102 (94%)	7 (6%)	0	100	100
All	All	6610/11883 (56%)	6416 (97%)	194 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	130/334 (39%)	116 (89%)	14 (11%)	5	19
2	3	330/356 (93%)	311 (94%)	19 (6%)	17	38
3	4	221/1213 (18%)	213 (96%)	8 (4%)	30	51
4	A	1200/1212 (99%)	1194 (100%)	6 (0%)	86	90
5	B	963/988 (98%)	956 (99%)	7 (1%)	81	87
6	C	299/302 (99%)	297 (99%)	2 (1%)	81	87
7	D	114/136 (84%)	114 (100%)	0	100	100
8	E	191/192 (100%)	191 (100%)	0	100	100
9	F	66/111 (60%)	66 (100%)	0	100	100
10	G	149/181 (82%)	148 (99%)	1 (1%)	81	87
11	H	129/131 (98%)	129 (100%)	0	100	100
12	I	48/93 (52%)	48 (100%)	0	100	100
13	J	53/56 (95%)	52 (98%)	1 (2%)	52	70
14	K	92/119 (77%)	91 (99%)	1 (1%)	70	80
15	L	43/55 (78%)	43 (100%)	0	100	100
16	M	377/622 (61%)	377 (100%)	0	100	100
17	N	131/347 (38%)	131 (100%)	0	100	100
18	O	458/476 (96%)	457 (100%)	1 (0%)	92	94
19	P	269/280 (96%)	268 (100%)	1 (0%)	89	91
20	Q	84/195 (43%)	83 (99%)	1 (1%)	67	79
21	U	153/293 (52%)	147 (96%)	6 (4%)	27	49
22	V	301/365 (82%)	294 (98%)	7 (2%)	45	64
23	W	102/2381 (4%)	96 (94%)	6 (6%)	16	38
All	All	5903/10438 (57%)	5822 (99%)	81 (1%)	62	76

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	31	GLU
1	1	34	ARG
1	1	45	ARG
1	1	90	LEU

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Mol	Chain	Res	Type
1	1	91	CYS
1	1	92	GLN
1	1	94	LYS
1	1	95	GLN
1	1	96	LYS
1	1	102	LYS
1	1	137	PHE
1	1	142	LYS
1	1	144	LEU
1	1	146	TYR
2	3	55	LEU
2	3	56	ARG
2	3	61	LEU
2	3	108	LYS
2	3	109	LEU
2	3	110	LYS
2	3	130	LEU
2	3	146	ILE
2	3	158	GLU
2	3	195	HIS
2	3	198	HIS
2	3	199	LYS
2	3	201	TYR
2	3	241	HIS
2	3	343	LEU
2	3	344	ILE
2	3	345	LYS
2	3	374	GLU
2	3	377	CYS
3	4	151	LYS
3	4	177	GLU
3	4	178	GLU
3	4	228	ARG
3	4	246	ASN
3	4	289	HIS
3	4	359	GLN
3	4	387	LEU
4	A	428	MET
4	A	492	VAL
4	A	494	THR
4	A	767	CYS
4	A	776	SER

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Mol	Chain	Res	Type
4	A	1007	THR
5	B	203	VAL
5	B	214	THR
5	B	292	ARG
5	B	304	THR
5	B	406	MET
5	B	460	GLU
5	B	680	SER
6	C	162	LEU
6	C	236	LEU
10	G	128	VAL
13	J	30	THR
14	K	29	MET
18	O	55	CYS
19	P	134	LYS
20	Q	60	LEU
21	U	205	ARG
21	U	296	ILE
21	U	297	LYS
21	U	299	ARG
21	U	300	ILE
21	U	323	GLU
22	V	195	GLU
22	V	242	ARG
22	V	243	LEU
22	V	247	LEU
22	V	356	LEU
22	V	357	LEU
22	V	384	ILE
23	W	288	THR
23	W	289	THR
23	W	291	TYR
23	W	301	LYS
23	W	351	ARG
23	W	357	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	95	GLN
1	1	118	GLN
2	3	38	ASN

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Mol	Chain	Res	Type
2	3	162	HIS
2	3	195	HIS
2	3	210	GLN
2	3	226	GLN
2	3	319	HIS
3	4	162	ASN
3	4	171	GLN
3	4	234	GLN
3	4	268	ASN
3	4	295	GLN
3	4	340	HIS
3	4	369	HIS
4	A	17	HIS
4	A	40	ASN
4	A	119	GLN
4	A	158	HIS
4	A	296	HIS
4	A	374	ASN
4	A	415	HIS
4	A	423	GLN
4	A	469	HIS
4	A	739	GLN
4	A	1054	HIS
4	A	1180	ASN
4	A	1213	HIS
4	A	1364	HIS
4	A	1371	ASN
5	B	100	HIS
5	B	253	GLN
5	B	260	HIS
5	B	395	GLN
5	B	552	HIS
5	B	692	GLN
5	B	737	GLN
5	B	1115	GLN
8	E	108	GLN
8	E	132	GLN
11	H	29	HIS
11	H	131	ASN
12	I	40	ASN
13	J	26	GLN
16	M	266	ASN

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Mol	Chain	Res	Type
16	M	412	HIS
18	O	34	GLN
18	O	68	HIS
18	O	249	GLN
18	O	374	HIS
18	O	377	GLN
18	O	407	GLN
18	O	457	ASN
18	O	497	GLN
18	O	534	GLN
19	P	297	HIS
21	U	164	GLN
21	U	166	GLN
22	V	84	GLN
22	V	235	GLN
22	V	406	GLN
23	W	357	GLN
23	W	383	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	Z	8/9 (88%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
30	SF4	P	401	19	0,12,12	-	-	-		
29	3AT	B	1202	-	25,32,32	1.01	1 (4%)	28,50,50	1.63	5 (17%)
31	GTP	Z	101	26	26,34,34	1.11	2 (7%)	32,54,54	1.58	7 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SF4	P	401	19	-	-	0/6/5/5
31	GTP	Z	101	26	-	7/18/38/38	0/3/3/3
29	3AT	B	1202	-	-	6/18/34/34	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Z	101	GTP	C5-C6	-3.97	1.39	1.47
29	B	1202	3AT	C5-C4	2.54	1.47	1.40
31	Z	101	GTP	C2-N3	2.23	1.38	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Z	101	GTP	PB-O3B-PG	-3.77	119.90	132.83
29	B	1202	3AT	PA-O3A-PB	-3.62	120.40	132.83
29	B	1202	3AT	PB-O3B-PG	-3.59	120.50	132.83
29	B	1202	3AT	N3-C2-N1	-3.17	123.72	128.68
31	Z	101	GTP	C5-C6-N1	3.16	119.54	113.95
31	Z	101	GTP	PA-O3A-PB	-3.15	122.03	132.83
31	Z	101	GTP	C3'-C2'-C1'	3.01	105.52	100.98
31	Z	101	GTP	C8-N7-C5	2.99	108.68	102.99
31	Z	101	GTP	C2-N1-C6	-2.87	119.81	125.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	1202	3AT	C4-C5-N7	-2.68	106.60	109.40
29	B	1202	3AT	O4'-C4'-C3'	2.21	107.92	105.07
31	Z	101	GTP	O6-C6-C5	-2.08	120.31	124.37

There are no chirality outliers.

