



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 01:00 PM UTC

PDB ID : 7W5W / pdb_00007w5w
EMDB ID : EMD-32322
Title : Cryo-EM structure of SoxS-dependent transcription activation complex with micF promoter DNA
Authors : Lin, W.; Feng, Y.
Deposited on : 2021-11-30
Resolution : 4.55 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

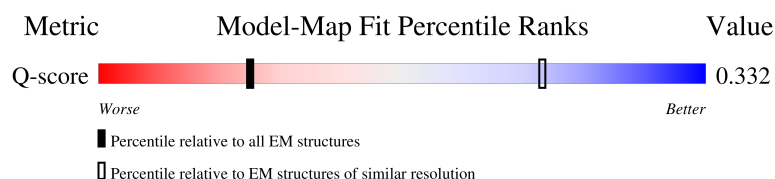
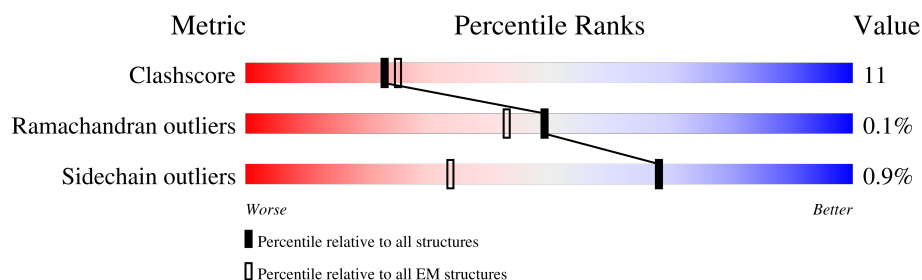
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.55 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2458 (4.05 - 5.04)

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

Mol	Chain	Length	Quality of chain
1	A	329	
1	B	329	
2	C	1342	
3	D	1407	

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Mol	Chain	Length	Quality of chain
4	E	91	77% 10% 13%
5	F	613	64% 14% 22%
6	1	70	37% 53% 10%
7	2	70	39% 51% 10%
8	J	107	69% 31%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 33053 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	311	Total	C	N	O	S	0	0
			2418	1512	425	473	8		
1	B	228	Total	C	N	O	S	0	0
			1767	1100	312	349	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1336	Total	C	N	O	S	0	0
			10528	6605	1831	2049	43		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	516	VAL	ASP	engineered mutation	UNP P0A8V2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1335	Total	C	N	O	S	0	0
			10344	6495	1846	1954	49		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	79	Total	C	N	O	S	0	0
			627	382	118	126	1		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	481	Total	C	N	O	S	0	0
			3861	2408	689	741	23		

- Molecule 6 is a DNA chain called micF promoter DNA forward strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1	63	Total	C	N	O	P	0	0
			1288	614	247	365	62		

- Molecule 7 is a DNA chain called micF promoter DNA reverse strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	2	63	Total	C	N	O	P	0	0
			1305	622	233	387	63		

- Molecule 8 is a protein called Regulatory protein SoxS.

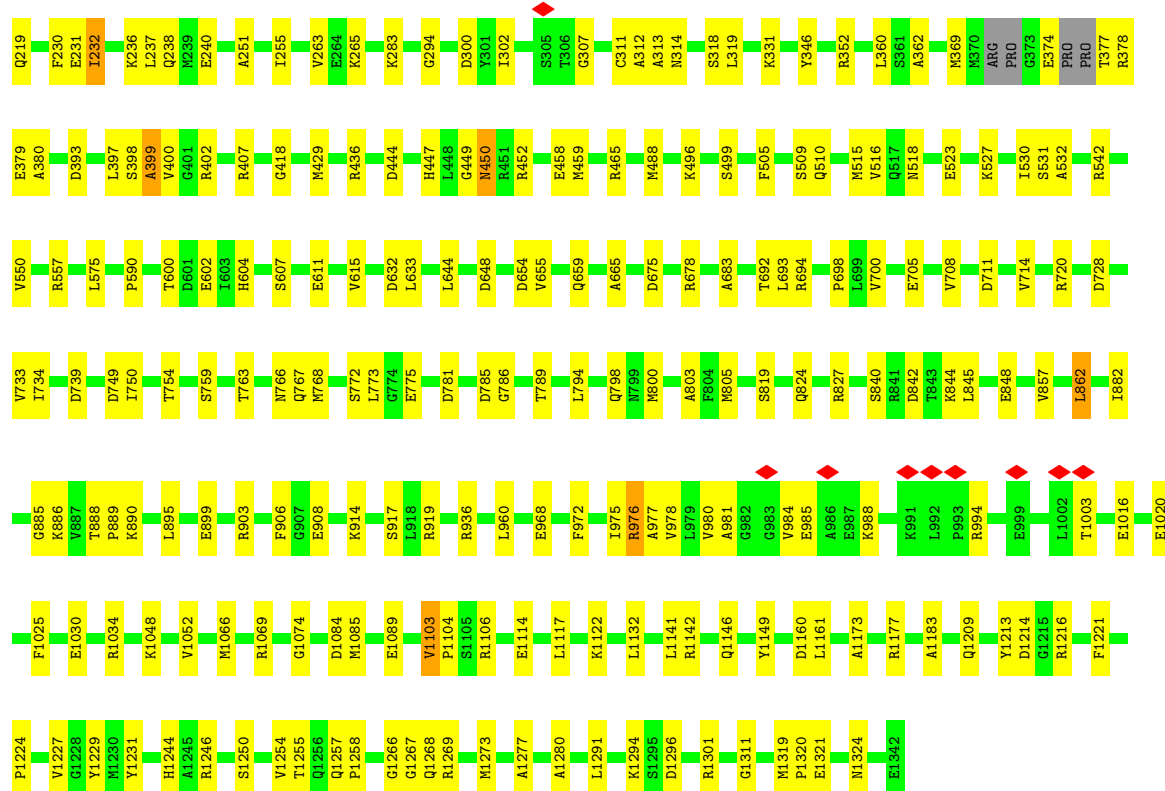
Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	107	Total	C	N	O	S	0	0
			912	579	170	160	3		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

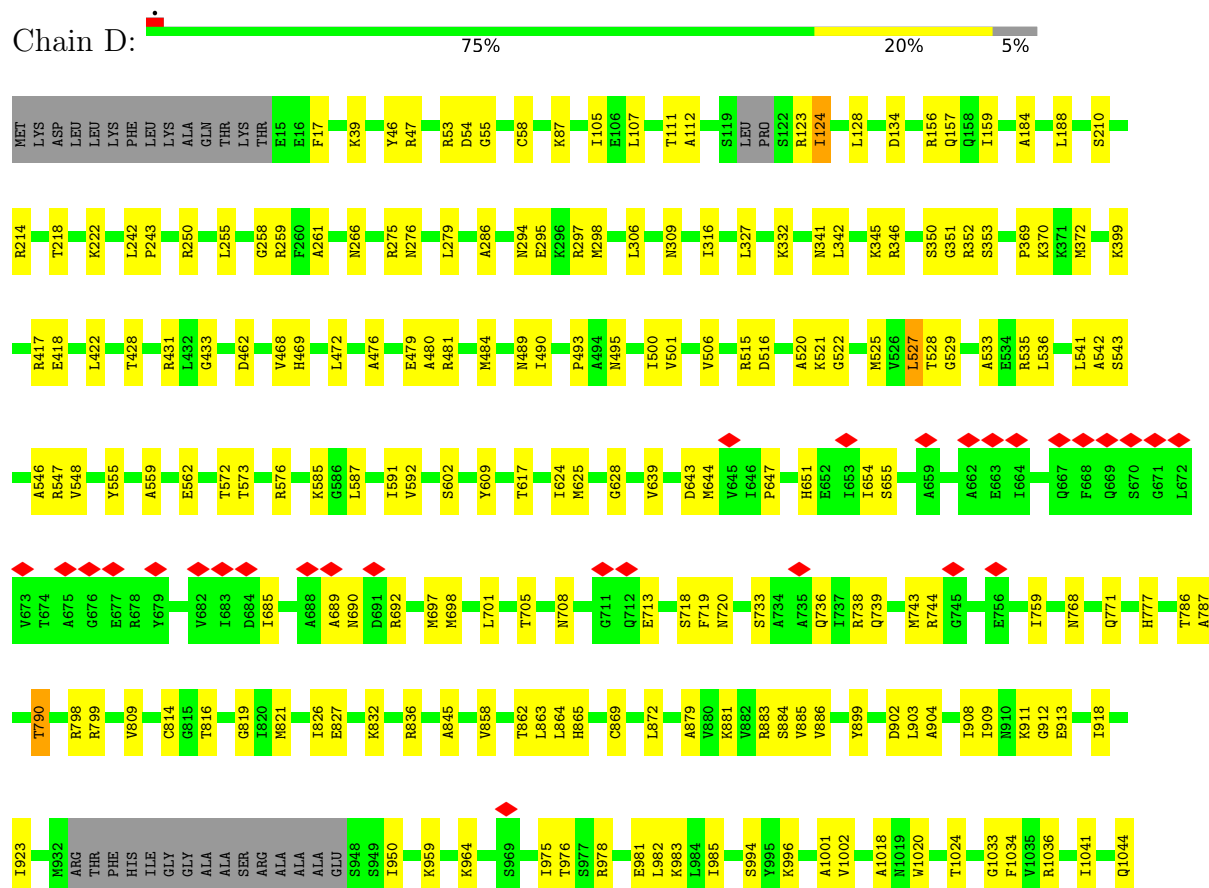
Mol	Chain	Residues	Atoms		AltConf
9	D	2	Total	Zn	0
			2	2	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

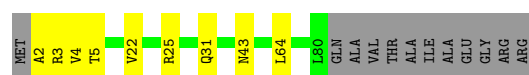
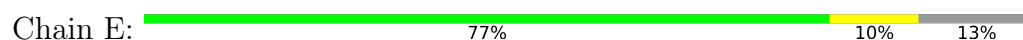
Mol	Chain	Residues	Atoms		AltConf
10	D	1	Total	Mg	0
			1	1	



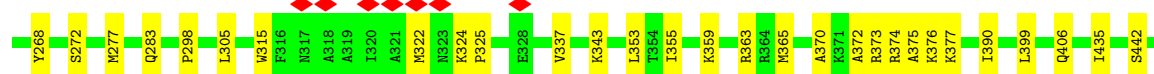
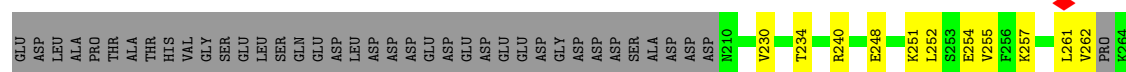
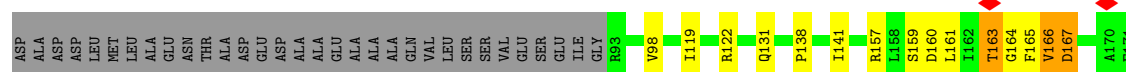
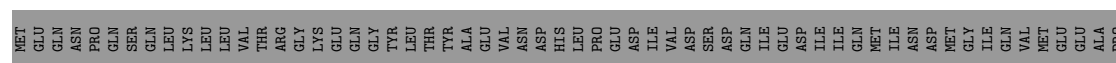
• Molecule 3: DNA-directed RNA polymerase subunit beta'



- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor RpoD

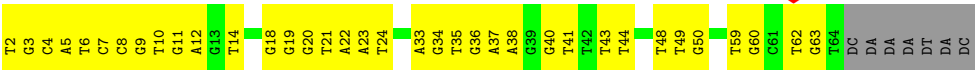


- Molecule 6: micF promoter DNA forward strand

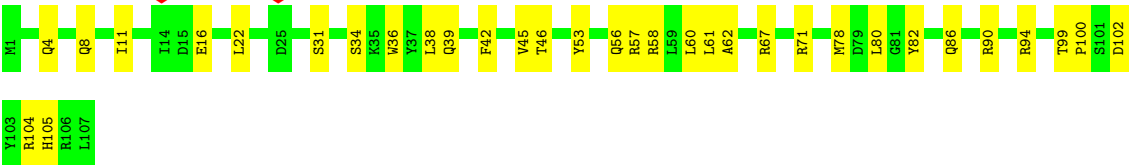




● Molecule 7: micF promoter DNA reverse strand



● Molecule 8: Regulatory protein SoxS



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	89000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.068	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.005	Depositor
Map size ($\text{\AA}$)	264.0, 264.0, 264.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/2449	0.61	0/3318
1	B	0.29	0/1789	0.55	0/2425
2	C	0.34	0/10692	0.62	4/14421 (0.0%)
3	D	0.32	0/10497	0.64	6/14171 (0.0%)
4	E	0.25	0/629	0.54	0/847
5	F	0.26	0/3910	0.65	4/5256 (0.1%)
6	1	0.34	0/1448	0.50	0/2231
7	2	0.33	0/1463	0.50	0/2261
8	J	0.25	0/932	0.62	0/1256
All	All	0.32	0/33809	0.61	14/46186 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	166	VAL	N-CA-C	8.94	119.73	110.62
2	C	41	GLN	CA-C-N	8.27	132.65	121.74
2	C	41	GLN	C-N-CA	8.27	132.65	121.74
3	D	500	ILE	N-CA-C	-6.31	106.29	111.91
5	F	163	THR	N-CA-C	-6.07	104.66	111.28
5	F	502	LYS	CA-C-N	6.00	132.21	122.48
5	F	502	LYS	C-N-CA	6.00	132.21	122.48
3	D	490	ILE	N-CA-C	-5.79	107.11	113.43
3	D	1186	TYR	N-CA-C	5.72	118.53	110.23
2	C	346	TYR	N-CA-C	-5.67	107.35	114.56
3	D	124	ILE	N-CA-C	-5.44	107.55	112.12
3	D	1184	ASP	CA-C-N	-5.12	113.36	119.05
3	D	1184	ASP	C-N-CA	-5.12	113.36	119.05
2	C	294	GLY	N-CA-C	-5.05	108.00	114.37

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2418	0	2467	53	0
1	B	1767	0	1789	30	0
2	C	10528	0	10531	174	0
3	D	10344	0	10527	192	0
4	E	627	0	634	7	0
5	F	3861	0	3871	71	0
6	1	1288	0	707	117	0
7	2	1305	0	716	147	0
8	J	912	0	917	31	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
All	All	33053	0	32159	715	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 11.

