Full wwPDB EM Validation Report

Mar 9, 2026 – 12:40 PM UTC

PDB ID	:	9GDS / pdb_00009gds
EMDB ID	:	EMD-51277
Title	:	Cryo-EM structure of Vibrio cholerae RNA polymerase Transcription Activation Complex with ToxR and TcpP transcription factors and a toxT promoter DNA fragment
Authors	:	Alcaide-Jimenez, A.; Baudin, F.; Canals, A.; Machon, C.; Murciano, B.; Fabrega-Ferrer, M.; Bantysh, O.; Perez-Luque, R.; Krukonis, E.S.; Muller, C.W.; Coll, M.
Deposited on	:	2024-08-06
Resolution	:	2.90 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:

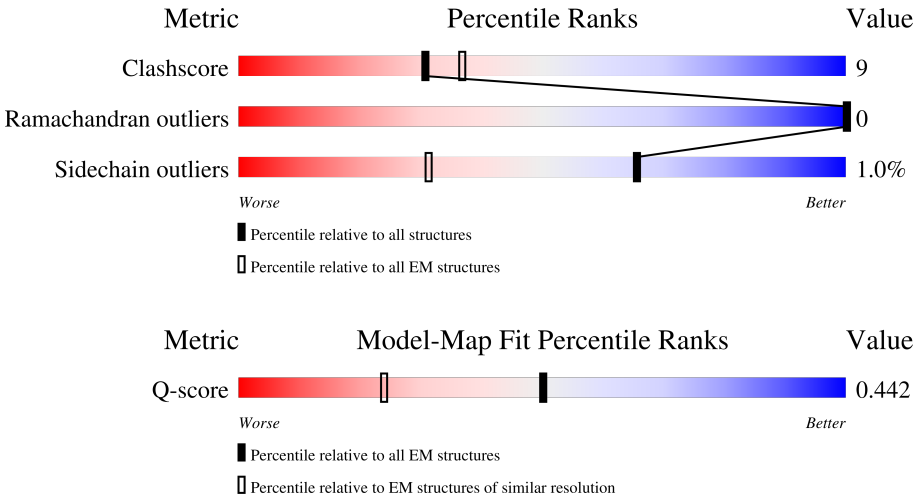
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & 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 2.90 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	13054 (2.40 - 3.40)

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 <=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	H	115	70% 26%
1	K	115	12% 60% 35% 5%
2	N	110	14% 30% 42% 28%
3	T	110	13% 35% 35% 29%

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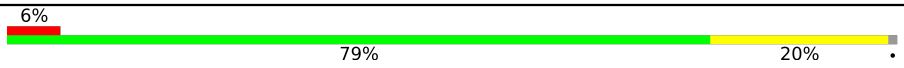
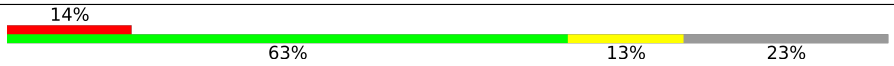
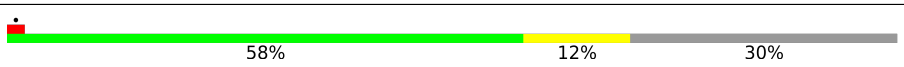
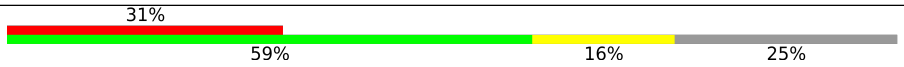
Mol	Chain	Length	Quality of chain
4	C	1341	
5	D	1401	
6	E	90	
7	A	330	
7	B	330	
7	G	330	
8	F	621	
9	I	110	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 34162 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 Toxin co-regulated pilus biosynthesis protein P.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	112	Total	C	N	O	S	0	0
			928	601	158	165	4		
1	K	109	Total	C	N	O	S	0	0
			898	581	152	161	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	19	ALA	CYS	engineered mutation	UNP A0A0H3AHV1
K	19	ALA	CYS	engineered mutation	UNP A0A0H3AHV1

- Molecule 2 is a DNA chain called toxT promoter non-template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	79	Total	C	N	O	P	0	0
			1621	784	266	492	79		

- Molecule 3 is a DNA chain called toxT promoter template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	78	Total	C	N	O	P	0	0
			1603	769	314	443	77		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	1328	Total	C	N	O	S	1	0
			10421	6547	1811	2025	38		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	1202	Total	C	N	O	S	0	0
			9408	5912	1675	1774	47		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	69	Total	C	N	O	S	0	0
			545	332	102	110	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	231	Total	C	N	O	S	0	0
			1776	1111	312	348	5		
7	B	222	Total	C	N	O	S	0	0
			1697	1064	295	333	5		
7	G	70	Total	C	N	O	S	0	0
			550	348	97	103	2		

- Molecule 8 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	468	Total	C	N	O	S	0	0
			3810	2384	690	719	17		

- Molecule 9 is a protein called Cholera toxin transcriptional activator.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	110	Total	C	N	O	S	0	0
			902	571	155	174	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	6	MET	-	initiating methionine	UNP P15795