All (13) torsion outliers are listed below:

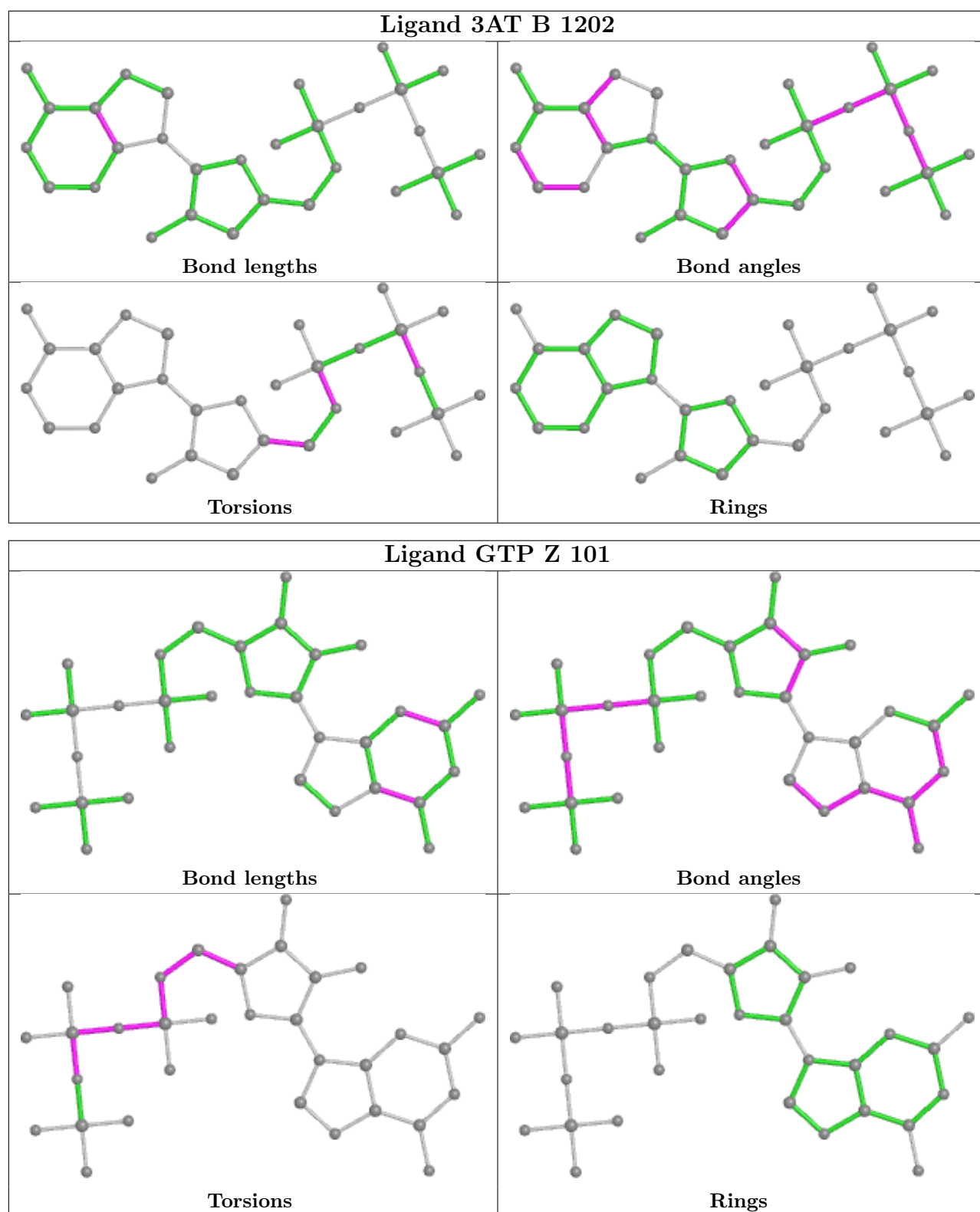
Mol	Chain	Res	Type	Atoms
29	B	1202	3AT	C5'-O5'-PA-O3A
29	B	1202	3AT	O4'-C4'-C5'-O5'
29	B	1202	3AT	C3'-C4'-C5'-O5'
31	Z	101	GTP	C4'-C5'-O5'-PA
29	B	1202	3AT	C5'-O5'-PA-O2A
29	B	1202	3AT	PG-O3B-PB-O2B
31	Z	101	GTP	PG-O3B-PB-O2B
31	Z	101	GTP	PB-O3A-PA-O2A
31	Z	101	GTP	PG-O3B-PB-O1B
29	B	1202	3AT	PG-O3B-PB-O1B
31	Z	101	GTP	PA-O3A-PB-O2B
31	Z	101	GTP	C5'-O5'-PA-O1A
31	Z	101	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	P	401	SF4	3	0
29	B	1202	3AT	7	0
31	Z	101	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

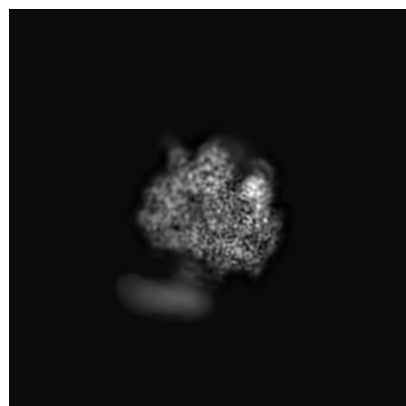
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62012. These allow visual inspection of the internal detail of the map and identification of artifacts.