All (715) 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)
7:2:40:DG:C8	7:2:41:DT:H71	1.78	1.18
7:2:22:DA:H2''	7:2:23:DA:OP1	1.44	1.17
7:2:21:DT:H73	7:2:21:DT:OP2	1.47	1.13
6:1:86:DT:N3	6:1:87:DG:C5	2.17	1.12
6:1:73:DG:N7	6:1:74:DA:N1	1.98	1.11
3:D:520:ALA:HB3	3:D:546:ALA:HB2	1.33	1.07
7:2:37:DA:C2	7:2:38:DA:C5	2.41	1.07
2:C:975:ILE:HD12	2:C:994:ARG:HH22	1.14	1.05
6:1:86:DT:C2	6:1:87:DG:C8	2.43	1.05
7:2:23:DA:H8	7:2:24:DT:H72	1.17	1.05
1:A:591:LEU:HD21	1:A:631:GLU:HB3	1.37	1.03
1:A:593:VAL:HG12	8:J:16:GLU:HG2	1.41	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1:84:DG:C8	6:1:85:DA:N7	2.29	1.00
2:C:377:THR:HG23	2:C:380:ALA:H	1.21	1.00
3:D:527:LEU:HD12	3:D:533:ALA:HA	1.44	1.00
7:2:40:DG:C4	7:2:41:DT:C6	2.51	0.98
1:B:193:GLU:N	1:B:193:GLU:OE2	1.97	0.98
7:2:37:DA:N3	7:2:38:DA:C8	2.31	0.98
7:2:37:DA:C2	7:2:38:DA:C4	2.52	0.98
6:1:83:DG:N2	7:2:9:DG:C2	2.32	0.97
1:A:591:LEU:HG	1:A:592:THR:H	1.30	0.96
2:C:374:GLU:N	2:C:374:GLU:OE2	1.99	0.94
7:2:35:DT:H6	7:2:35:DT:H5''	1.32	0.94
6:1:84:DG:N2	7:2:8:DC:C2	2.36	0.94
7:2:36:DG:C6	7:2:37:DA:N6	2.36	0.93
1:B:191:ARG:HG2	1:B:191:ARG:HH11	1.34	0.92
6:1:56:DA:C2	7:2:35:DT:O4	2.23	0.91
7:2:36:DG:C5	7:2:37:DA:N6	2.39	0.91
5:F:166:VAL:O	5:F:167:ASP:HB3	1.70	0.91
6:1:84:DG:N7	6:1:85:DA:N7	2.20	0.89
7:2:2:DT:C6	7:2:3:DG:N7	2.41	0.88
7:2:33:DA:C2	7:2:34:DG:C2	2.61	0.88
7:2:23:DA:C8	7:2:24:DT:H72	2.08	0.88
2:C:977:ALA:O	2:C:980:VAL:HG12	1.74	0.88
6:1:84:DG:N2	7:2:8:DC:N3	2.21	0.87
1:A:593:VAL:HG12	8:J:16:GLU:CG	2.04	0.86
6:1:86:DT:C2	6:1:87:DG:N7	2.43	0.86
6:1:84:DG:O6	6:1:85:DA:N6	2.09	0.86
7:2:40:DG:C8	7:2:41:DT:C7	2.59	0.86
1:A:591:LEU:HD21	1:A:631:GLU:CB	2.05	0.86
7:2:21:DT:OP2	7:2:21:DT:C7	2.24	0.85
2:C:976:ARG:NH2	2:C:984:VAL:HG21	1.92	0.85
6:1:73:DG:C8	6:1:74:DA:C2	2.64	0.85
6:1:43:DA:C2	7:2:49:DT:N3	2.46	0.84
3:D:521:LYS:O	3:D:542:ALA:CB	2.26	0.83
7:2:43:DT:H4'	7:2:44:DT:OP1	1.78	0.83
2:C:975:ILE:HD12	2:C:994:ARG:NH2	1.93	0.82
6:1:73:DG:N7	6:1:74:DA:C2	2.47	0.82
6:1:81:DA:C2	7:2:10:DT:N3	2.47	0.82
6:1:81:DA:N1	7:2:10:DT:C4	2.47	0.82
2:C:975:ILE:O	2:C:978:VAL:HG12	1.80	0.81
7:2:8:DC:H2''	7:2:9:DG:C8	2.16	0.81
6:1:84:DG:C8	6:1:85:DA:C8	2.69	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:20:DG:H5''	7:2:20:DG:H8	1.47	0.79
7:2:35:DT:H5''	7:2:35:DT:C6	2.17	0.79
7:2:40:DG:C5	7:2:41:DT:C5	2.70	0.79
6:1:83:DG:N2	7:2:9:DG:N3	2.31	0.78
1:A:593:VAL:HG12	8:J:16:GLU:CB	2.14	0.78
5:F:98:VAL:CB	6:1:72:DG:H21	1.97	0.78
5:F:166:VAL:HA	5:F:262:VAL:HG12	1.64	0.78
6:1:81:DA:C6	7:2:9:DG:C6	2.72	0.77
7:2:37:DA:H2	7:2:38:DA:C4	1.99	0.77
3:D:525:MET:O	3:D:548:VAL:CB	2.33	0.77
7:2:20:DG:H5''	7:2:20:DG:C8	2.20	0.77
1:B:191:ARG:HG2	1:B:191:ARG:NH1	2.00	0.76
3:D:521:LYS:O	3:D:542:ALA:HB1	1.83	0.76
6:1:86:DT:O4	6:1:87:DG:O6	2.04	0.76
1:A:591:LEU:CD2	1:A:631:GLU:HB3	2.16	0.76
6:1:86:DT:C2	6:1:87:DG:C5	2.74	0.75
6:1:80:DC:O2	7:2:11:DG:N1	2.20	0.75
7:2:43:DT:C5	7:2:44:DT:C4	2.75	0.75
2:C:377:THR:HG22	2:C:380:ALA:CB	2.18	0.74
6:1:84:DG:C6	6:1:85:DA:N6	2.55	0.74
6:1:86:DT:N3	6:1:87:DG:N7	2.34	0.74
3:D:1179:PRO:HG2	3:D:1183:SER:O	1.88	0.74
3:D:1179:PRO:CD	3:D:1184:ASP:HA	2.18	0.74
7:2:40:DG:N7	7:2:41:DT:C7	2.52	0.73
6:1:51:DC:H1'	6:1:52:DC:H5'	1.69	0.73
6:1:58:DT:C2	7:2:34:DG:N2	2.57	0.72
6:1:86:DT:O2	6:1:87:DG:C8	2.40	0.72
6:1:81:DA:N1	7:2:10:DT:O4	2.22	0.72
2:C:377:THR:HG22	2:C:380:ALA:HB3	1.71	0.72
6:1:86:DT:C4	6:1:87:DG:C6	2.79	0.71
1:A:591:LEU:HG	1:A:592:THR:N	2.02	0.71
5:F:164:GLY:O	5:F:262:VAL:HB	1.90	0.70
6:1:43:DA:H2	7:2:49:DT:N3	1.87	0.70
6:1:86:DT:C4	7:2:5:DA:N1	2.59	0.70
6:1:86:DT:O2	6:1:87:DG:N9	2.24	0.70
7:2:2:DT:N1	7:2:3:DG:C8	2.60	0.70
5:F:161:LEU:O	5:F:164:GLY:CA	2.39	0.70
6:1:86:DT:N3	6:1:87:DG:C6	2.58	0.70
6:1:56:DA:N6	7:2:34:DG:O6	2.25	0.70
6:1:83:DG:C2	7:2:9:DG:C2	2.80	0.70
7:2:20:DG:H2''	7:2:21:DT:C7	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:200:ARG:HB2	6:1:79:DT:H3	1.57	0.69
3:D:521:LYS:O	3:D:542:ALA:HB2	1.92	0.69
5:F:166:VAL:O	5:F:167:ASP:CB	2.40	0.69
7:2:2:DT:H1'	7:2:3:DG:C8	2.28	0.69
7:2:35:DT:H2''	7:2:36:DG:O5'	1.93	0.69
2:C:1254:VAL:HG23	2:C:1255:THR:HG23	1.74	0.69
5:F:505:ILE:CG2	7:2:21:DT:C7	2.71	0.69
5:F:596:ARG:HD2	5:F:599:ARG:HE	1.57	0.69
1:A:58:GLU:HB3	1:A:145:LYS:HB3	1.75	0.68
1:A:591:LEU:CG	1:A:592:THR:H	2.03	0.68
7:2:21:DT:OP2	7:2:21:DT:C6	2.46	0.68
7:2:40:DG:N3	7:2:41:DT:O4'	2.26	0.68
6:1:81:DA:H2	7:2:10:DT:H3	1.32	0.68
7:2:20:DG:H2''	7:2:21:DT:H72	1.75	0.68
2:C:377:THR:CG2	2:C:380:ALA:H	2.01	0.68
6:1:58:DT:O2	7:2:34:DG:N2	2.27	0.68
2:C:377:THR:HG23	2:C:380:ALA:N	2.04	0.67
7:2:20:DG:H8	7:2:20:DG:C5'	2.06	0.67
1:A:591:LEU:HD11	1:A:631:GLU:HB3	1.77	0.67
2:C:360:LEU:HD11	2:C:378:ARG:HD2	1.75	0.67
1:A:182:ARG:HB3	1:A:206:GLU:HB3	1.77	0.67
7:2:43:DT:C4	7:2:44:DT:N3	2.63	0.67
7:2:21:DT:OP2	7:2:21:DT:H6	1.78	0.67
2:C:633:LEU:HD12	2:C:644:LEU:HB3	1.76	0.67
3:D:816:THR:H	3:D:883:ARG:HH22	1.44	0.66
7:2:33:DA:N1	7:2:34:DG:C2	2.64	0.66
7:2:50:DG:N7	8:J:90:ARG:NH1	2.43	0.66
3:D:790:THR:HB	7:2:12:DA:C6	2.31	0.66
5:F:161:LEU:O	5:F:164:GLY:N	2.29	0.66
3:D:827:GLU:HG2	3:D:994:SER:HB3	1.78	0.65
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.79	0.64
3:D:643:ASP:HB3	3:D:720:ASN:HD21	1.62	0.64
7:2:35:DT:H2''	7:2:36:DG:O4'	1.98	0.64
7:2:43:DT:C2	7:2:44:DT:C2	2.85	0.64
1:B:92:VAL:HG13	1:B:148:ARG:HH21	1.63	0.64
2:C:516:VAL:HG23	2:C:516:VAL:O	1.98	0.64
7:2:23:DA:H2'	7:2:24:DT:H72	1.80	0.64
7:2:2:DT:C1'	7:2:3:DG:C8	2.80	0.64
1:A:33:ARG:HH21	1:B:150:ARG:HG3	1.63	0.64
2:C:985:GLU:HB3	2:C:988:LYS:HB3	1.81	0.64
6:1:51:DC:C4	6:1:52:DC:C5	2.86	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:37:DA:C2	7:2:38:DA:C8	2.86	0.63
1:A:37:HIS:HB2	1:B:45:ARG:HH22	1.62	0.63
2:C:255:ILE:HB	2:C:263:VAL:HB	1.81	0.63
4:E:22:VAL:HG12	4:E:25:ARG:HH22	1.63	0.63
7:2:20:DG:H2''	7:2:21:DT:OP2	1.98	0.63
3:D:520:ALA:CB	3:D:546:ALA:HB2	2.21	0.63
6:1:58:DT:N3	7:2:34:DG:N2	2.47	0.63
6:1:53:DT:H3'	6:1:54:DT:H71	1.82	0.62
3:D:279:LEU:HD13	3:D:295:GLU:HG2	1.82	0.62
7:2:23:DA:H2'	7:2:24:DT:C7	2.29	0.62
2:C:976:ARG:HH22	2:C:984:VAL:HG21	1.62	0.62
1:B:99:ILE:HD11	1:B:143:ARG:HB3	1.81	0.62
1:A:593:VAL:HG12	8:J:16:GLU:HB3	1.83	0.61
6:1:86:DT:C4	6:1:87:DG:C5	2.87	0.61
6:1:84:DG:C6	6:1:85:DA:C6	2.88	0.61
7:2:8:DC:H2''	7:2:9:DG:H8	1.66	0.61
3:D:1179:PRO:HD2	3:D:1184:ASP:CB	2.31	0.61
3:D:1179:PRO:HD2	3:D:1184:ASP:HA	1.83	0.61
6:1:51:DC:N3	6:1:52:DC:C5	2.69	0.61
1:B:166:ARG:HD2	1:B:170:ARG:HH21	1.65	0.61
3:D:515:ARG:NH2	3:D:718:SER:O	2.34	0.61
3:D:294:ASN:HD22	5:F:406:GLN:HE21	1.49	0.60
2:C:91:THR:HG22	2:C:138:ILE:HA	1.84	0.60
7:2:40:DG:N3	7:2:41:DT:C6	2.69	0.60
3:D:814:CYS:SG	3:D:883:ARG:NH2	2.75	0.60
7:2:37:DA:C2	7:2:38:DA:N7	2.69	0.60
5:F:119:ILE:HG23	5:F:375:ALA:HB1	1.83	0.60
6:1:86:DT:O4	6:1:87:DG:C6	2.55	0.60
7:2:2:DT:C6	7:2:3:DG:C8	2.90	0.60
3:D:353:SER:HB3	3:D:372:MET:HE1	1.84	0.59
3:D:527:LEU:HD12	3:D:533:ALA:CA	2.27	0.59
7:2:2:DT:C5	7:2:3:DG:N7	2.70	0.59
1:A:79:LEU:HD11	2:C:693:LEU:HD11	1.85	0.59
2:C:314:ASN:O	2:C:352:ARG:NH1	2.35	0.59
6:1:80:DC:N3	7:2:11:DG:O6	2.35	0.59
2:C:848:GLU:HG2	2:C:888:THR:HG22	1.84	0.59
3:D:1368:ASP:OD1	3:D:1371:ARG:NH1	2.36	0.59
6:1:84:DG:C5	6:1:85:DA:C5	2.90	0.59
8:J:71:ARG:O	8:J:104:ARG:NH2	2.35	0.59
3:D:884:SER:OG	3:D:885:VAL:N	2.35	0.58
1:B:41:ASN:ND2	2:C:1216:ARG:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:98:VAL:CB	6:1:72:DG:N2	2.66	0.58
7:2:40:DG:C5	7:2:41:DT:C6	2.91	0.58
3:D:527:LEU:CD1	3:D:533:ALA:HA	2.28	0.58
6:1:73:DG:C8	6:1:74:DA:N1	2.65	0.58
1:A:64:VAL:HG11	1:A:171:LEU:HD11	1.85	0.58
2:C:1294:LYS:HE2	3:D:472:LEU:HD23	1.85	0.58
6:1:72:DG:H2''	6:1:73:DG:O4'	2.02	0.58
7:2:43:DT:C5	7:2:44:DT:O4	2.57	0.58
3:D:105:ILE:HD11	3:D:242:LEU:HD23	1.86	0.58
5:F:166:VAL:CA	5:F:262:VAL:HG12	2.33	0.58
2:C:180:ARG:NH2	2:C:393:ASP:O	2.37	0.58
7:2:34:DG:H2''	7:2:35:DT:OP2	2.03	0.58
4:E:25:ARG:HE	4:E:64:LEU:HD22	1.68	0.58
6:1:73:DG:N7	6:1:74:DA:C6	2.70	0.57
3:D:845:ALA:HB3	3:D:881:LYS:HB3	1.84	0.57
2:C:886:LYS:H	2:C:917:SER:HB2	1.69	0.57
3:D:47:ARG:NH2	6:1:60:DG:OP1	2.37	0.57
3:D:902:ASP:HB2	3:D:909:ILE:HB	1.85	0.57
7:2:37:DA:N3	7:2:38:DA:N7	2.52	0.57
2:C:199:ASP:HB3	6:1:78:DG:H22	1.68	0.57
3:D:809:VAL:HG23	3:D:912:GLY:H	1.70	0.57
3:D:826:ILE:HG22	3:D:832:LYS:H	1.70	0.57
5:F:160:ASP:O	5:F:163:THR:HB	2.05	0.57
6:1:54:DT:C4	6:1:55:DC:C5	2.92	0.57
7:2:36:DG:H2'	7:2:37:DA:C8	2.40	0.57
3:D:493:PRO:HB3	3:D:904:ALA:HB2	1.85	0.57
3:D:821:MET:HE2	3:D:879:ALA:HB1	1.86	0.57
7:2:59:DT:H72	8:J:39:GLN:HB3	1.86	0.57
1:B:193:GLU:H	1:B:193:GLU:CD	2.11	0.57
2:C:360:LEU:HD21	2:C:378:ARG:HD3	1.86	0.57
3:D:428:THR:HG23	3:D:433:GLY:HA3	1.87	0.57
7:2:33:DA:N1	7:2:34:DG:N1	2.53	0.57
3:D:250:ARG:O	3:D:266:ASN:ND2	2.38	0.56
3:D:259:ARG:HG3	5:F:502:LYS:HG2	1.87	0.56
7:2:20:DG:C8	7:2:20:DG:C5'	2.85	0.56
7:2:23:DA:H2''	7:2:24:DT:H5'	1.87	0.56
2:C:1142:ARG:NH1	2:C:1161:LEU:O	2.38	0.56
6:1:84:DG:H2'	6:1:85:DA:C8	2.40	0.56
2:C:360:LEU:HD11	2:C:378:ARG:CD	2.34	0.56
3:D:572:THR:OG1	3:D:573:THR:N	2.39	0.56
6:1:81:DA:C6	7:2:9:DG:O6	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:505:ILE:HG23	7:2:21:DT:C7	2.35	0.56
2:C:318:SER:OG	2:C:319:LEU:N	2.38	0.56
2:C:557:ARG:NH2	2:C:607:SER:O	2.39	0.56
8:J:53:TYR:HA	8:J:56:GLN:HB2	1.88	0.56
3:D:644:MET:HE1	3:D:701:LEU:HD11	1.87	0.56
7:2:43:DT:C7	7:2:44:DT:O4	2.54	0.56
3:D:17:PHE:O	3:D:1355:ARG:NH1	2.39	0.56
1:A:606:TYR:OH	1:A:654:SER:O	2.24	0.56
3:D:286:ALA:O	5:F:373:ARG:NH1	2.39	0.56
6:1:77:DT:H73	6:1:77:DT:OP2	2.06	0.56
2:C:633:LEU:HB3	2:C:644:LEU:HD22	1.87	0.55
8:J:67:ARG:NH1	8:J:104:ARG:O	2.38	0.55
2:C:89:GLY:HA2	2:C:140:GLY:HA3	1.86	0.55
2:C:1311:GLY:O	4:E:31:GLN:NE2	2.39	0.55
3:D:156:ARG:HG2	3:D:157:GLN:HG3	1.88	0.55
3:D:959:LYS:HD2	3:D:985:ILE:HG13	1.88	0.55
3:D:1089:LEU:HD13	3:D:1094:ASP:HA	1.88	0.55
3:D:1179:PRO:HD2	3:D:1184:ASP:CA	2.36	0.55
4:E:4:VAL:HG13	4:E:5:THR:HG23	1.88	0.55
8:J:8:GLN:HA	8:J:11:ILE:HD12	1.87	0.55
3:D:1262:ARG:O	3:D:1279:GLN:NE2	2.40	0.55
3:D:522:GLY:O	3:D:525:MET:HG2	2.07	0.55
3:D:950:ILE:HB	3:D:1018:ALA:HB3	1.89	0.55
5:F:138:PRO:HD2	5:F:353:LEU:HD13	1.87	0.55
2:C:1296:ASP:O	2:C:1301:ARG:NH2	2.40	0.55
7:2:40:DG:C2	7:2:41:DT:N1	2.75	0.55
6:1:81:DA:N6	7:2:9:DG:C6	2.75	0.55
2:C:968:GLU:O	2:C:972:PHE:N	2.38	0.55
3:D:1163:VAL:HG23	3:D:1177:ILE:HG22	1.88	0.55
5:F:161:LEU:C	5:F:164:GLY:H	2.15	0.54
1:B:124:VAL:HG21	1:B:210:THR:HG22	1.88	0.54
3:D:1268:ASN:ND2	3:D:1301:THR:OG1	2.40	0.54
5:F:592:ALA:HA	5:F:595:LEU:HD12	1.90	0.54