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

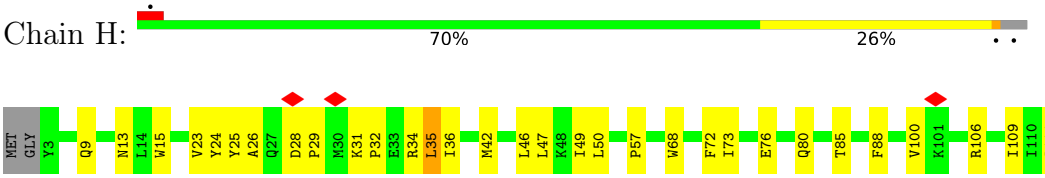
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
11	D	2	2	2	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

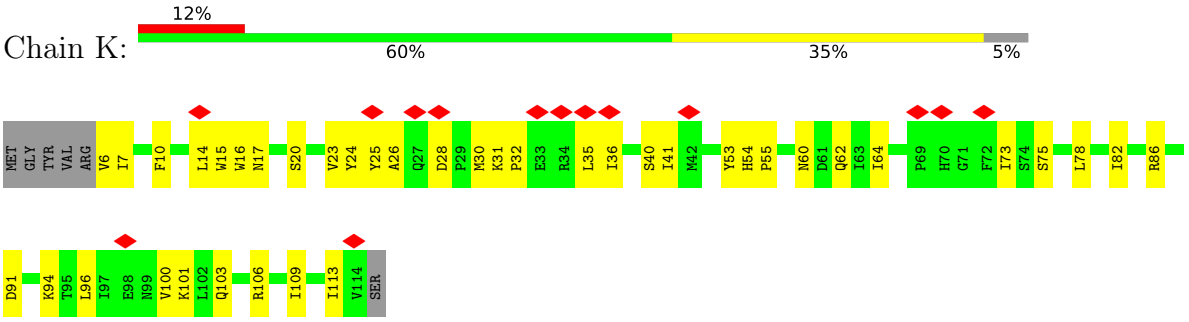
• Molecule 1: Toxin co-regulated pilus biosynthesis protein P

Chain H:



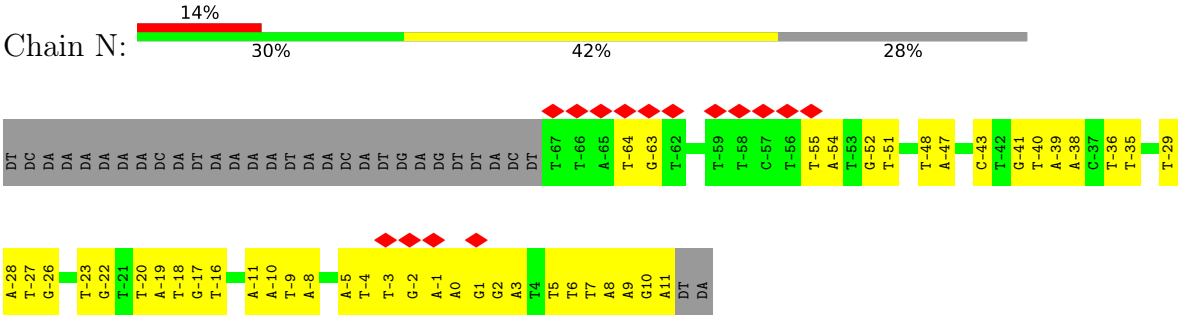
• Molecule 1: Toxin co-regulated pilus biosynthesis protein P

Chain K:



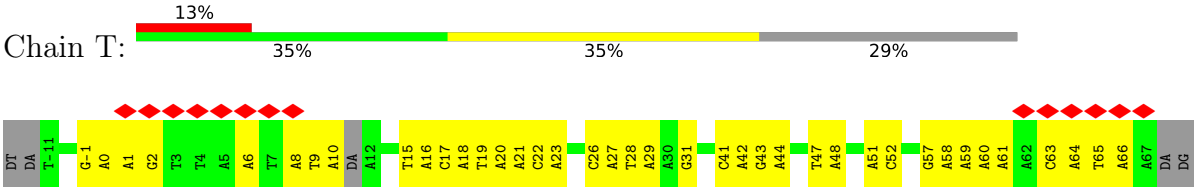
• Molecule 2: toxT promoter non-template DNA strand

Chain N:

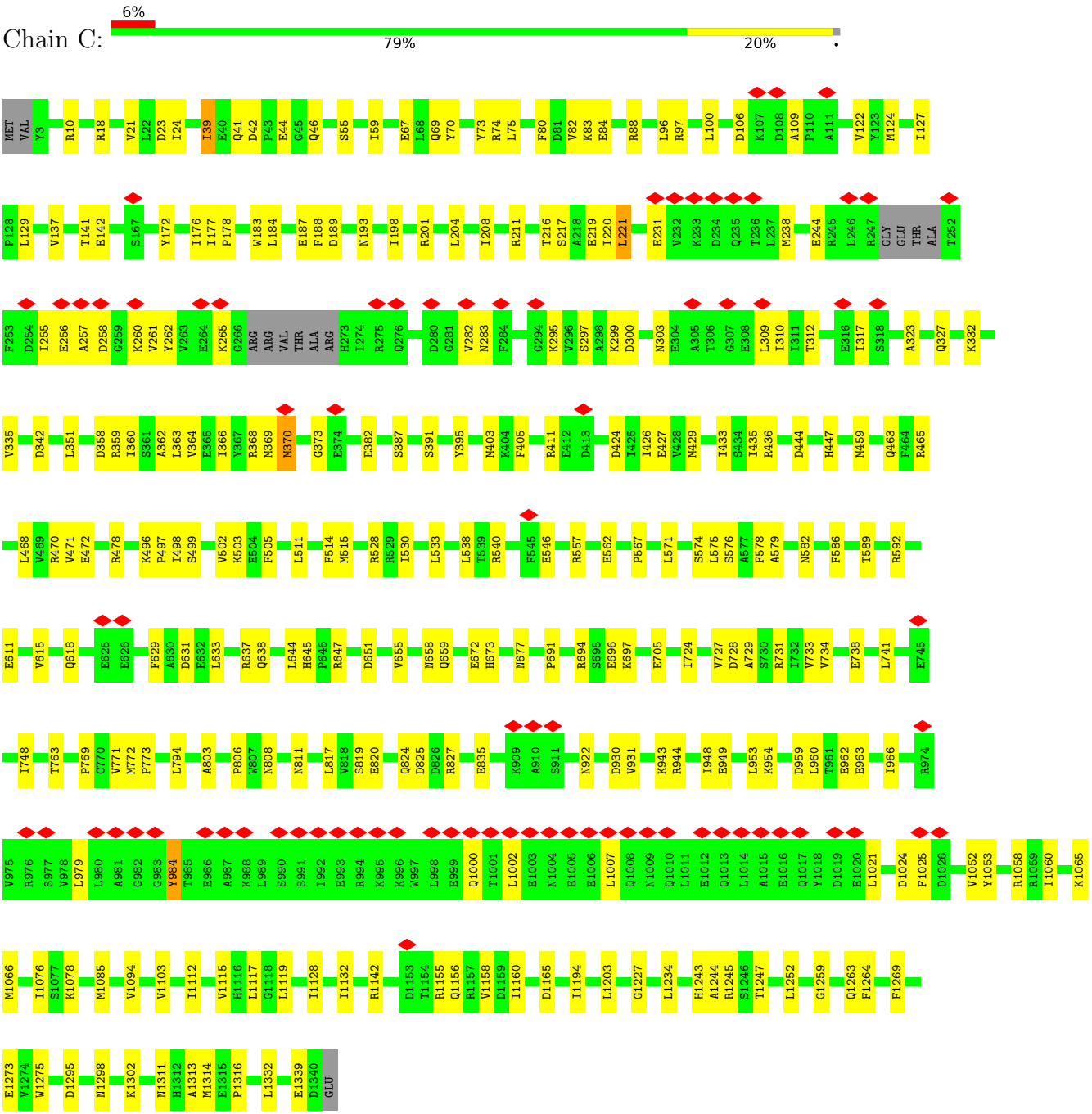


• Molecule 3: toxT promoter template DNA strand

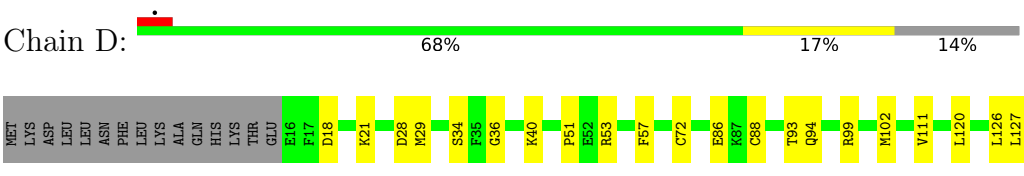
Chain T:

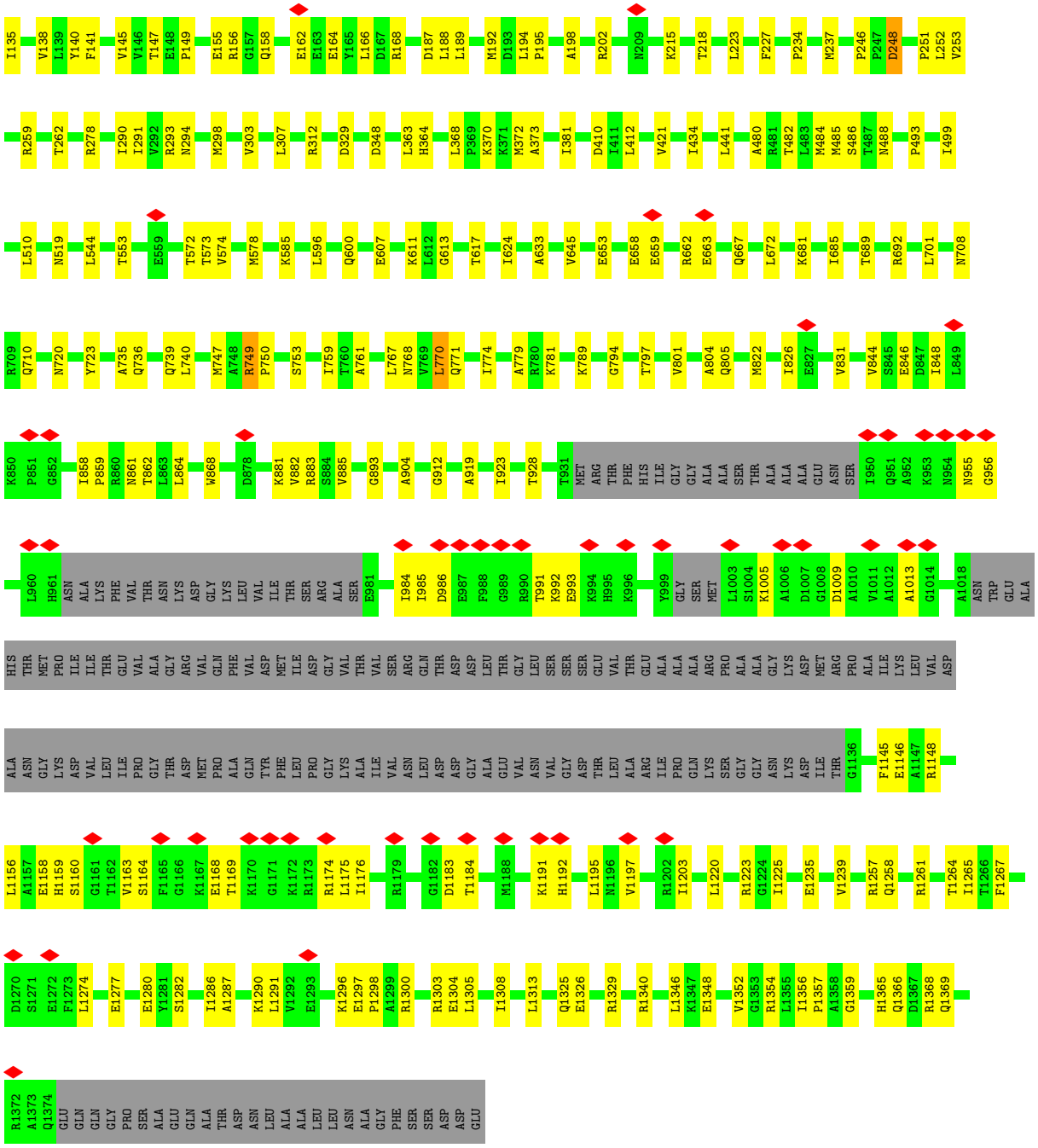


• Molecule 4: DNA-directed RNA polymerase subunit beta



• Molecule 5: DNA-directed RNA polymerase subunit beta'

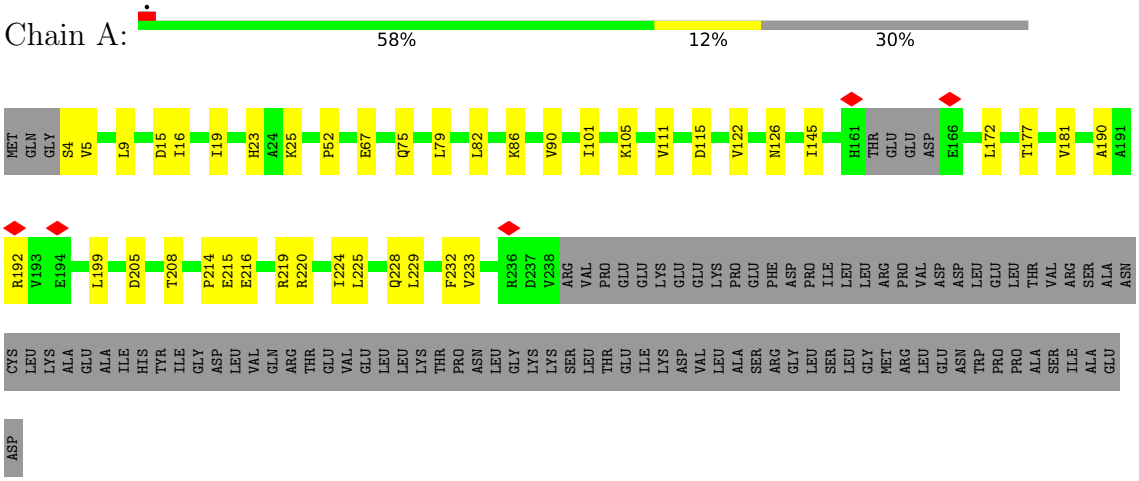




• Molecule 6: DNA-directed RNA polymerase subunit omega

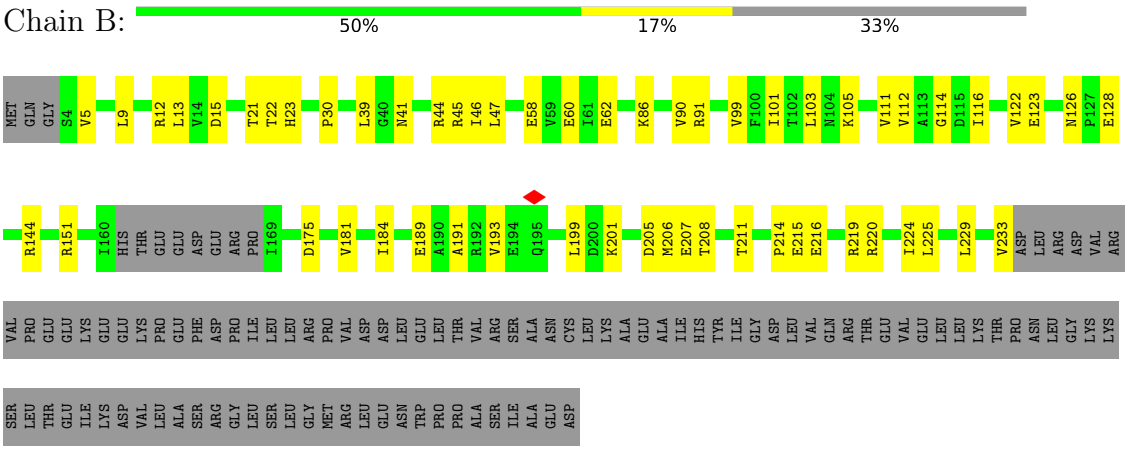
• Molecule 7: DNA-directed RNA polymerase subunit alpha