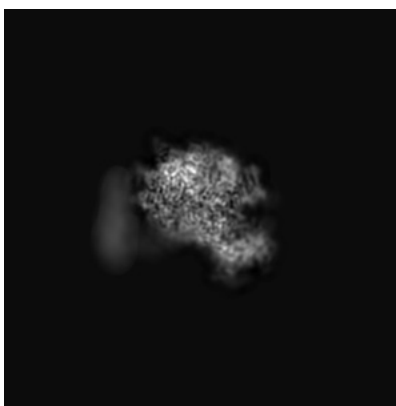
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

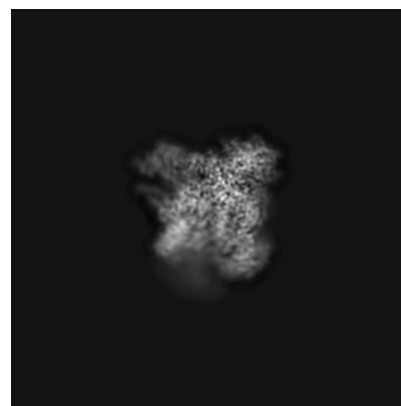
6.1.1 Primary map



X

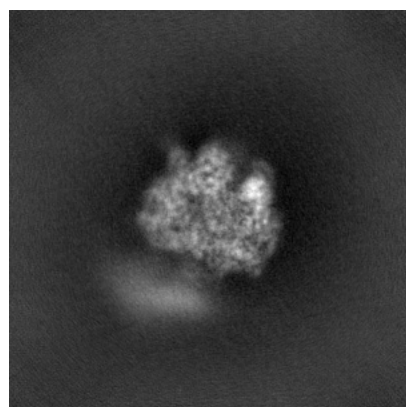


Y

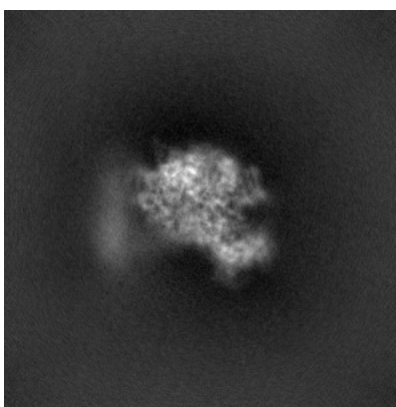


Z

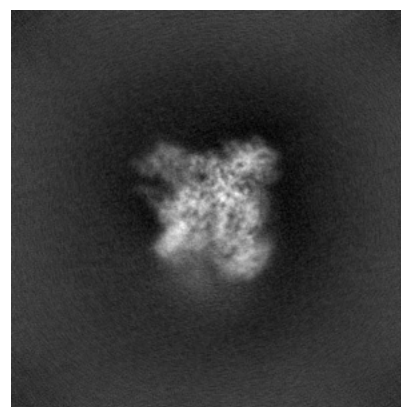
6.1.2 Raw map



X



Y

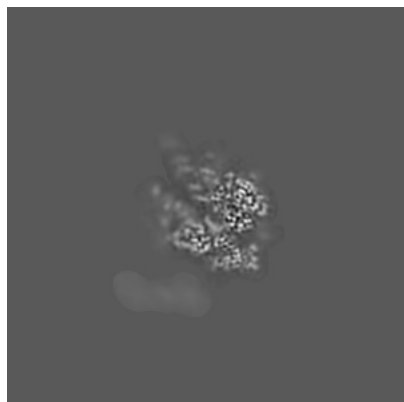


Z

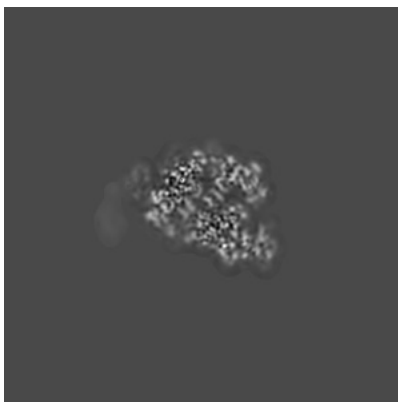
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

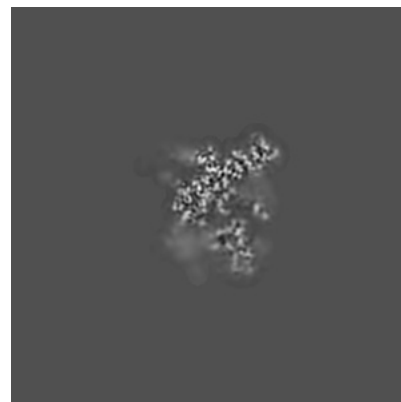
6.2.1 Primary map



X Index: 160

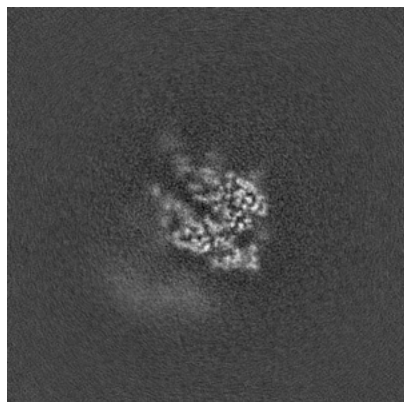


Y Index: 160

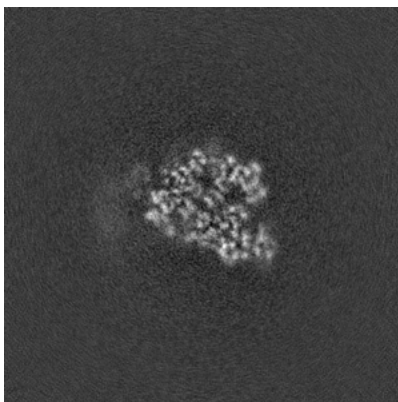


Z Index: 160

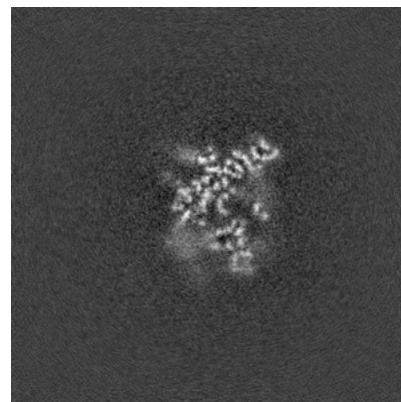
6.2.2 Raw map



X Index: 160



Y Index: 160

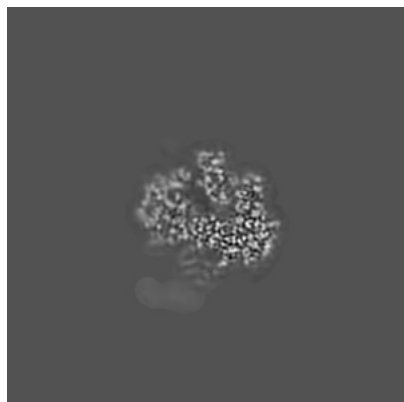


Z Index: 160

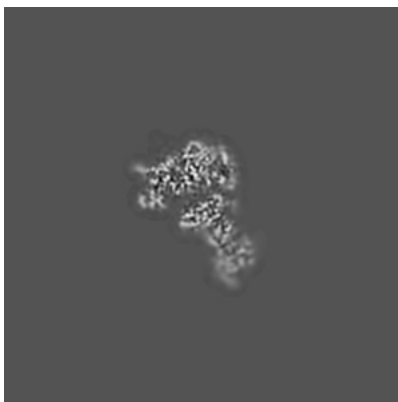
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