2:C:459:MET:HE3	2:C:505:PHE:HZ	1.71	0.54
4:E:2:ALA:N	4:E:5:THR:O	2.40	0.54
2:C:360:LEU:CD2	2:C:378:ARG:HD3	2.37	0.54
6:1:81:DA:H1'	6:1:82:DC:C6	2.43	0.54
3:D:790:THR:HB	7:2:12:DA:C5	2.43	0.54
7:2:20:DG:C2'	7:2:21:DT:H72	2.38	0.54
3:D:332:LYS:HA	3:D:1328:THR:HG21	1.89	0.54
6:1:81:DA:N6	7:2:9:DG:O6	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:379:GLU:OE1	2:C:379:GLU:HA	2.07	0.54
6:1:51:DC:N3	6:1:52:DC:C4	2.75	0.54
3:D:733:SER:H	3:D:736:GLN:HB2	1.72	0.54
6:1:86:DT:N3	7:2:5:DA:C2	2.76	0.54
1:A:235:ARG:HA	1:B:218:ARG:HE	1.73	0.54
2:C:1069:ARG:NH2	2:C:1114:GLU:OE2	2.37	0.54
3:D:476:ALA:HA	3:D:479:GLU:HB2	1.89	0.54
5:F:161:LEU:O	5:F:164:GLY:HA3	2.08	0.54
2:C:191:LYS:O	2:C:193:ASN:ND2	2.41	0.53
2:C:1132:LEU:HD13	2:C:1177:ARG:HH21	1.72	0.53
3:D:799:ARG:HB3	3:D:1309:ILE:HD12	1.91	0.53
5:F:251:LYS:HA	5:F:254:GLU:HB2	1.91	0.53
2:C:675:ASP:OD2	3:D:744:ARG:NH1	2.41	0.53
7:2:2:DT:N1	7:2:3:DG:N7	2.55	0.53
6:1:56:DA:H1'	7:2:36:DG:H22	1.74	0.53
2:C:678:ARG:HD3	2:C:1106:ARG:HD2	1.90	0.53
3:D:214:ARG:HH12	3:D:218:THR:HB	1.74	0.53
2:C:93:SER:OG	2:C:94:ALA:N	2.40	0.53
2:C:1016:GLU:O	2:C:1020:GLU:N	2.34	0.53
3:D:369:PRO:HG2	3:D:372:MET:HB3	1.89	0.53
6:1:58:DT:H3	7:2:34:DG:N2	2.05	0.53
6:1:86:DT:O4	7:2:5:DA:N1	2.42	0.53
8:J:57:ARG:HD2	8:J:60:LEU:HD12	1.91	0.53
1:A:9:LEU:O	1:B:227:GLN:NE2	2.41	0.53
2:C:805:MET:SD	2:C:805:MET:N	2.82	0.53
3:D:46:TYR:OH	3:D:47:ARG:NH2	2.42	0.53
2:C:240:GLU:HB3	2:C:283:LYS:HZ1	1.73	0.53
2:C:450:ASN:N	2:C:450:ASN:OD1	2.42	0.53
2:C:1268:GLN:OE1	3:D:352:ARG:NH1	2.42	0.53
5:F:505:ILE:HG23	7:2:21:DT:H73	1.91	0.53
1:A:592:THR:CG2	1:A:595:SER:HB2	2.39	0.52
2:C:1273:MET:HB3	3:D:428:THR:HB	1.91	0.52
3:D:275:ARG:HH11	3:D:298:MET:HB3	1.74	0.52
3:D:909:ILE:HD11	3:D:913:GLU:HB3	1.90	0.52
5:F:322:MET:N	5:F:322:MET:SD	2.83	0.52
1:A:23:HIS:HE1	1:A:25:LYS:HE3	1.74	0.52
1:A:597:ASN:OD1	1:A:600:LYS:NZ	2.42	0.52
1:A:91:ARG:HB3	1:A:122:GLU:HB3	1.91	0.52
2:C:232:ILE:HG23	2:C:237:LEU:HD13	1.91	0.52
2:C:772:SER:OG	2:C:775:GLU:OE1	2.28	0.52
2:C:1319:MET:HE1	2:C:1324:ASN:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:589:GLN:NE2	8:J:82:TYR:O	2.43	0.52
2:C:692:THR:OG1	2:C:694:ARG:O	2.27	0.52
3:D:547:ARG:HA	3:D:573:THR:HA	1.92	0.52
5:F:254:GLU:HA	5:F:257:LYS:HB2	1.92	0.52
7:2:7:DC:H2''	7:2:8:DC:C6	2.44	0.52
3:D:1046:ILE:HG21	3:D:1061:VAL:HA	1.92	0.52
6:1:84:DG:N2	7:2:8:DC:C4	2.78	0.52
7:2:19:DG:C2	7:2:20:DG:C6	2.98	0.52
2:C:720:ARG:NH2	2:C:749:ASP:OD1	2.43	0.51
3:D:1048:ARG:HH11	3:D:1059:LEU:HD23	1.75	0.51
5:F:161:LEU:O	5:F:165:PHE:N	2.42	0.51
6:1:86:DT:C2	6:1:87:DG:C4	2.98	0.51
2:C:230:PHE:HB3	2:C:237:LEU:HD11	1.92	0.51
6:1:37:DA:OP2	8:J:94:ARG:NH1	2.42	0.51
6:1:81:DA:C6	7:2:10:DT:O4	2.63	0.51
7:2:21:DT:H6	7:2:21:DT:P	2.34	0.51
2:C:886:LYS:HB3	2:C:917:SER:HA	1.92	0.51
3:D:1024:THR:HA	3:D:1125:PRO:HA	1.93	0.51
6:1:82:DC:C4	6:1:83:DG:C6	2.98	0.51
2:C:1296:ASP:OD2	3:D:345:LYS:NZ	2.43	0.51
3:D:123:ARG:HH21	3:D:1334:GLU:HG2	1.75	0.51
3:D:1173:ARG:HB2	3:D:1192:LYS:HD2	1.92	0.51
1:A:114:ASP:OD1	1:A:114:ASP:N	2.40	0.51
2:C:733:VAL:HG12	2:C:750:ILE:HA	1.92	0.51
3:D:124:ILE:O	3:D:128:LEU:N	2.41	0.51
6:1:76:DC:H3'	6:1:77:DT:H72	1.93	0.51
6:1:83:DG:N2	7:2:9:DG:C4	2.79	0.51
3:D:798:ARG:NH1	7:2:11:DG:OP1	2.44	0.51
7:2:40:DG:C5	7:2:41:DT:C7	2.94	0.51
3:D:53:ARG:NH2	3:D:87:LYS:O	2.44	0.51
3:D:1179:PRO:HD3	3:D:1184:ASP:HA	1.92	0.51
2:C:602:GLU:OE2	2:C:604:HIS:NE2	2.43	0.51
2:C:705:GLU:HB3	2:C:794:LEU:H	1.74	0.51
3:D:242:LEU:HD21	3:D:306:LEU:HD22	1.92	0.51
7:2:43:DT:N3	7:2:44:DT:N3	2.59	0.51
2:C:1103:VAL:HG13	2:C:1104:PRO:HD3	1.93	0.50
3:D:744:ARG:H	3:D:759:ILE:HD13	1.76	0.50
5:F:575:GLU:O	5:F:578:LYS:NZ	2.40	0.50
2:C:903:ARG:HG3	2:C:908:GLU:HB3	1.94	0.50
3:D:647:PRO:HG3	3:D:697:MET:HG2	1.93	0.50
3:D:708:ASN:HB3	3:D:713:GLU:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:252:LEU:HA	5:F:255:VAL:HG12	1.93	0.50
6:1:84:DG:C5	6:1:85:DA:N7	2.79	0.50
6:1:84:DG:H2'	6:1:85:DA:H8	1.75	0.50
7:2:59:DT:C7	8:J:39:GLN:HB3	2.41	0.50
1:A:51:MET:HE3	1:A:52:PRO:HD2	1.94	0.50
2:C:739:ASP:OD1	2:C:739:ASP:N	2.42	0.50
2:C:857:VAL:HG11	2:C:862:LEU:HD23	1.93	0.50
2:C:976:ARG:CZ	2:C:984:VAL:HG21	2.41	0.50
3:D:431:ARG:HD2	3:D:493:PRO:HG3	1.93	0.50
6:1:47:DA:N6	7:2:43:DT:O4	2.45	0.50
7:2:40:DG:C4	7:2:41:DT:C5	2.92	0.50
7:2:40:DG:C2	7:2:41:DT:C1'	2.94	0.50
2:C:798:GLN:HG2	2:C:827:ARG:HB3	1.93	0.50
3:D:690:ASN:O	3:D:738:ARG:NH1	2.43	0.50
5:F:359:LYS:O	5:F:363:ARG:NH1	2.44	0.50
6:1:55:DC:H2'	6:1:55:DC:O2	2.12	0.50
1:B:60:GLU:HG3	1:B:143:ARG:HE	1.77	0.49
2:C:377:THR:CG2	2:C:380:ALA:CB	2.89	0.49
2:C:1209:GLN:HG2	2:C:1224:PRO:HB2	1.94	0.49
3:D:651:HIS:HA	3:D:654:ILE:HB	1.94	0.49
5:F:283:GLN:HE22	5:F:343:LYS:HG2	1.77	0.49
6:1:29:DA:H5''	8:J:34:SER:HB3	1.93	0.49
2:C:518:ASN:OD1	2:C:518:ASN:N	2.45	0.49
3:D:899:TYR:O	3:D:1251:LYS:NZ	2.37	0.49
3:D:983:LYS:HB3	3:D:985:ILE:HD11	1.94	0.49
6:1:86:DT:C4	6:1:87:DG:O6	2.64	0.49
6:1:51:DC:H2''	6:1:52:DC:O5'	2.12	0.49
7:2:43:DT:C4	7:2:44:DT:C4	3.00	0.49
3:D:107:LEU:HA	3:D:276:ASN:HD21	1.77	0.49
5:F:591:GLU:O	5:F:595:LEU:N	2.42	0.49
5:F:157:ARG:NH1	5:F:159:SER:OG	2.40	0.49
7:2:60:DG:O6	8:J:36:TRP:NE1	2.45	0.49
2:C:125:GLY:HA2	2:C:499:SER:HB2	1.94	0.49
2:C:848:GLU:HG3	2:C:889:PRO:HD2	1.93	0.49
3:D:1175:LEU:HB2	3:D:1190:ILE:HD12	1.93	0.49
5:F:593:LYS:HD3	5:F:596:ARG:HB2	1.95	0.49
6:1:86:DT:O4	7:2:5:DA:C6	2.66	0.49
7:2:3:DG:H2''	7:2:4:DC:O4'	2.12	0.49
2:C:55:SER:OG	2:C:465:ARG:NH1	2.45	0.49
1:A:591:LEU:CD1	1:A:631:GLU:HB3	2.43	0.49
2:C:842:ASP:OD1	2:C:842:ASP:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:21:DT:OP2	7:2:21:DT:C5	2.66	0.49
2:C:164:THR:HG23	2:C:171:LEU:HD11	1.95	0.48
2:C:648:ASP:OD1	2:C:648:ASP:N	2.42	0.48
3:D:242:LEU:HD12	3:D:243:PRO:HD2	1.95	0.48
3:D:417:ARG:NH2	4:E:43:ASN:O	2.43	0.48
3:D:1273:ASP:N	3:D:1273:ASP:OD1	2.46	0.48
3:D:743:MET:HB2	3:D:759:ILE:HG23	1.94	0.48
1:A:593:VAL:CG1	8:J:16:GLU:HB3	2.42	0.48
2:C:890:LYS:HB2	2:C:914:LYS:HB2	1.95	0.48
3:D:468:VAL:O	3:D:469:HIS:ND1	2.46	0.48
3:D:555:TYR:HD2	3:D:585:LYS:HB3	1.79	0.48
3:D:787:ALA:HA	3:D:790:THR:OG1	2.13	0.48
3:D:1002:VAL:H	3:D:1020:TRP:HB3	1.78	0.48
7:2:40:DG:N7	7:2:41:DT:H73	2.29	0.48
2:C:632:ASP:N	2:C:632:ASP:OD1	2.42	0.48
3:D:1048:ARG:HE	3:D:1050:THR:HG22	1.79	0.48
3:D:1258:ARG:O	3:D:1258:ARG:NH1	2.45	0.48
6:1:83:DG:H2''	6:1:84:DG:O5'	2.14	0.48
2:C:530:ILE:HD11	2:C:575:LEU:HD23	1.95	0.48
2:C:975:ILE:CD1	2:C:994:ARG:HH22	2.04	0.48
3:D:1159:ILE:HG21	3:D:1179:PRO:HG3	1.95	0.48
3:D:1230:THR:HA	3:D:1233:ILE:HD12	1.95	0.48
2:C:1122:LYS:HD3	2:C:1229:TYR:CZ	2.49	0.48
5:F:555:GLU:HG3	5:F:590:ILE:HD12	1.94	0.48
7:2:37:DA:C2	7:2:38:DA:N9	2.81	0.48
2:C:14:ASP:OD2	2:C:15:PHE:N	2.47	0.48
2:C:1146:GLN:HE22	2:C:1160:ASP:HA	1.79	0.48
3:D:417:ARG:HG2	3:D:418:GLU:HG2	1.96	0.48
3:D:689:ALA:HB2	3:D:692:ARG:HH21	1.79	0.48
3:D:982:LEU:O	3:D:994:SER:OG	2.24	0.48
7:2:40:DG:N2	7:2:41:DT:H1'	2.29	0.48
2:C:557:ARG:NH1	2:C:611:GLU:OE2	2.46	0.48
3:D:294:ASN:OD1	3:D:297:ARG:NH1	2.47	0.48
5:F:399:LEU:HD22	5:F:447:ALA:HB2	1.95	0.48
1:A:593:VAL:CG1	8:J:16:GLU:CB	2.88	0.47
3:D:255:LEU:HD11	3:D:261:ALA:HB2	1.96	0.47
5:F:234:THR:HG21	5:F:248:GLU:HG2	1.96	0.47
1:A:617:GLU:HA	1:A:620:LYS:HB2	1.96	0.47
2:C:444:ASP:N	2:C:444:ASP:OD1	2.46	0.47
5:F:131:GLN:HB2	5:F:261:LEU:HD21	1.95	0.47
6:1:43:DA:H2	7:2:49:DT:C2	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1:51:DC:H42	6:1:52:DC:H41	1.62	0.47
6:1:87:DG:H2''	6:1:88:DC:H6	1.79	0.47
5:F:119:ILE:HA	5:F:122:ARG:HB2	1.95	0.47
2:C:30:ILE:HD13	2:C:575:LEU:HD21	1.95	0.47
2:C:231:GLU:O	2:C:238:GLN:N	2.46	0.47
2:C:1258:PRO:HG2	3:D:346:ARG:HB2	1.95	0.47
3:D:624:ILE:O	3:D:628:GLY:N	2.48	0.47
5:F:492:ASP:OD1	5:F:492:ASP:N	2.47	0.47
6:1:88:DC:H2''	6:1:89:DA:H5'	1.97	0.47
2:C:397:LEU:HB2	2:C:418:GLY:HA2	1.96	0.47
3:D:1067:ARG:HH12	3:D:1076:PRO:HG3	1.80	0.47
6:1:43:DA:C2	7:2:49:DT:C2	3.03	0.47
6:1:82:DC:H42	7:2:9:DG:H1	1.61	0.47
3:D:685:ILE:O	3:D:692:ARG:NH2	2.46	0.47
6:1:85:DA:H2''	6:1:86:DT:H73	1.97	0.47
3:D:786:THR:HG23	3:D:787:ALA:N	2.28	0.47
3:D:1081:VAL:HB	3:D:1085:GLY:HA2	1.96	0.47
5:F:305:LEU:HB3	5:F:315:TRP:HB2	1.96	0.47
5:F:480:PRO:HA	5:F:483:LEU:HD12	1.96	0.47
5:F:492:ASP:O	5:F:496:LYS:N	2.47	0.47
5:F:589:GLN:HG2	8:J:78:MET:HB2	1.97	0.47
3:D:903:LEU:HD22	3:D:1249:ASN:HD22	1.79	0.47
8:J:22:LEU:H	8:J:58:ARG:HH22	1.62	0.47
2:C:899:GLU:O	2:C:903:ARG:N	2.44	0.47
6:1:42:DA:C2	6:1:43:DA:C4	3.02	0.47
7:2:33:DA:C6	7:2:34:DG:N1	2.83	0.47
3:D:134:ASP:HB3	3:D:159:ILE:HD11	1.96	0.47
3:D:1034:PHE:HB2	3:D:1081:VAL:HG23	1.97	0.47
1:A:585:PRO:HA	1:A:606:TYR:HA	1.98	0.46
3:D:768:ASN:HB3	3:D:771:GLN:HG3	1.96	0.46
8:J:62:ALA:HB2	8:J:80:LEU:HD21	1.96	0.46
2:C:975:ILE:HD13	2:C:994:ARG:HH12	1.79	0.46
5:F:305:LEU:HD12	5:F:315:TRP:HA	1.96	0.46
7:2:33:DA:C2	7:2:34:DG:N3	2.83	0.46
2:C:208:ILE:HG23	2:C:362:ALA:HB1	1.97	0.46
3:D:1109:LEU:HD13	3:D:1113:VAL:HB	1.96	0.46
6:1:55:DC:O2	6:1:55:DC:C2'	2.62	0.46
1:B:191:ARG:NH1	1:B:191:ARG:CG	2.73	0.46
2:C:654:ASP:OD1	2:C:659:GLN:NE2	2.48	0.46
3:D:1148:ARG:NH1	6:1:83:DG:OP1	2.48	0.46
5:F:268:TYR:O	5:F:272:SER:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:LEU:HD21	1:B:180:VAL:HG11	1.97	0.46
2:C:980:VAL:HG13	2:C:981:ALA:N	2.30	0.46
8:J:58:ARG:HB3	8:J:80:LEU:HG	1.97	0.46
2:C:447:HIS:HD2	2:C:449:GLY:H	1.62	0.46
5:F:581:ASP:OD1	5:F:581:ASP:N	2.49	0.46
1:A:630:THR:OG1	1:A:631:GLU:OE1	2.31	0.46
1:B:191:ARG:HD2	1:B:192:VAL:N	2.30	0.46
3:D:886:VAL:HA	3:D:1258:ARG:HD3	1.98	0.46
3:D:978:ARG:NH2	3:D:1197:ASN:OD1	2.42	0.46
2:C:251:ALA:O	2:C:265:LYS:NZ	2.41	0.46
3:D:495:ASN:OD1	3:D:495:ASN:N	2.48	0.46
3:D:1220:ILE:HG22	3:D:1229:VAL:HG22	1.98	0.46
6:1:84:DG:N2	7:2:7:DC:C2	2.84	0.46
1:A:648:GLU:HG2	1:A:649:ASN:H	1.80	0.46
1:B:16:ILE:HG12	1:B:26:VAL:HG12	1.98	0.46
3:D:591:ILE:HG23	3:D:592:VAL:HG13	1.98	0.46
3:D:705:THR:HG21	3:D:719:PHE:H	1.80	0.46
1:A:207:THR:OG1	1:A:208:ASN:N	2.49	0.45
1:A:604:ILE:HD11	1:A:613:ARG:HG2	1.97	0.45
1:B:13:LEU:HD21	1:B:16:ILE:HD11	1.98	0.45
1:B:207:THR:OG1	1:B:208:ASN:N	2.49	0.45
2:C:786:GLY:H	2:C:789:THR:HB	1.81	0.45
3:D:342:LEU:HD11	3:D:1352:ILE:HB	1.98	0.45
3:D:559:ALA:HB3	3:D:562:GLU:HB3	1.97	0.45
3:D:625:MET:HE2	3:D:625:MET:HB2	1.74	0.45
1:A:75:GLN:HB2	1:A:132:HIS:HB2	1.97	0.45
2:C:840:SER:HG	2:C:1048:LYS:H	1.63	0.45
3:D:836:ARG:HG3	3:D:869:CYS:HB3	1.98	0.45
3:D:964:LYS:O	3:D:976:THR:OG1	2.28	0.45
8:J:31:SER:HB3	8:J:38:LEU:HD22	1.99	0.45
1:A:614:THR:HG23	1:A:617:GLU:H	1.81	0.45