Chain A:



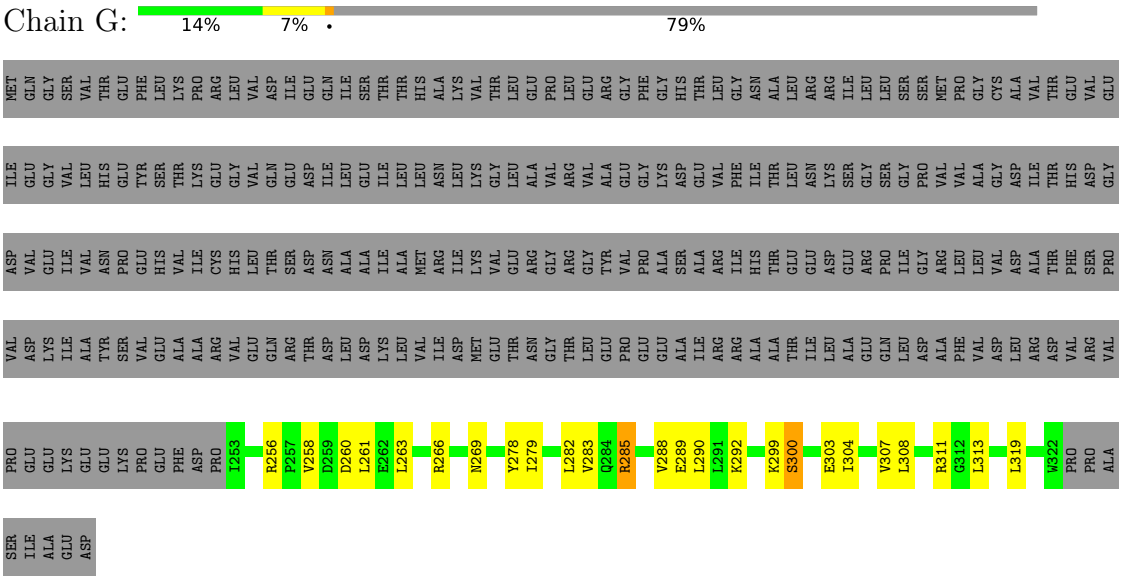
• Molecule 7: DNA-directed RNA polymerase subunit alpha

Chain B:



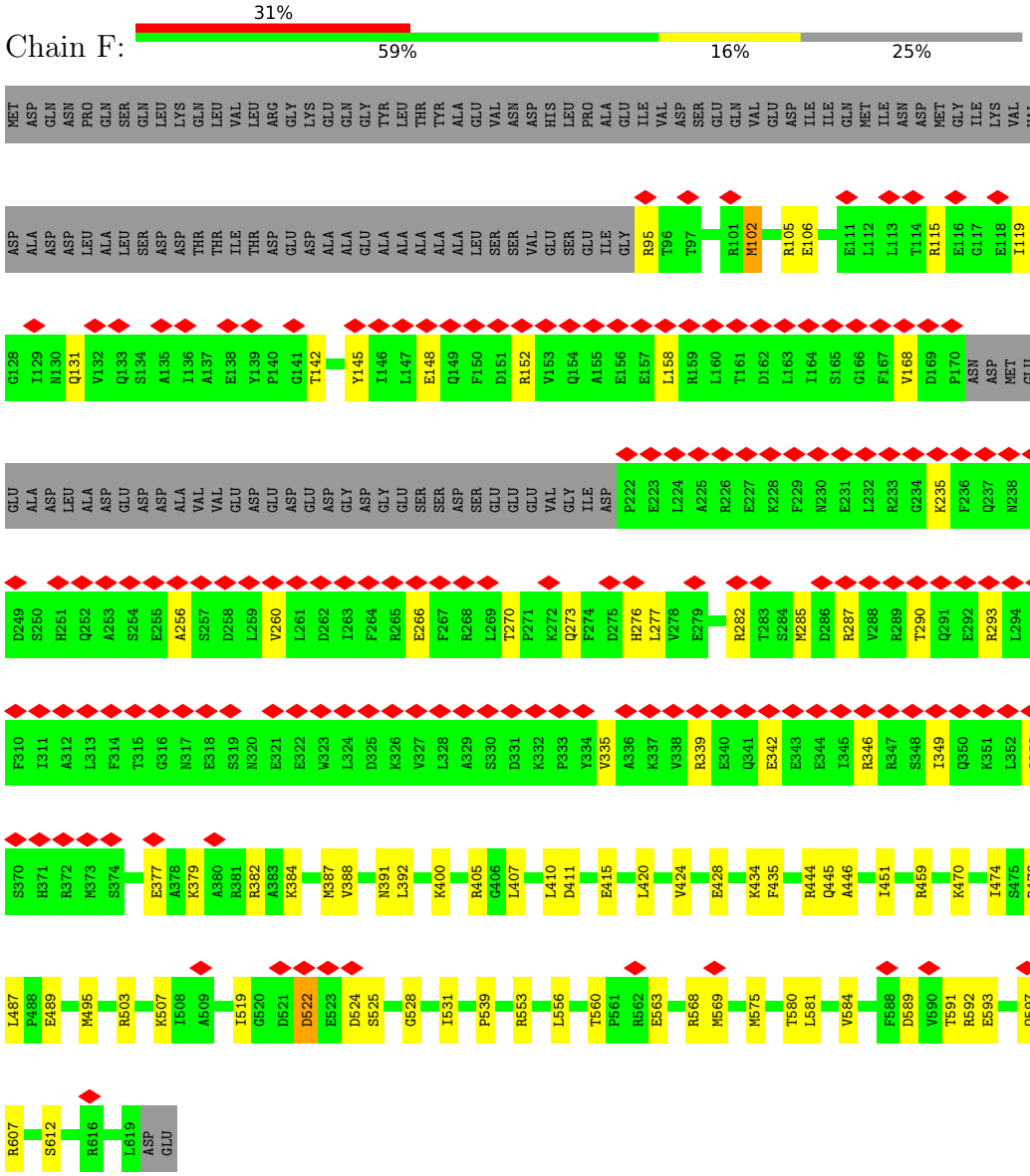
• Molecule 7: DNA-directed RNA polymerase subunit alpha