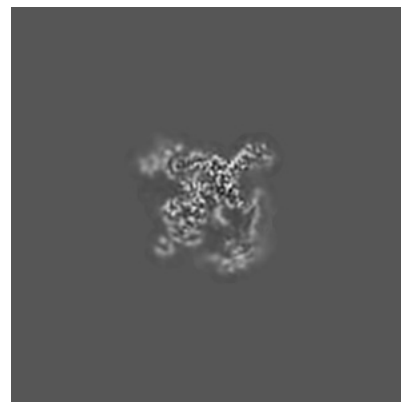
6.3.1 Primary map



X Index: 182

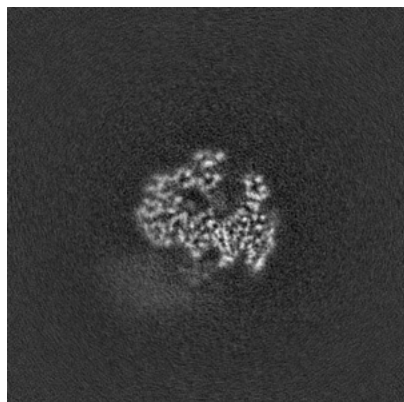


Y Index: 198

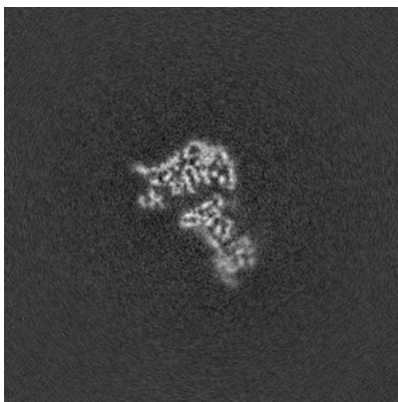


Z Index: 173

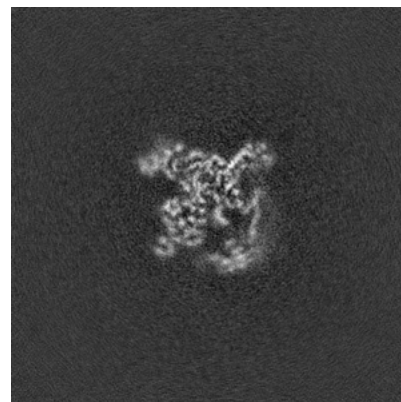
6.3.2 Raw map



X Index: 187



Y Index: 199

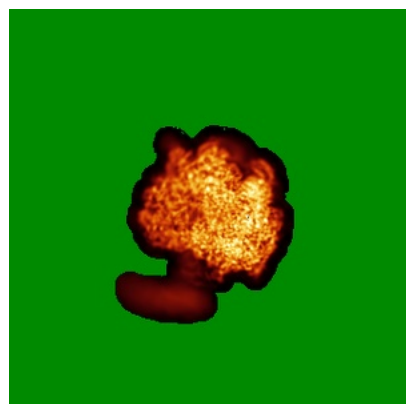


Z Index: 173

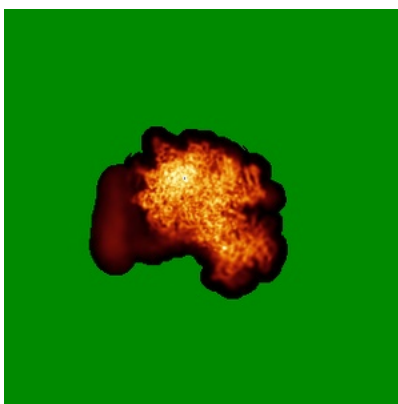
The images above show the largest variance slices of the map in three orthogonal directions.

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

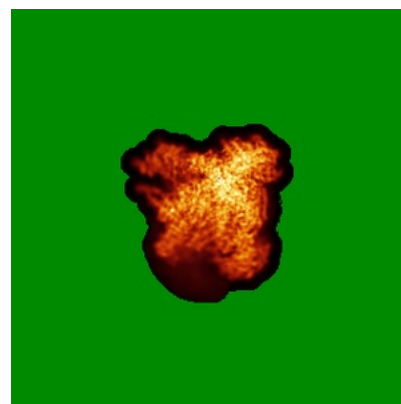
6.4.1 Primary map



X

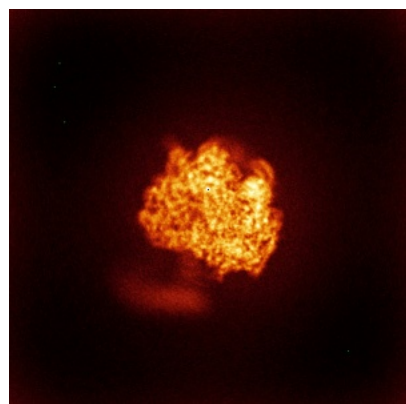


Y

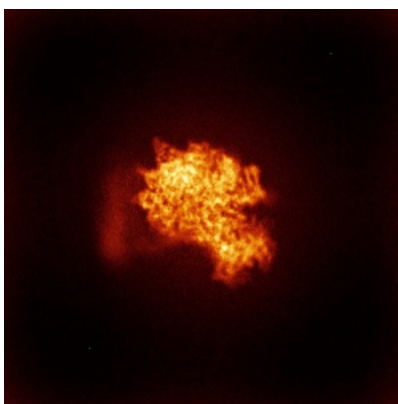


Z

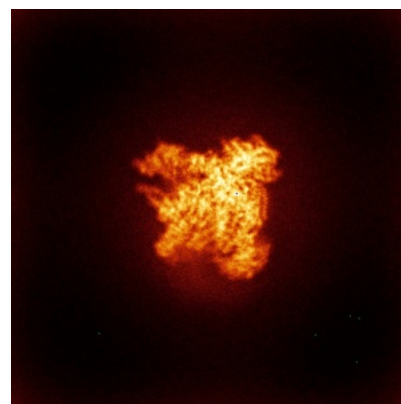
6.4.2 Raw map



X



Y

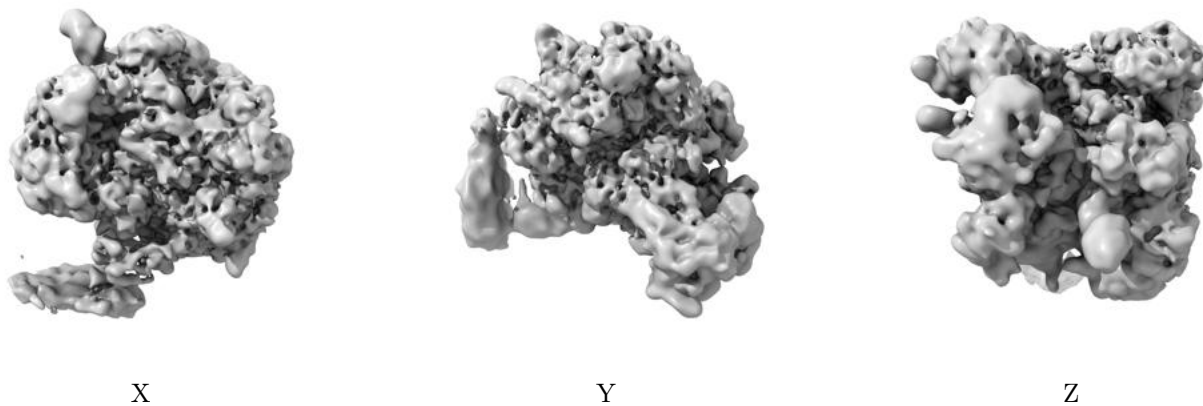


Z

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.