3:D:520:ALA:HB2	3:D:543:SER:HB3	1.98	0.45
3:D:1063:ASP:HA	3:D:1103:GLY:HA3	1.98	0.45
1:B:48:LEU:HD11	3:D:535:ARG:HG2	1.98	0.45
6:1:84:DG:C5	6:1:85:DA:C6	3.04	0.45
1:A:51:MET:HE2	1:A:216:ALA:HA	1.99	0.45
1:A:215:GLU:HA	1:A:218:ARG:HB3	1.97	0.45
2:C:120:GLN:HE22	2:C:488:MET:HB3	1.82	0.45
6:1:88:DC:H2"	6:1:89:DA:C8	2.52	0.45
7:2:43:DT:C6	7:2:44:DT:C4	3.04	0.45
6:1:44:DA:C6	6:1:45:DA:N1	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:22:DA:C2'	7:2:23:DA:OP1	2.32	0.45
7:2:37:DA:N3	7:2:38:DA:N9	2.64	0.45
2:C:377:THR:HG22	2:C:380:ALA:HB2	1.94	0.45
5:F:456:MET:O	5:F:459:THR:OG1	2.32	0.45
2:C:803:ALA:HB1	2:C:805:MET:HE1	1.97	0.45
3:D:697:MET:HB2	3:D:698:MET:HE2	1.97	0.45
3:D:1261:LEU:HD21	3:D:1306:LEU:HD12	1.99	0.45
2:C:216:THR:H	2:C:219:GLN:HB2	1.81	0.45
2:C:1141:LEU:HD21	2:C:1173:ALA:HB2	1.99	0.45
6:1:51:DC:H42	6:1:52:DC:N4	2.15	0.45
6:1:86:DT:O2	6:1:87:DG:C4	2.69	0.45
8:J:99:THR:OG1	8:J:102:ASP:OD2	2.35	0.45
3:D:528:THR:OG1	3:D:529:GLY:N	2.49	0.45
3:D:816:THR:O	3:D:883:ARG:NH1	2.47	0.45
6:1:51:DC:H1'	6:1:52:DC:C5'	2.44	0.45
3:D:609:TYR:HB3	3:D:617:THR:HG21	1.97	0.44
3:D:1057:SER:OG	3:D:1058:SER:N	2.50	0.44
2:C:206:ALA:HB1	2:C:429:MET:HE1	1.99	0.44
3:D:1036:ARG:HE	3:D:1081:VAL:HG11	1.81	0.44
3:D:1307:LEU:HD11	3:D:1311:LYS:HD2	1.99	0.44
5:F:372:ALA:O	5:F:376:LYS:NZ	2.50	0.44
1:B:207:THR:HG1	1:B:208:ASN:H	1.66	0.44
2:C:515:MET:HE1	2:C:527:LYS:HE3	1.99	0.44
2:C:800:MET:HE2	2:C:800:MET:HB3	1.79	0.44
3:D:259:ARG:NH2	5:F:499:LYS:O	2.50	0.44
3:D:975:ILE:HD13	3:D:1001:ALA:HB3	1.99	0.44
3:D:1033:GLY:HA2	3:D:1114:GLN:HE21	1.81	0.44
3:D:1041:ILE:HB	3:D:1044:GLN:HB2	2.00	0.44
7:2:43:DT:H71	7:2:44:DT:O4	2.17	0.44
2:C:960:LEU:HB3	2:C:1025:PHE:HE1	1.82	0.44
3:D:309:ASN:ND2	3:D:316:ILE:O	2.37	0.44
2:C:665:ALA:HB2	2:C:683:ALA:HB2	2.00	0.44
3:D:1181:ASP:OD1	3:D:1181:ASP:N	2.51	0.44
6:1:86:DT:O2	6:1:87:DG:O4'	2.36	0.44
1:A:73:GLY:H	2:C:728:ASP:CG	2.25	0.44
2:C:550:VAL:O	3:D:777:HIS:NE2	2.37	0.44
5:F:442:SER:OG	5:F:446:GLN:OE1	2.35	0.44
6:1:41:DC:H42	7:2:50:DG:H1	1.65	0.44
2:C:496:LYS:HB3	2:C:496:LYS:HE2	1.79	0.44
2:C:734:ILE:HG22	2:C:749:ASP:HB2	2.00	0.44
2:C:819:SER:HB3	2:C:1085:MET:HE2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:THR:HB	2:C:773:LEU:HD22	1.98	0.44
1:B:82:LEU:HD13	1:B:85:LEU:HD12	1.99	0.44
2:C:13:LYS:HD2	2:C:1149:TYR:HB2	1.99	0.44
2:C:452:ARG:NH2	2:C:458:GLU:OE2	2.50	0.44
6:1:84:DG:O6	7:2:6:DT:O4	2.35	0.44
2:C:436:ARG:O	2:C:436:ARG:NH1	2.50	0.43
3:D:210:SER:O	3:D:214:ARG:N	2.51	0.43
3:D:863:LEU:HD22	3:D:865:HIS:HD2	1.83	0.43
8:J:104:ARG:HD2	8:J:105:HIS:CE1	2.53	0.43
2:C:759:SER:HG	2:C:763:THR:H	1.61	0.43
2:C:917:SER:O	2:C:919:ARG:NH1	2.51	0.43
2:C:936:ARG:HH12	5:F:495:ARG:HD3	1.83	0.43
2:C:1066:MET:HB3	2:C:1066:MET:HE3	1.85	0.43
2:C:1277:ALA:HB2	3:D:428:THR:HG21	1.99	0.43
6:1:84:DG:H2''	6:1:85:DA:O4'	2.18	0.43
7:2:19:DG:N1	7:2:20:DG:O6	2.51	0.43
1:A:212:ASP:OD2	1:A:215:GLU:N	2.51	0.43
2:C:232:ILE:HG13	2:C:331:LYS:HA	2.00	0.43
2:C:1280:ALA:O	3:D:431:ARG:NH2	2.45	0.43
3:D:350:SER:OG	3:D:351:GLY:N	2.52	0.43
2:C:302:ILE:HD12	2:C:307:GLY:HA2	2.01	0.43
5:F:376:LYS:HE2	5:F:376:LYS:HB2	1.87	0.43
2:C:14:ASP:HA	2:C:1183:ALA:HB3	2.00	0.43
6:1:86:DT:H2''	6:1:87:DG:O5'	2.18	0.43
7:2:59:DT:C7	8:J:39:GLN:CB	2.97	0.43
1:A:29:GLU:HA	1:A:30:PRO:HA	1.82	0.43
5:F:161:LEU:HD12	5:F:164:GLY:HA3	2.00	0.43
7:2:2:DT:C1'	7:2:3:DG:H8	2.28	0.43
1:A:110:VAL:HB	1:A:131:CYS:H	1.83	0.43
1:A:591:LEU:CG	1:A:631:GLU:HB3	2.49	0.43
1:B:61:ILE:HG23	1:B:142:MET:HB3	2.01	0.43
2:C:67:GLU:OE2	2:C:105:TYR:OH	2.36	0.43
2:C:705:GLU:HA	2:C:708:VAL:HG12	2.01	0.43
2:C:1103:VAL:HG11	3:D:639:VAL:HG11	2.01	0.43
3:D:399:LYS:HA	3:D:399:LYS:HD2	1.85	0.43
2:C:844:LYS:HD2	2:C:845:LEU:HG	2.00	0.43
2:C:895:LEU:HD13	2:C:899:GLU:HB2	2.00	0.43
3:D:1164:SER:HB2	3:D:1176:VAL:HG23	2.01	0.43
3:D:39:LYS:NZ	3:D:54:ASP:OD2	2.39	0.43
3:D:981:GLU:HB2	3:D:996:LYS:HA	2.01	0.43
6:1:83:DG:C2	7:2:9:DG:N2	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1269:ARG:HB3	7:2:14:DT:H5'	2.00	0.43
3:D:573:THR:HG23	3:D:576:ARG:H	1.83	0.43
6:1:84:DG:H2''	6:1:85:DA:C5'	2.48	0.43
2:C:1244:HIS:NE2	2:C:1266:GLY:O	2.52	0.42
3:D:258:GLY:O	3:D:259:ARG:NH1	2.52	0.42
3:D:481:ARG:NH1	4:E:3:ARG:O	2.52	0.42
3:D:1259:GLN:HE21	3:D:1262:ARG:HE	1.67	0.42
1:B:40:GLY:O	1:B:44:ARG:N	2.46	0.42
2:C:509:SER:OG	2:C:510:GLN:N	2.52	0.42
3:D:422:LEU:HB2	3:D:469:HIS:HB2	2.01	0.42
3:D:516:ASP:OD1	3:D:516:ASP:N	2.47	0.42
3:D:739:GLN:HB3	3:D:744:ARG:HB3	2.01	0.42
7:2:18:DG:C8	7:2:19:DG:C8	3.07	0.42
2:C:300:ASP:OD1	2:C:313:ALA:N	2.51	0.42
2:C:754:THR:N	2:C:767:GLN:OE1	2.50	0.42
3:D:370:LYS:HE2	3:D:370:LYS:HB2	1.70	0.42
3:D:480:ALA:HA	3:D:484:MET:HG3	2.01	0.42
5:F:572:THR:H	5:F:575:GLU:HB2	1.83	0.42
8:J:4:GLN:HG3	8:J:45:VAL:HG13	2.02	0.42
2:C:975:ILE:CD1	2:C:994:ARG:HH12	2.32	0.42
3:D:1061:VAL:HB	3:D:1105:ALA:HB3	2.02	0.42
5:F:138:PRO:HA	5:F:141:ILE:HD12	2.01	0.42
7:2:4:DC:N4	7:2:5:DA:N6	2.68	0.42
1:A:78:ILE:HA	1:A:81:ILE:HD12	2.02	0.42
1:A:232:VAL:HA	1:B:218:ARG:HG3	2.02	0.42
1:A:591:LEU:CG	1:A:592:THR:N	2.73	0.42
3:D:536:LEU:HG	3:D:541:LEU:HB2	2.02	0.42
3:D:787:ALA:O	3:D:790:THR:OG1	2.33	0.42
5:F:240:ARG:HH12	5:F:353:LEU:HA	1.84	0.42
2:C:202:ARG:HH12	7:2:6:DT:H3'	1.84	0.42
2:C:360:LEU:CD1	2:C:378:ARG:CD	2.98	0.42
3:D:184:ALA:O	3:D:188:LEU:N	2.49	0.42
3:D:1318:SER:OG	3:D:1319:PHE:N	2.53	0.42
1:B:25:LYS:HE3	1:B:204:GLU:HG3	2.01	0.42
3:D:858:VAL:HG23	3:D:862:THR:HG23	2.00	0.42
3:D:863:LEU:HD12	3:D:908:ILE:HG23	2.02	0.42
6:1:86:DT:C2	6:1:87:DG:N9	2.80	0.42
3:D:786:THR:CG2	3:D:787:ALA:N	2.83	0.42
2:C:1257:GLN:OE1	3:D:341:ASN:ND2	2.53	0.41
3:D:479:GLU:OE2	3:D:1361:THR:OG1	2.32	0.41
3:D:489:ASN:OD1	3:D:489:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:651:HIS:O	3:D:655:SER:N	2.48	0.41
5:F:390:ILE:HD12	5:F:435:ILE:HD11	2.02	0.41
8:J:99:THR:HA	8:J:100:PRO:HD3	1.93	0.41
2:C:542:ARG:NH1	6:1:79:DT:OP1	2.52	0.41
2:C:906:PHE:HD2	5:F:611:LEU:HG	1.86	0.41
2:C:1214:ASP:HB2	2:C:1221:PHE:HE2	1.84	0.41
3:D:501:VAL:HG23	3:D:602:SER:HB3	2.01	0.41
6:1:88:DC:C2'	6:1:89:DA:C8	3.03	0.41
7:2:33:DA:C6	7:2:34:DG:C6	3.08	0.41
2:C:398:SER:O	2:C:400:VAL:N	2.54	0.41
2:C:768:MET:O	2:C:785:ASP:N	2.47	0.41
2:C:803:ALA:HA	2:C:1227:VAL:HG22	2.02	0.41
2:C:1066:MET:O	2:C:1074:GLY:N	2.53	0.41
2:C:1296:ASP:HB3	2:C:1321:GLU:H	1.86	0.41
3:D:218:THR:O	3:D:222:LYS:N	2.46	0.41
8:J:42:PHE:O	8:J:46:THR:OG1	2.37	0.41
3:D:55:GLY:H	3:D:58:CYS:HB2	1.84	0.41
1:A:594:ARG:HH12	1:A:625:GLY:HA3	1.85	0.41
2:C:515:MET:HE3	2:C:523:GLU:HB2	2.03	0.41
3:D:462:ASP:N	3:D:462:ASP:OD1	2.52	0.41
3:D:522:GLY:O	3:D:525:MET:SD	2.79	0.41
3:D:799:ARG:NH2	3:D:1146:GLU:OE1	2.54	0.41
5:F:513:ASP:OD1	5:F:513:ASP:N	2.52	0.41
7:2:62:DT:H2'	7:2:63:DG:C8	2.56	0.41
1:A:7:GLU:O	1:B:150:ARG:NH2	2.53	0.41
2:C:1089:GLU:HA	2:C:1213:TYR:HE2	1.86	0.41
3:D:911:LYS:HE2	3:D:911:LYS:HB3	1.83	0.41
5:F:365:MET:HE3	5:F:365:MET:HB3	1.90	0.41
5:F:462:LYS:HD3	5:F:465:ARG:HH21	1.85	0.41
2:C:1291:LEU:HD13	3:D:345:LYS:HD2	2.02	0.41
3:D:214:ARG:HD2	3:D:214:ARG:HA	1.87	0.41
5:F:355:ILE:HG22	5:F:359:LYS:HE3	2.03	0.41
6:1:68:DA:H2''	6:1:69:DA:H5'	2.03	0.41
2:C:74:ARG:N	2:C:97:ARG:O	2.54	0.41
2:C:369:MET:HE2	2:C:369:MET:HB3	1.84	0.41
2:C:882:ILE:HD11	2:C:885:GLY:HA2	2.03	0.41
2:C:1246:ARG:HD2	2:C:1267:GLY:N	2.35	0.41
5:F:557:LYS:HB2	5:F:560:ARG:HH21	1.86	0.41
7:2:37:DA:C4	7:2:38:DA:C8	3.07	0.41
1:B:133:LEU:HD23	1:B:133:LEU:HA	1.87	0.41
2:C:236:LYS:HD3	2:C:236:LYS:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:711:ASP:OD1	2:C:711:ASP:N	2.48	0.41
2:C:1319:MET:HA	2:C:1320:PRO:HD3	1.96	0.41
3:D:111:THR:OG1	3:D:112:ALA:N	2.54	0.41
3:D:819:GLY:O	3:D:881:LYS:NZ	2.45	0.41
3:D:1284:ARG:HA	3:D:1287:ILE:HG12	2.03	0.41
5:F:315:TRP:HZ2	5:F:337:VAL:HG11	1.86	0.41
5:F:505:ILE:CG2	7:2:21:DT:H73	2.45	0.41
6:1:86:DT:C4	6:1:87:DG:N7	2.88	0.41
7:2:4:DC:N3	7:2:5:DA:C5	2.89	0.41
7:2:40:DG:N3	7:2:41:DT:C1'	2.83	0.41
2:C:1117:LEU:HD23	2:C:1117:LEU:HA	1.90	0.41
3:D:1348:LYS:HD3	3:D:1348:LYS:HA	1.90	0.41
8:J:61:LEU:HD12	8:J:61:LEU:HA	1.92	0.41
1:A:59:VAL:HG11	1:A:82:LEU:HD11	2.03	0.40
1:A:139:SER:OG	1:A:140:ILE:N	2.54	0.40
1:A:152:TYR:CZ	2:C:824:GLN:HG2	2.55	0.40
2:C:1084:ASP:HB2	2:C:1216:ARG:HG2	2.02	0.40
3:D:923:ILE:HD11	3:D:1253:ILE:HG12	2.02	0.40
5:F:277:MET:HE1	5:F:365:MET:HE2	2.04	0.40
2:C:311:CYS:SG	2:C:312:ALA:N	2.95	0.40
2:C:766:ASN:OD1	2:C:767:GLN:N	2.53	0.40
2:C:1030:GLU:O	2:C:1034:ARG:N	2.52	0.40
5:F:157:ARG:HA	5:F:157:ARG:HD3	1.91	0.40
5:F:374:ARG:HA	5:F:377:LYS:HG3	2.02	0.40
6:1:44:DA:N1	6:1:45:DA:C2	2.89	0.40
6:1:56:DA:C2	7:2:35:DT:C4	3.04	0.40
6:1:87:DG:C2	7:2:5:DA:C2	3.09	0.40
7:2:40:DG:N9	7:2:41:DT:H71	2.26	0.40
1:B:171:LEU:HD23	1:B:171:LEU:HA	1.89	0.40
2:C:399:ALA:HA	2:C:402:ARG:HB3	2.02	0.40
6:1:43:DA:C2	7:2:49:DT:C4	3.08	0.40
7:2:48:DT:O4	8:J:86:GLN:NE2	2.41	0.40
2:C:13:LYS:HB2	2:C:1149:TYR:HB2	2.03	0.40
2:C:407:ARG:HD3	2:C:407:ARG:HA	1.82	0.40
2:C:531:SER:OG	2:C:532:ALA:N	2.54	0.40
2:C:698:PRO:HB3	2:C:1231:TYR:CZ	2.56	0.40
5:F:370:ALA:HA	5:F:373:ARG:HB3	2.03	0.40
6:1:35:DG:H2'	6:1:36:DA:C8	2.57	0.40
2:C:1246:ARG:NH2	2:C:1250:SER:O	2.54	0.40
3:D:327:LEU:HD23	3:D:327:LEU:HA	1.82	0.40
3:D:864:LEU:HD21	3:D:872:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1054:THR:HG23	3:D:1056:LEU:H	1.86	0.40
3:D:1247:LYS:HE2	3:D:1247:LYS:HB2	1.84	0.40
3:D:1332:LEU:O	3:D:1336:ALA:N	2.54	0.40
5:F:324:LYS:HA	5:F:325:PRO:HD3	1.90	0.40
6:1:72:DG:H2''	6:1:73:DG:C5'	2.51	0.40
7:2:35:DT:H2'	7:2:36:DG:C8	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	307/329 (93%)	282 (92%)	25 (8%)	0	100	100
1	B	226/329 (69%)	211 (93%)	15 (7%)	0	100	100
2	C	1330/1342 (99%)	1252 (94%)	77 (6%)	1 (0%)	48	83
3	D	1327/1407 (94%)	1237 (93%)	89 (7%)	1 (0%)	48	83
4	E	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
5	F	473/613 (77%)	427 (90%)	43 (9%)	3 (1%)	21	58
8	J	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
All	All	3845/4218 (91%)	3585 (93%)	255 (7%)	5 (0%)	49	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	399	ALA
5	F	507	MET
5	F	298	PRO
3	D	1184	ASP
5	F	167	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/286 (94%)	266 (99%)	3 (1%)	65	74
1	B	196/286 (68%)	190 (97%)	6 (3%)	35	56
2	C	1149/1157 (99%)	1136 (99%)	13 (1%)	65	74
3	D	1107/1168 (95%)	1101 (100%)	6 (0%)	81	81
4	E	67/75 (89%)	67 (100%)	0	100	100
5	F	415/540 (77%)	413 (100%)	2 (0%)	81	81
8	J	99/99 (100%)	99 (100%)	0	100	100
All	All	3302/3611 (91%)	3272 (99%)	30 (1%)	68	76