Chain G:



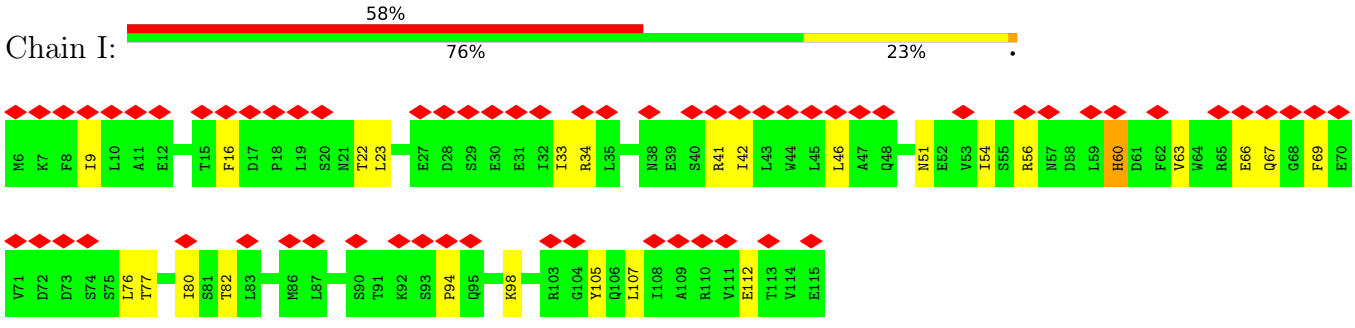
• Molecule 8: RNA polymerase sigma factor RpoD

Chain F:



• Molecule 9: Cholera toxin transcriptional activator

Chain I:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88323	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 ($e^-/Å^2$)	50.71	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	112.047	Depositor
Minimum map value	-3.276	Depositor
Average map value	0.011	Depositor
Map value standard deviation	1.107	Depositor
Recommended contour level	3.84	Depositor
Map size (Å)	374.272, 374.272, 374.272	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.731, 0.731, 0.731	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	H	0.16	0/953	0.48	0/1297
1	K	0.12	0/922	0.38	0/1255
2	N	0.21	0/1812	0.45	0/2798
3	T	0.19	0/1806	0.37	0/2781
4	C	0.13	0/10585	0.35	1/14288 (0.0%)
5	D	0.12	0/9552	0.32	0/12881
6	E	0.08	0/547	0.20	0/734
7	A	0.11	0/1798	0.29	0/2437
7	B	0.12	0/1717	0.31	0/2327
7	G	0.11	0/555	0.36	0/749
8	F	0.15	0/3861	0.36	0/5184
9	I	0.65	0/917	0.81	0/1237
All	All	0.17	0/35025	0.37	1/47968 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	211	ARG	N-CA-C	-5.83	104.83	111.07

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	H	928	0	932	22	0
1	K	898	0	901	30	0
2	N	1621	0	909	33	0
3	T	1603	0	879	31	0
4	C	10421	0	10444	174	0
5	D	9408	0	9588	155	0
6	E	545	0	551	6	0
7	A	1776	0	1802	26	0
7	B	1697	0	1728	39	0
7	G	550	0	584	21	0
8	F	3810	0	3891	82	0
9	I	902	0	910	24	0
10	D	1	0	0	0	0
11	D	2	0	0	0	0
All	All	34162	0	33119	600	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 9.