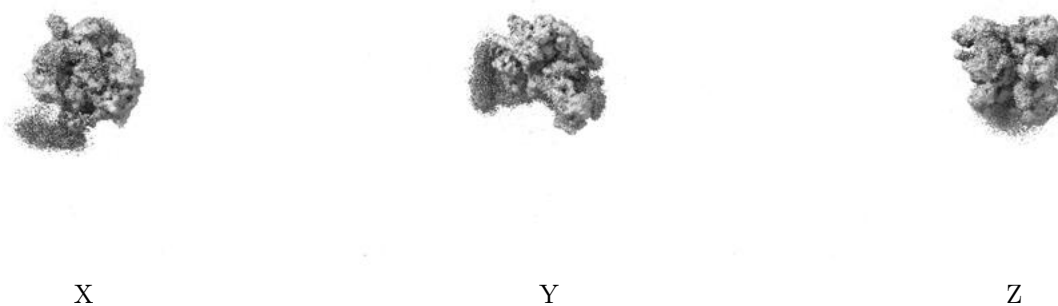
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

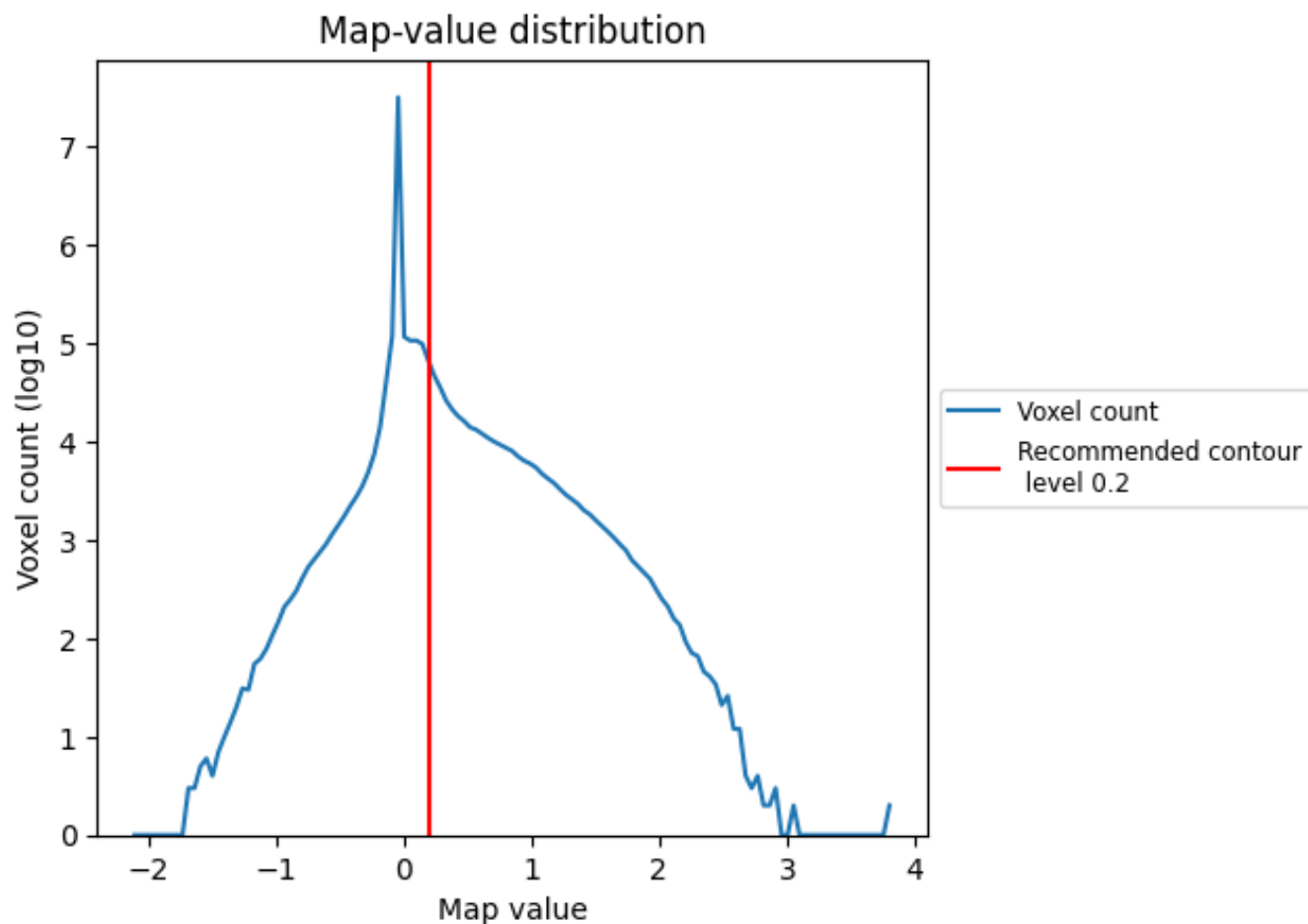
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