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	153	VAL
1	A	606	TYR
1	B	22	THR
1	B	70	THR
1	B	111	THR
1	B	191	ARG
1	B	193	GLU
1	B	196	THR
2	C	92	TYR
2	C	232	ILE
2	C	450	ASN
2	C	600	THR
2	C	615	VAL
2	C	700	VAL
2	C	714	VAL
2	C	781	ASP
2	C	862	LEU
2	C	976	ARG
2	C	1003	THR

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Mol	Chain	Res	Type
2	C	1052	VAL
2	C	1103	VAL
3	D	506	VAL
3	D	527	LEU
3	D	587	LEU
3	D	790	THR
3	D	918	ILE
3	D	1139	PRO
5	F	230	VAL
5	F	449	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	75	GLN
1	A	137	ASN
1	A	612	GLN
1	B	37	HIS
1	B	66	HIS
1	B	132	HIS
2	C	120	GLN
2	C	193	ASN
2	C	406	ASN
2	C	462	ASN
2	C	613	ASN
2	C	955	GLN
2	C	1070	HIS
2	C	1111	GLN
2	C	1136	GLN
2	C	1220	GLN
2	C	1257	GLN
3	D	157	GLN
3	D	206	ASN
3	D	232	ASN
3	D	277	ASN
3	D	300	GLN
3	D	341	ASN
3	D	430	HIS
3	D	488	ASN
3	D	606	ASN
3	D	623	GLN