All (600) 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)
3:T:57:DG:OP2	9:I:56:ARG:NH1	2.01	0.92
1:H:24:TYR:HB3	1:H:35:LEU:HD23	1.60	0.82
1:K:16:TRP:HD1	1:K:23:VAL:HG22	1.47	0.80
1:H:46:LEU:HD11	1:H:85:THR:HG21	1.65	0.78
1:H:28:ASP:HB2	1:H:31:LYS:HB3	1.66	0.77
1:K:10:PHE:HB2	1:K:14:LEU:HB3	1.67	0.76
1:K:6:VAL:HA	1:K:113:ILE:O	1.84	0.76
9:I:9:ILE:HB	9:I:112:GLU:HB2	1.69	0.75
3:T:58:DA:OP2	9:I:77:THR:HG23	1.85	0.75
2:N:-41:DG:H21	7:G:266:ARG:HH22	1.33	0.74
5:D:1280:GLU:OE2	5:D:1282:SER:OG	2.04	0.74
5:D:710:GLN:N	5:D:710:GLN:OE1	2.21	0.74
3:T:-1:DG:H2'	3:T:0:DA:H8	1.53	0.73
5:D:984:ILE:HB	5:D:993:GLU:HB2	1.70	0.73
4:C:297:SER:HB2	4:C:317:ILE:HD11	1.69	0.73
9:I:60:HIS:HB2	9:I:76:LEU:HD12	1.71	0.72
3:T:51:DA:H2"	3:T:52:DC:H5"	1.71	0.71
3:T:58:DA:OP2	9:I:77:THR:CG2	2.39	0.70
4:C:615:VAL:HG23	4:C:638:GLN:HB2	1.73	0.70
4:C:499:SER:O	4:C:503:LYS:HG3	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1169:THR:OG1	5:D:1174:ARG:NH1	2.25	0.69
4:C:44:GLU:OE1	4:C:44:GLU:N	2.26	0.69
7:A:181:VAL:HA	7:A:208:THR:HG22	1.73	0.69
4:C:201:ARG:HD3	4:C:369:MET:HE3	1.75	0.69
8:F:391:ASN:HB2	8:F:420:LEU:HD11	1.73	0.69
5:D:198:ALA:O	5:D:202:ARG:HG3	1.93	0.68
4:C:731:ARG:NH2	4:C:963:GLU:OE2	2.26	0.68
7:G:288:VAL:HG12	7:G:292:LYS:HE3	1.76	0.68
4:C:208:ILE:HG23	4:C:362:ALA:HB1	1.76	0.68
7:B:191:ALA:O	7:B:199:LEU:HB2	1.94	0.67
1:K:15:TRP:NE1	1:K:26:ALA:O	2.26	0.67
7:B:112:VAL:HG23	7:B:114:GLY:H	1.60	0.67
4:C:244:GLU:N	4:C:244:GLU:OE1	2.27	0.66
1:K:28:ASP:HB3	1:K:31:LYS:HB3	1.77	0.66
4:C:1103:VAL:HG11	4:C:1112:ILE:HD11	1.78	0.66
5:D:290:ILE:HD11	8:F:106:GLU:HB3	1.75	0.66
8:F:519:ILE:O	8:F:525:SER:OG	2.13	0.66
4:C:819:SER:HB2	4:C:1085:MET:HE2	1.78	0.66
7:B:86:LYS:HD3	7:B:175:ASP:HB2	1.77	0.66
4:C:748:ILE:HG13	4:C:966:ILE:HG22	1.78	0.65
4:C:728:ASP:OD1	4:C:729:ALA:N	2.29	0.65
4:C:738:GLU:HA	4:C:741:LEU:HD12	1.77	0.65
5:D:681:LYS:O	5:D:685:ILE:HG23	1.95	0.65
7:G:279:ILE:HG21	7:G:313:LEU:HD13	1.78	0.65
8:F:387:MET:HE2	8:F:391:ASN:HD21	1.60	0.65
4:C:429:MET:O	4:C:433:ILE:HG12	1.97	0.65
2:N:-5:DA:H2"	2:N:-4:DT:H5'	1.79	0.64
1:K:73:ILE:HG22	1:K:75:SER:H	1.62	0.64
1:H:34:ARG:NH2	1:H:35:LEU:O	2.30	0.64
1:K:10:PHE:HE1	1:K:109:ILE:HG12	1.62	0.64
2:N:10:DG:H2'	2:N:11:DA:C8	2.32	0.64
5:D:53:ARG:HH11	5:D:53:ARG:HB2	1.63	0.63
5:D:1264:THR:OG1	5:D:1304:GLU:OE2	2.16	0.63
4:C:959:ASP:OD1	4:C:960:LEU:N	2.31	0.63
4:C:258:ASP:HA	4:C:261:VAL:HG23	1.81	0.63
4:C:611:GLU:OE2	4:C:637:ARG:NH2	2.32	0.63
4:C:806:PRO:HA	4:C:811:ASN:HD21	1.63	0.63
4:C:589:THR:OG1	4:C:659:GLN:NE2	2.32	0.63
8:F:563:GLU:OE2	8:F:602:ALA:HB2	2.00	0.62
8:F:569:MET:HE3	8:F:584:VAL:HA	1.82	0.62
1:H:46:LEU:HA	1:H:49:ILE:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:5:VAL:O	7:B:151:ARG:NH1	2.33	0.62
4:C:67:GLU:OE2	4:C:69:GLN:NE2	2.32	0.61
5:D:1325:GLN:HG3	5:D:1326:GLU:HG3	1.81	0.61
3:T:63:DC:H2"	3:T:64:DA:C8	2.34	0.61