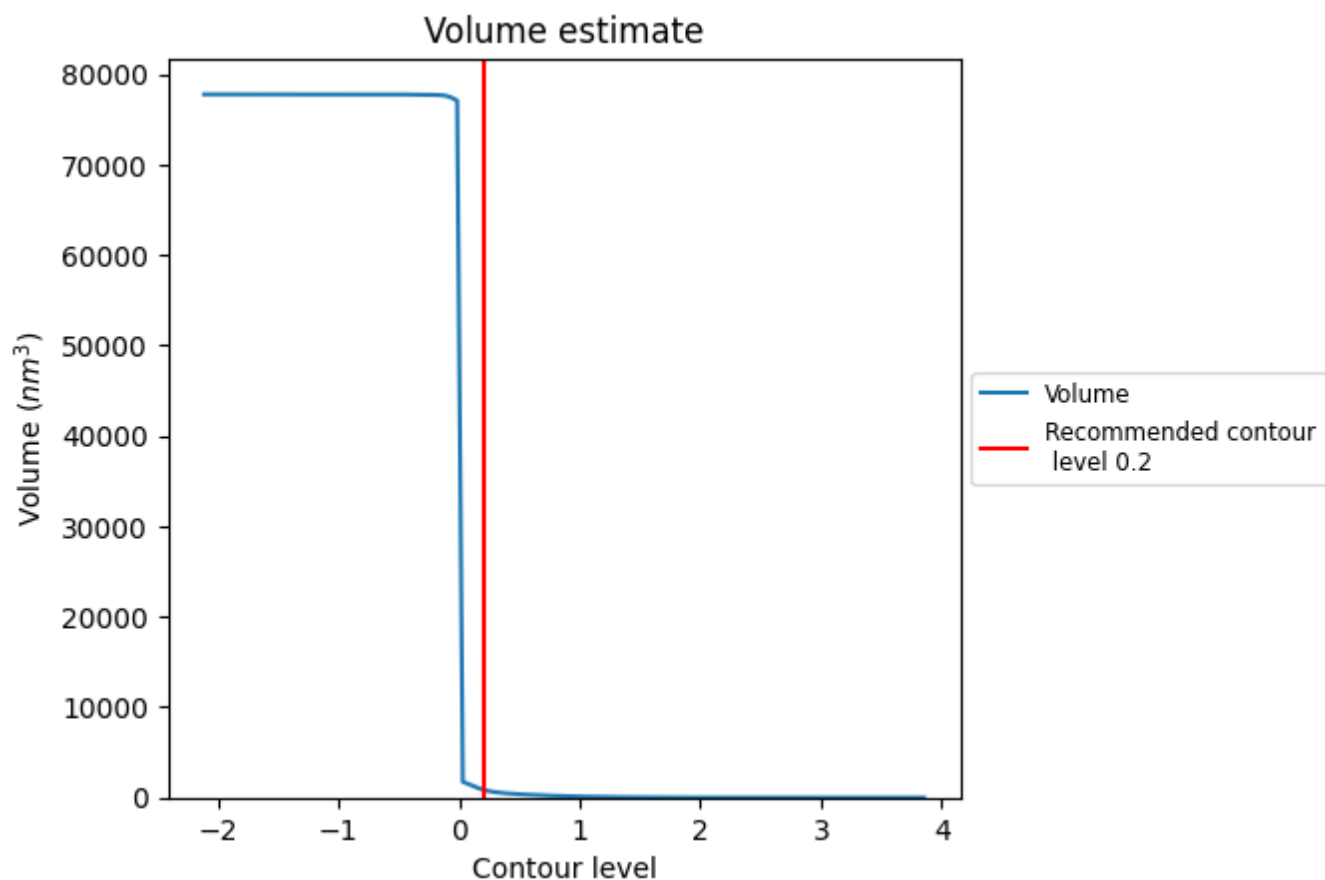
This section contains the results of statistical analysis of the map.

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.

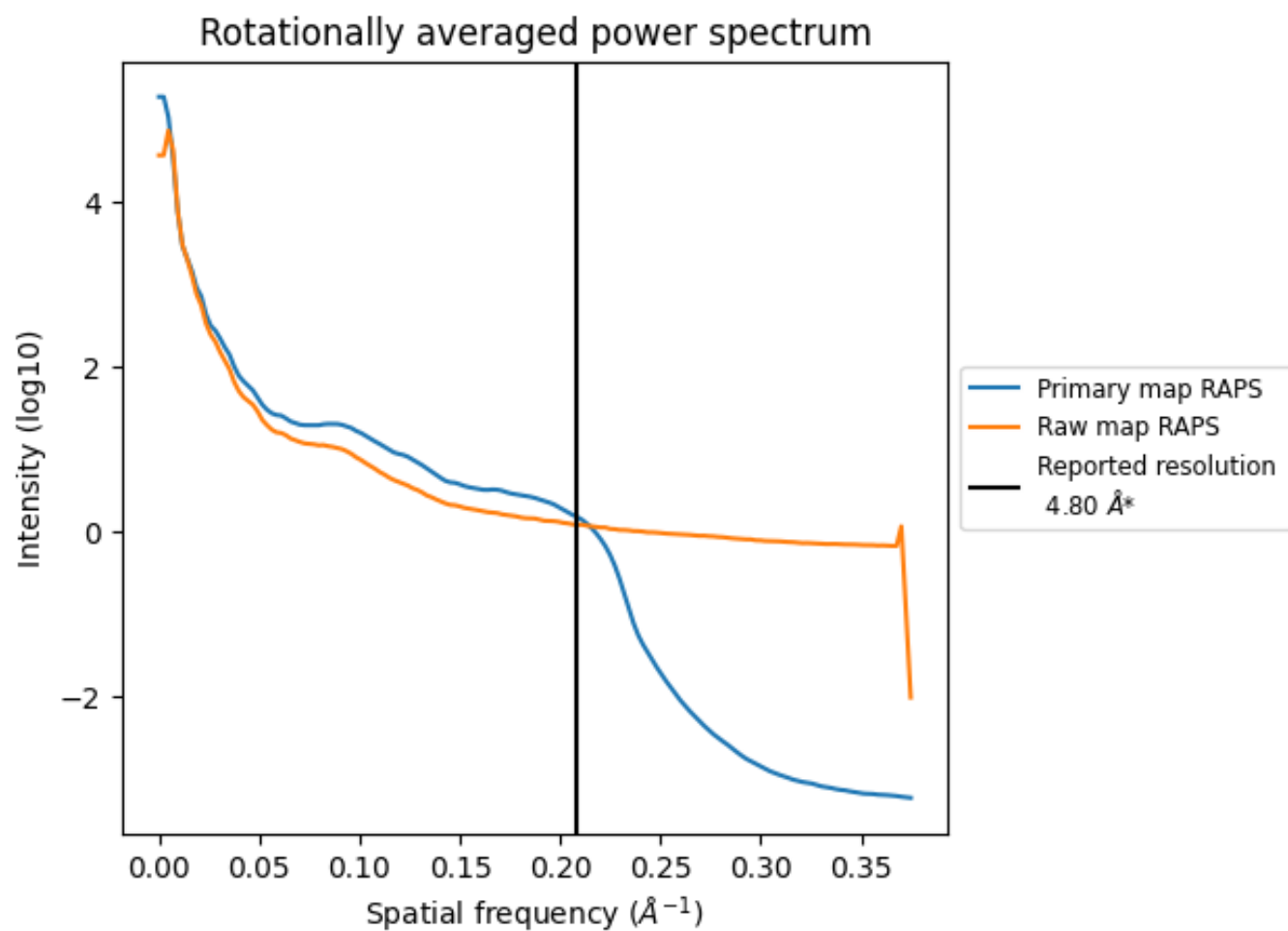
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 872 nm³; this corresponds to an approximate mass of 787 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 ⓘ