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Mol	Chain	Res	Type
3	D	651	HIS
3	D	716	GLN
3	D	720	ASN
3	D	739	GLN
3	D	1010	GLN
3	D	1114	GLN
3	D	1259	GLN
3	D	1268	ASN
3	D	1295	ASN
4	E	43	ASN
5	F	128	ASN
5	F	210	ASN
5	F	283	GLN
5	F	309	ASN
5	F	383	ASN
5	F	406	GLN
5	F	464	ASN
5	F	518	HIS
5	F	568	ASN
5	F	600	HIS
8	J	105	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

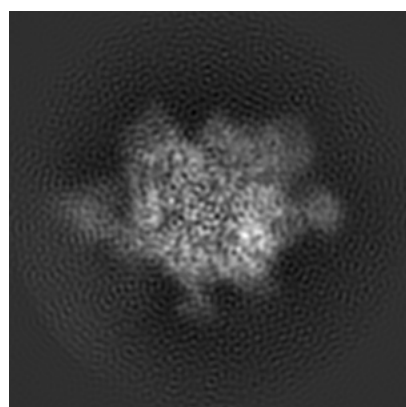
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32322. These allow visual inspection of the internal detail of the map and identification of artifacts.

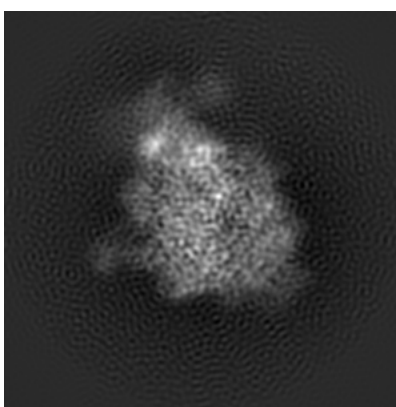
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

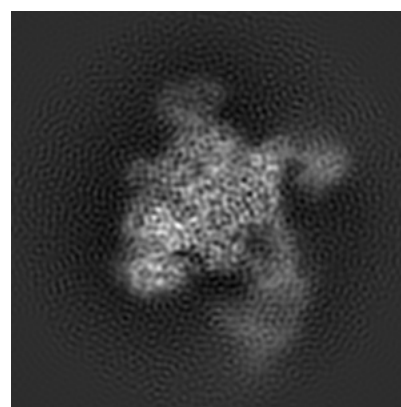
6.1.1 Primary map



X



Y

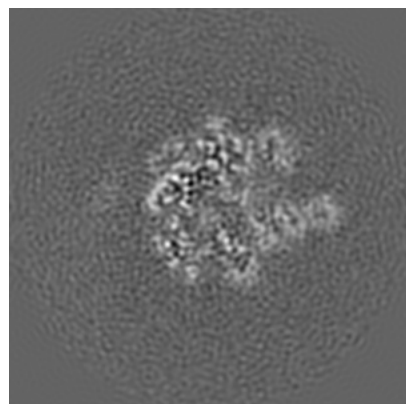


Z

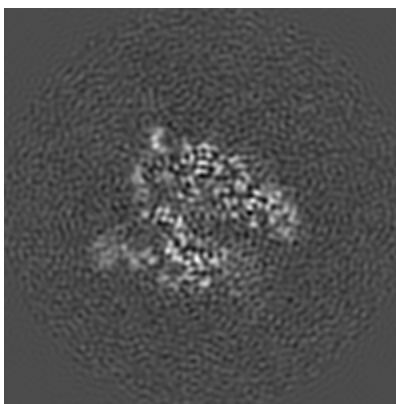
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