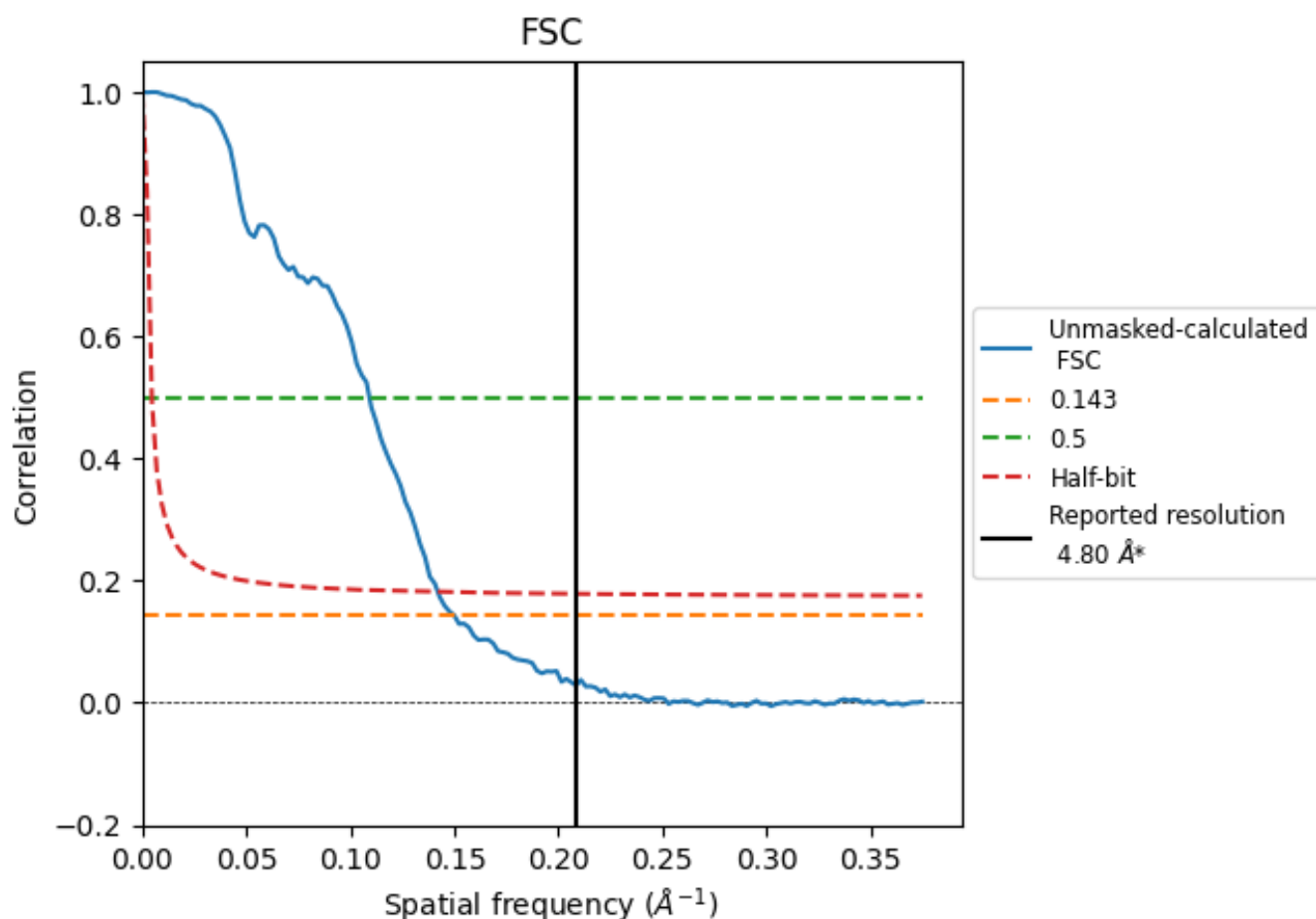


*Reported resolution corresponds to spatial frequency of 0.208 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.208 \AA^{-1}

8.2 Resolution estimates [i](#)

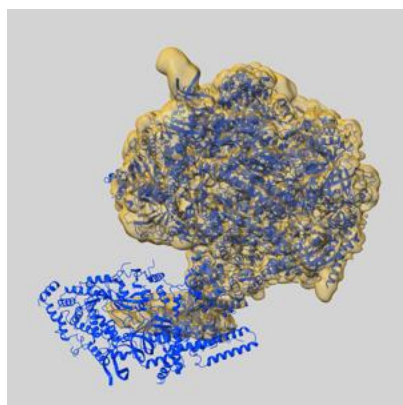
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.67	9.16	7.04

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.67 differs from the reported value 4.8 by more than 10 %

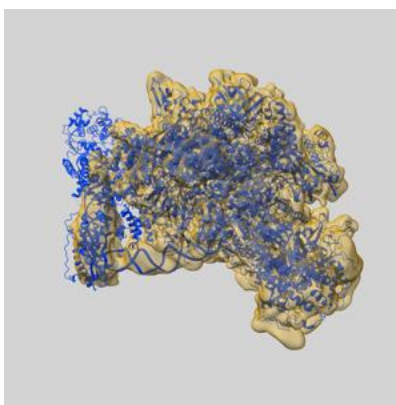
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62012 and PDB model 9K3B. Per-residue inclusion information can be found in section [3](#) on page [10](#).

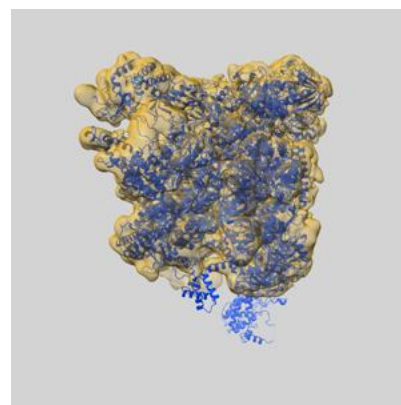
9.1 Map-model overlay [i](#)