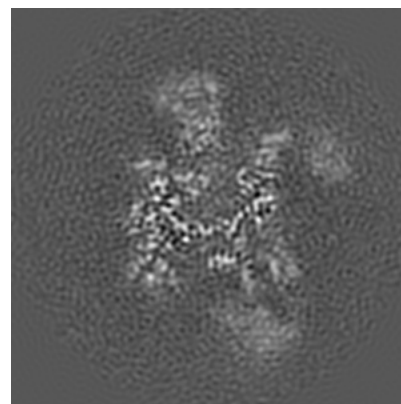
6.2.1 Primary map



X Index: 120



Y Index: 120

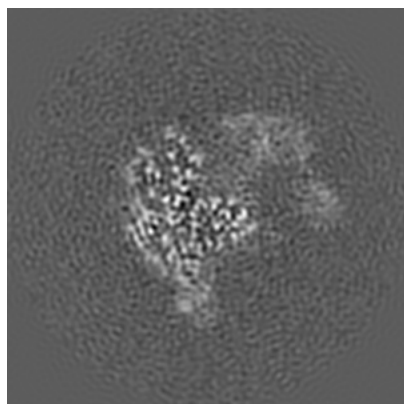


Z Index: 120

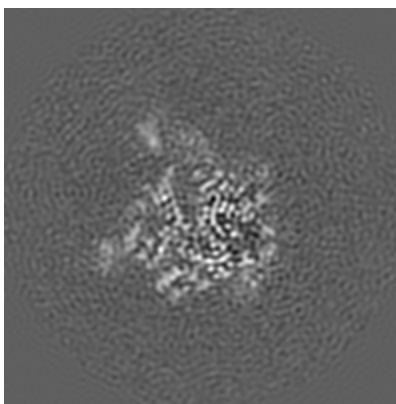
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

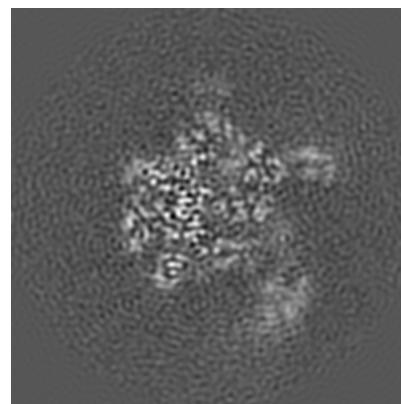
6.3.1 Primary map



X Index: 96



Y Index: 106

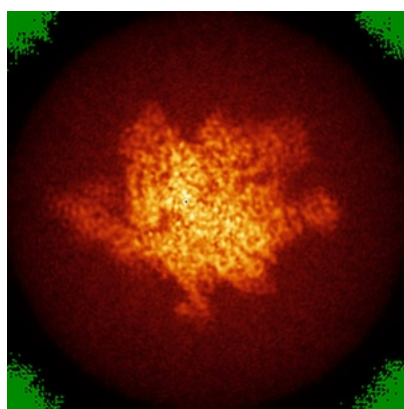


Z Index: 106

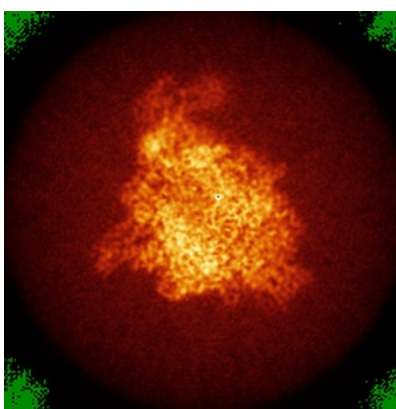
The images above show the largest variance slices of the map in three orthogonal directions.

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

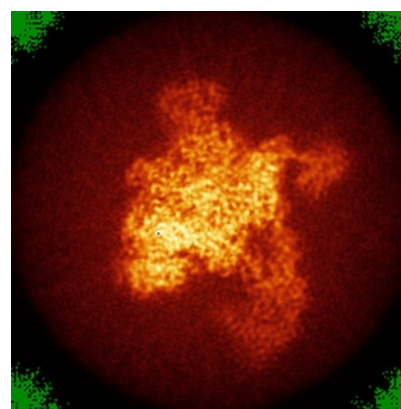
6.4.1 Primary map



X



Y

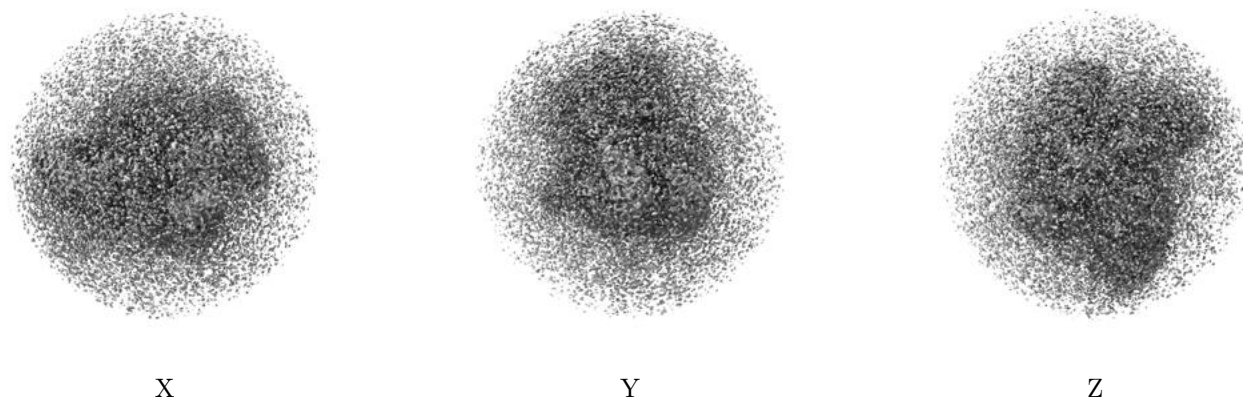


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

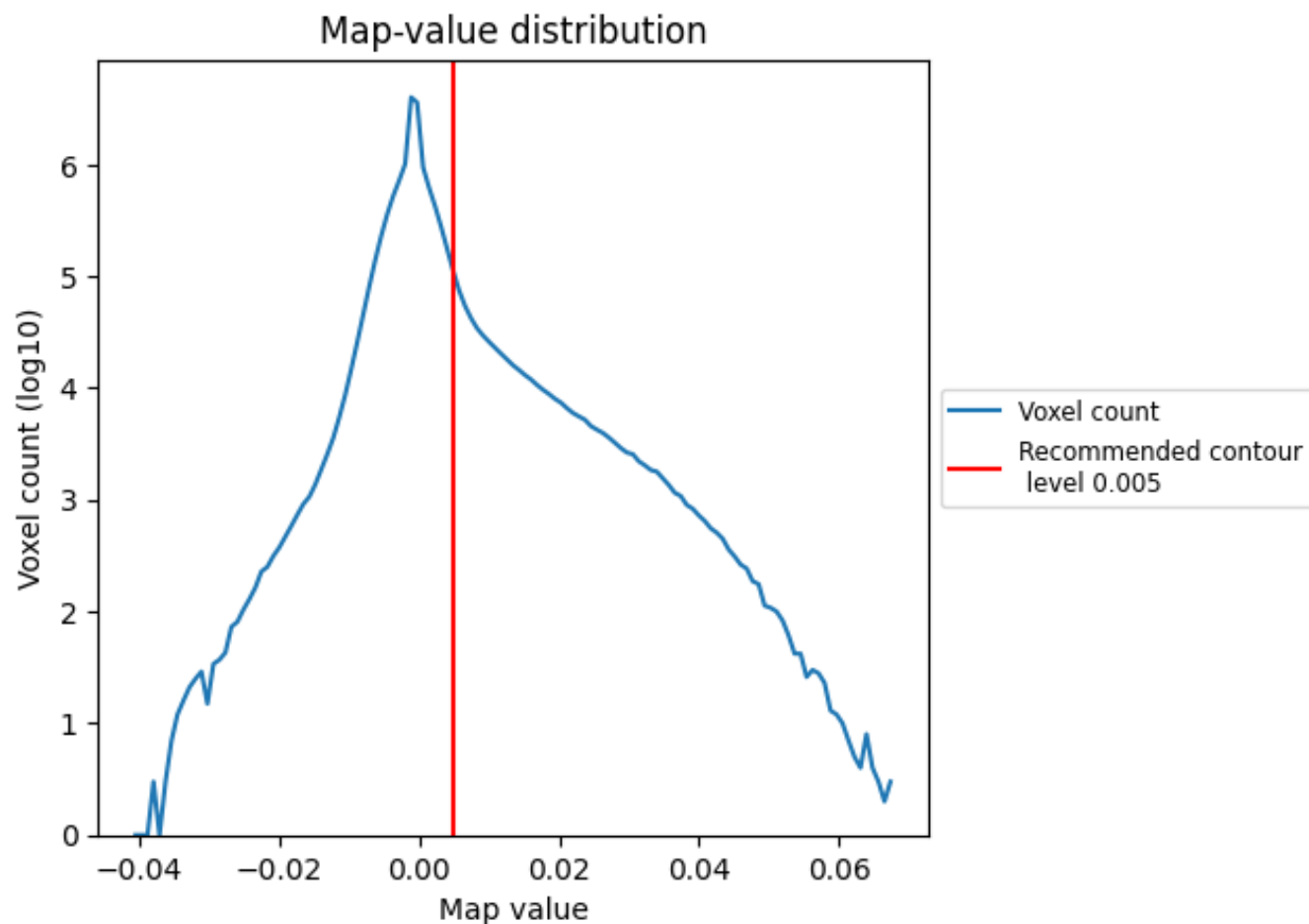
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

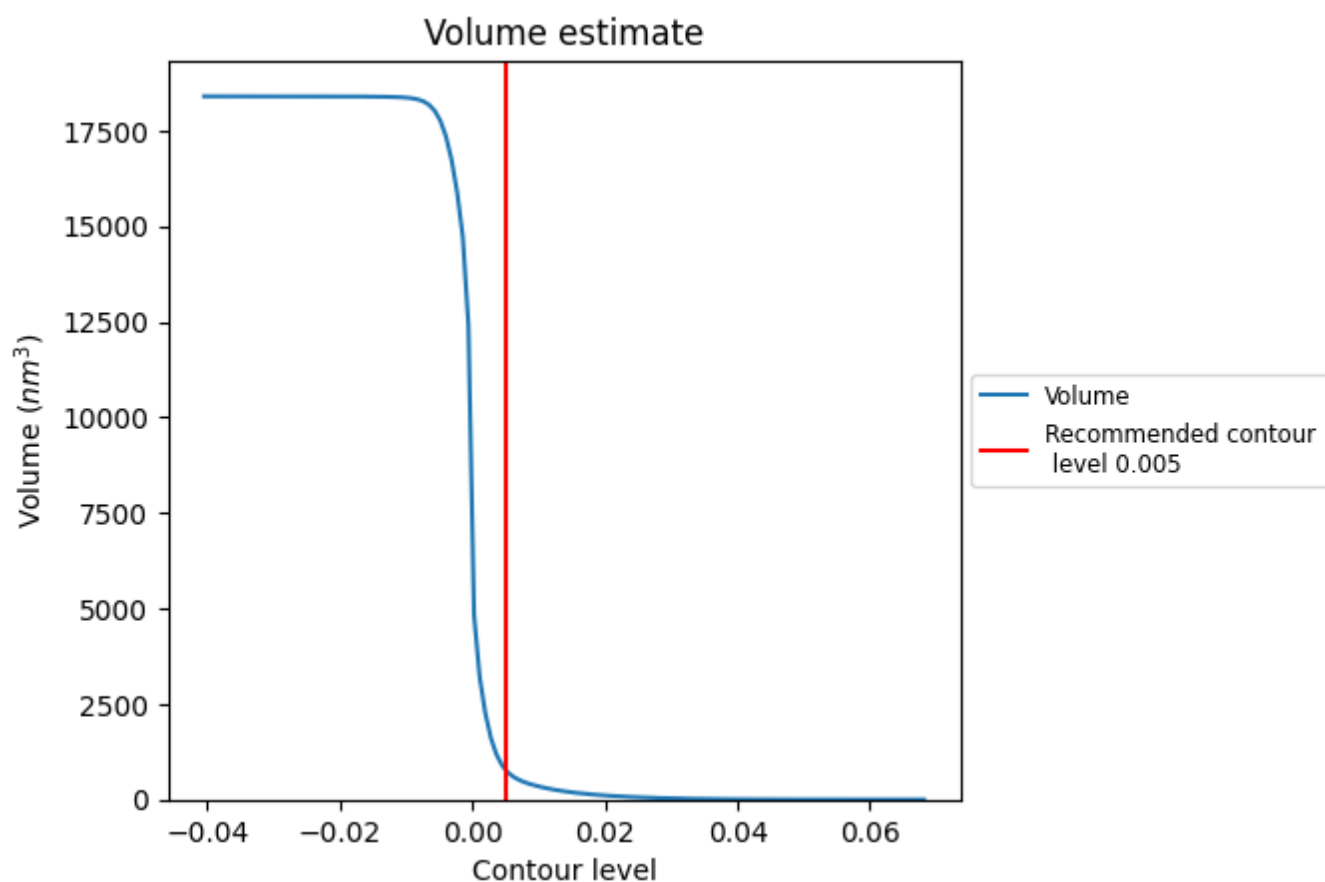
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