X



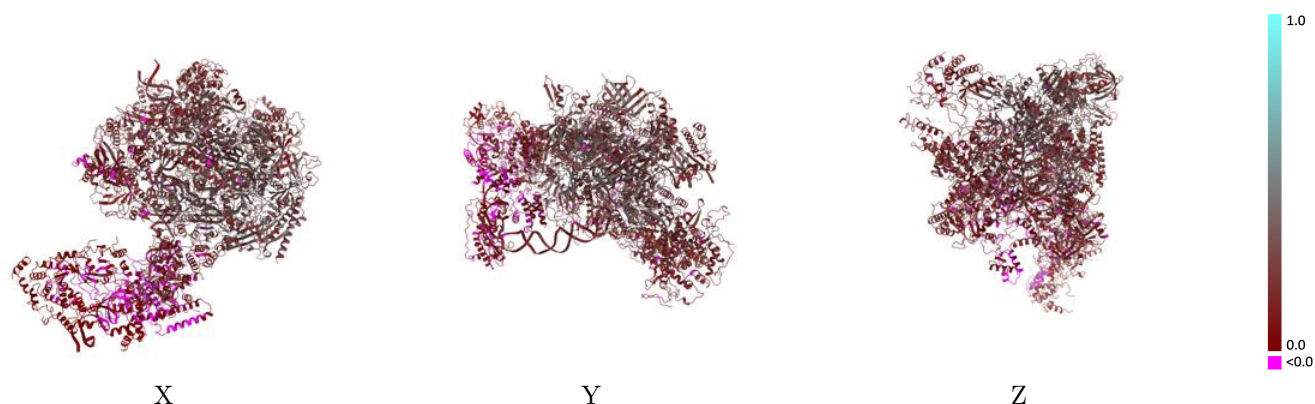
Y



Z

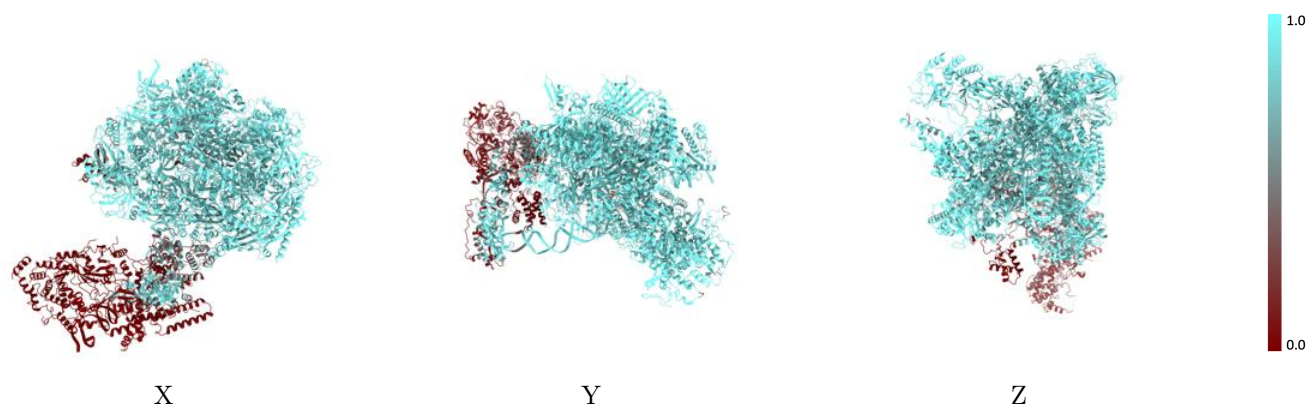
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



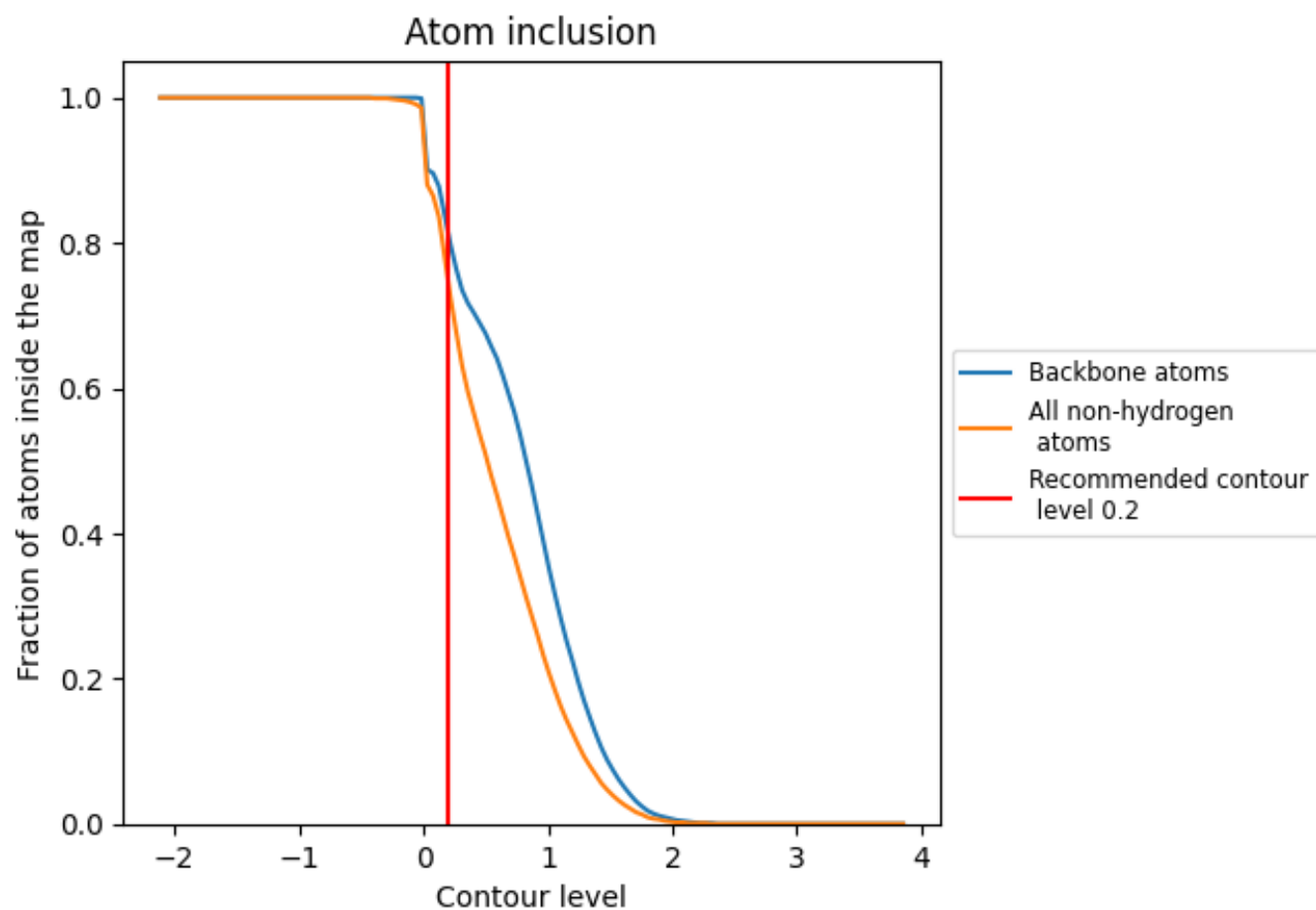
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 74% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7450	 0.2010
1	 0.0000	 -0.0070
3	 0.0050	 -0.0030
4	 0.0390	 0.0080
A	 0.9020	 0.2850
B	 0.9020	 0.2920
C	 0.9440	 0.3190
D	 0.9540	 0.1910
E	 0.9290	 0.2500
F	 0.9480	 0.3450
G	 0.9360	 0.2270
H	 0.9530	 0.3040
I	 0.9450	 0.2310
J	 0.9340	 0.3080
K	 0.9430	 0.3090
L	 0.9440	 0.2860
M	 0.6990	 0.1730
N	 0.9110	 0.1940
O	 0.9000	 0.1960
P	 0.7030	 0.1420
Q	 0.9290	 0.2260
U	 0.6790	 0.0630
V	 0.3370	 0.0420
W	 0.6700	 0.0260
X	 0.7120	 0.1160
Y	 0.7280	 0.1400
Z	 0.9170	 0.2800