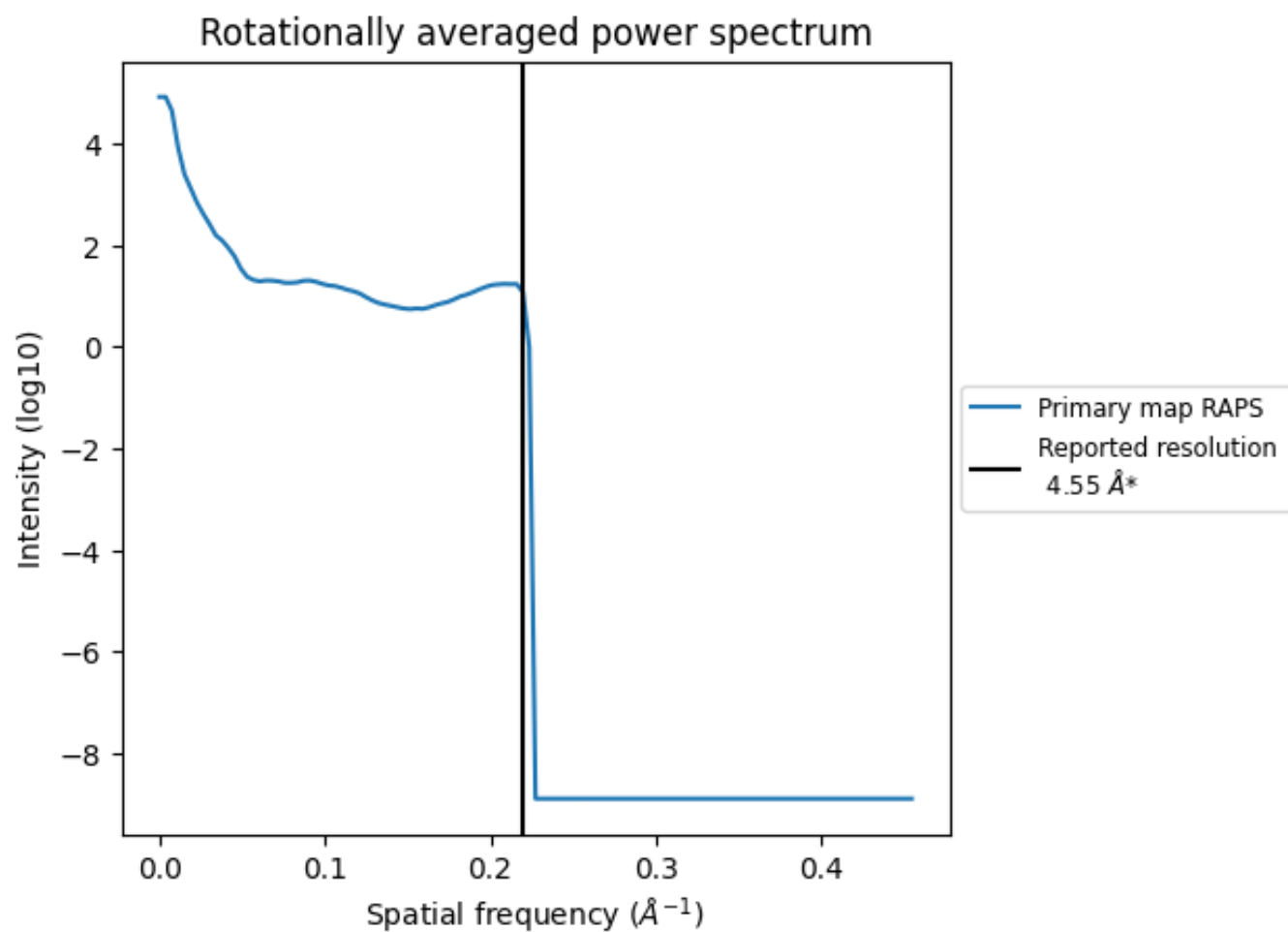
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 793 nm³; this corresponds to an approximate mass of 717 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 $0.220 \text{ \AA}^{-1}$

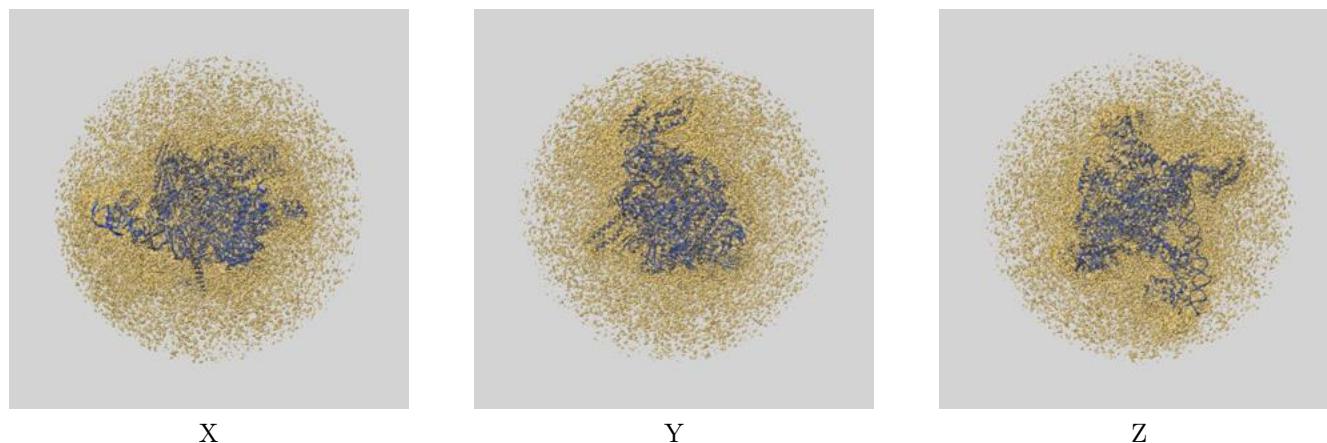
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

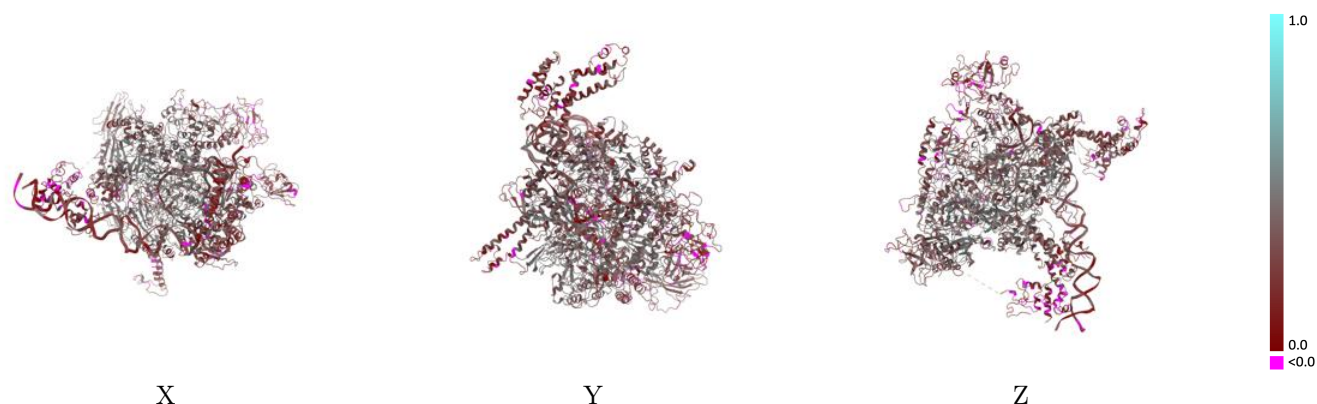
This section contains information regarding the fit between EMDB map EMD-32322 and PDB model 7W5W. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



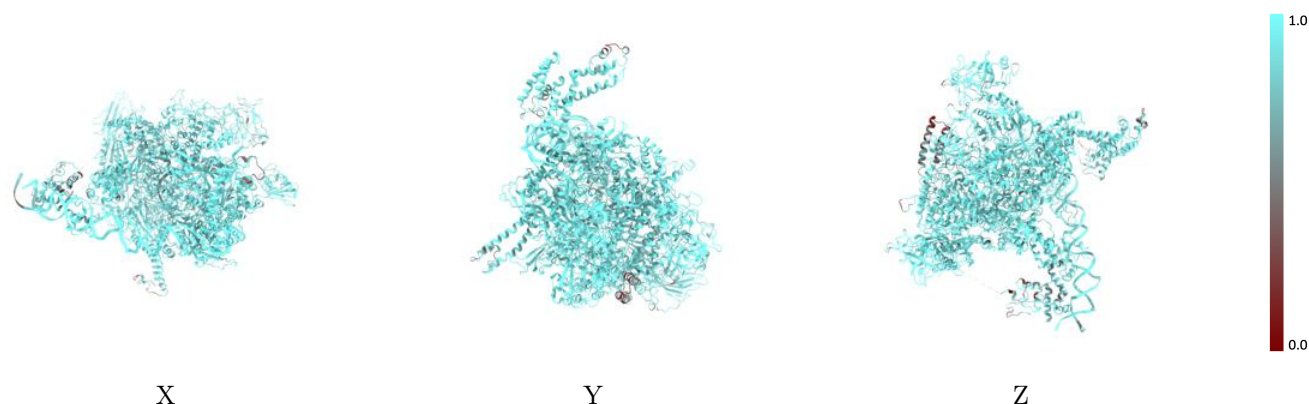
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



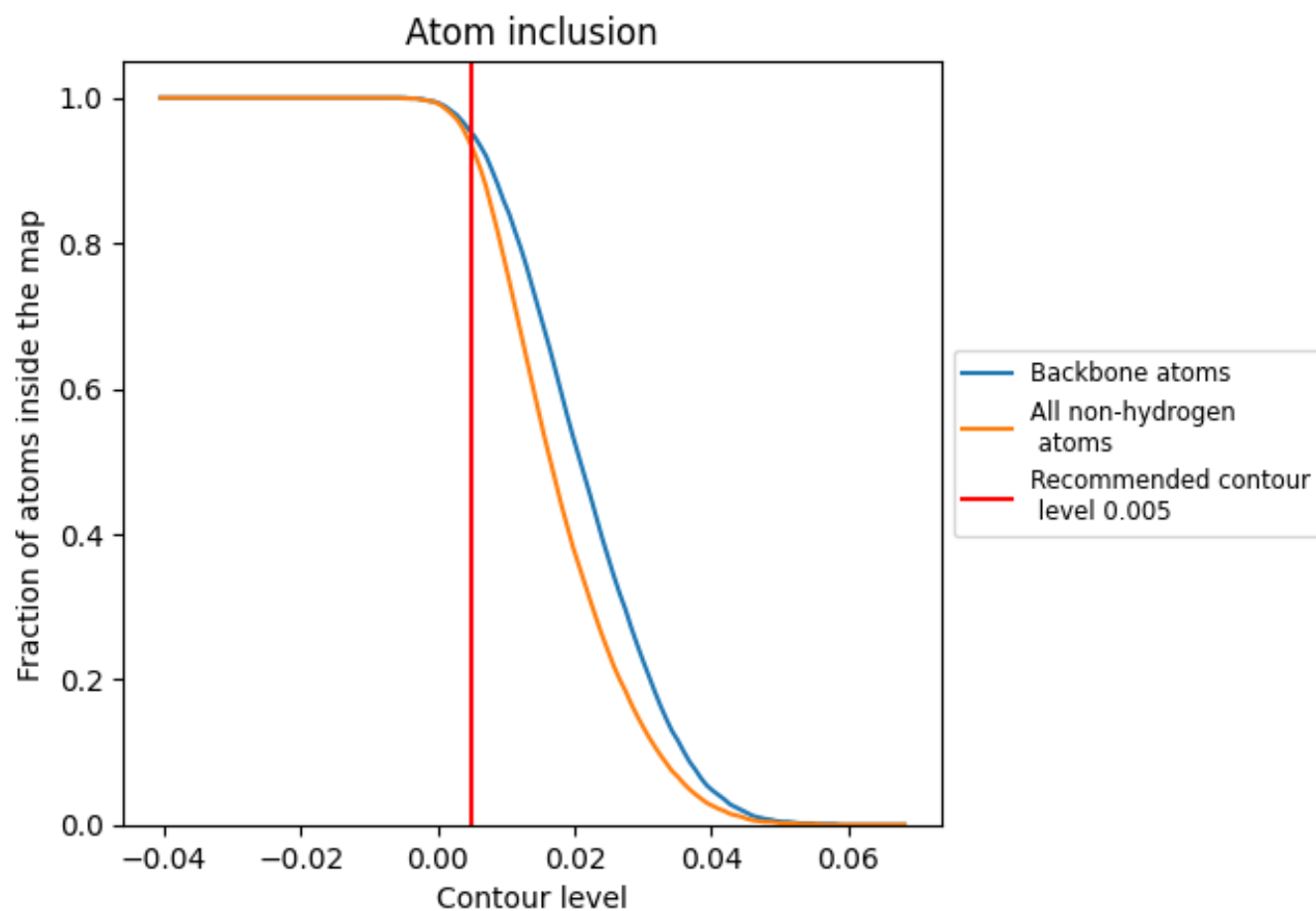
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 93% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9330	0.3320
1	0.9580	0.2510
2	0.9010	0.2420
A	0.8910	0.3260
B	0.9560	0.3410
C	0.9550	0.3760
D	0.9250	0.3420
E	0.9480	0.3640
F	0.9190	0.2740
J	0.8850	0.1670

1.0

0.0

<0.0