4:C:808:ASN:H	5:D:633:ALA:HB2	1.65	0.61
4:C:962:GLU:O	4:C:966:ILE:HG13	2.00	0.61
7:A:216:GLU:O	7:A:220:ARG:HG3	2.00	0.61
8:F:391:ASN:CB	8:F:420:LEU:HD11	2.30	0.61
4:C:463:GLN:HG3	4:C:505:PHE:HB2	1.83	0.61
5:D:1287:ALA:HA	5:D:1290:LYS:HD2	1.83	0.61
7:B:128:GLU:OE1	7:B:128:GLU:N	2.30	0.61
4:C:41:GLN:NE2	4:C:73:TYR:O	2.34	0.61
4:C:187:GLU:N	4:C:187:GLU:OE1	2.34	0.60
4:C:528:ARG:NH2	4:C:576:SER:O	2.32	0.60
4:C:631:ASP:O	4:C:647:ARG:NH1	2.34	0.60
9:I:56:ARG:HG3	9:I:76:LEU:HD13	1.84	0.60
3:T:28:DT:H2"	3:T:29:DA:C8	2.36	0.60
4:C:470:ARG:NH2	4:C:497:PRO:O	2.35	0.60
4:C:696:GLU:OE1	4:C:827:ARG:NH2	2.34	0.60
2:N:-10:DA:H2'	2:N:-9:DT:C6	2.37	0.60
7:B:47:LEU:HB3	7:B:181:VAL:HG21	1.84	0.60
4:C:705:GLU:HB3	4:C:794:LEU:H	1.68	0.59
2:N:-16:DT:OP1	8:F:459:ARG:NH2	2.34	0.59
5:D:1267:PHE:HB2	5:D:1300:ARG:HB2	1.84	0.59
7:B:41:ASN:O	7:B:45:ARG:HG3	2.01	0.59
4:C:387:SER:HA	4:C:391:SER:HB3	1.85	0.59
4:C:771:VAL:O	7:A:75:GLN:NE2	2.35	0.59
4:C:1298:ASN:O	4:C:1302:LYS:HG3	2.03	0.59
3:T:60:DA:H2"	3:T:61:DA:C8	2.38	0.59
4:C:444:ASP:HB3	4:C:447:HIS:HB2	1.85	0.59
7:A:190:ALA:O	7:A:192:ARG:NH1	2.36	0.59
8:F:339:ARG:HA	8:F:342:GLU:HG2	1.85	0.59
7:A:215:GLU:O	7:A:219:ARG:HG3	2.03	0.59
5:D:767:LEU:HB3	5:D:771:GLN:HB2	1.85	0.58
8:F:282:ARG:NH2	8:F:377:GLU:OE1	2.34	0.58
4:C:309:LEU:HD23	4:C:312:THR:HG22	1.86	0.58
5:D:86:GLU:H	5:D:86:GLU:CD	2.12	0.58
5:D:145:VAL:HG11	5:D:188:LEU:HD11	1.84	0.58
1:H:76:GLU:OE2	2:N:-38:DA:N6	2.21	0.58
4:C:24:ILE:HD11	4:C:658:ASN:HD21	1.67	0.58
9:I:80:ILE:HG21	9:I:105:TYR:HE2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:123:GLU:N	7:B:123:GLU:OE1	2.37	0.58
2:N:8:DA:H2"	2:N:9:DA:H5"	1.85	0.58
5:D:574:VAL:O	5:D:578:MET:HG3	2.03	0.58
4:C:359:ARG:O	4:C:363:LEU:HD12	2.04	0.57
4:C:979:LEU:HB3	4:C:984:TYR:HE2	1.69	0.57
7:B:12:ARG:HG2	7:B:30:PRO:HD3	1.86	0.57
4:C:299:LYS:HZ1	4:C:300:ASP:HB2	1.70	0.57
4:C:256:GLU:HG3	4:C:257:ALA:H	1.68	0.57
4:C:629:PHE:HB2	4:C:647:ARG:HD3	1.87	0.57
5:D:53:ARG:HB2	5:D:53:ARG:NH1	2.21	0.56
7:B:181:VAL:HG13	7:B:206:MET:HE3	1.85	0.56
4:C:733:VAL:HG11	4:C:966:ILE:HG21	1.87	0.56
5:D:127:LEU:HD13	5:D:223:LEU:HD23	1.88	0.56
4:C:592:ARG:HG3	4:C:655:VAL:HG12	1.87	0.56
5:D:1291:LEU:HD23	5:D:1298:PRO:HA	1.87	0.56
8:F:115:ARG:O	8:F:119:ILE:HG12	2.05	0.56
7:G:283:VAL:HG23	7:G:319:LEU:HD11	1.88	0.56
5:D:158:GLN:HE22	5:D:168:ARG:HH12	1.54	0.56
9:I:41:ARG:HG3	9:I:63:VAL:HG22	1.88	0.56
5:D:162:GLU:O	5:D:166:LEU:HD12	2.06	0.56
4:C:82:VAL:HG13	4:C:137:VAL:HG21	1.88	0.55
5:D:1368:ARG:HH11	5:D:1368:ARG:HG3	1.70	0.55
7:A:105:LYS:HG2	7:A:111:VAL:HG22	1.87	0.55
2:N:-36:DT:H2"	2:N:-35:DT:H5'	1.88	0.55
5:D:846:GLU:HG3	5:D:881:LYS:HD3	1.86	0.55
5:D:147:THR:HG21	5:D:187:ASP:HB3	1.87	0.55
8:F:420:LEU:O	8:F:424:VAL:HG23	2.06	0.55
8:F:601:LYS:O	8:F:605:LYS:HG3	2.07	0.55
2:N:-9:DT:O3'	8:F:434:LYS:NZ	2.38	0.55
5:D:1225:ILE:HD11	5:D:1303:ARG:HD3	1.89	0.55
4:C:1117:LEU:HD13	4:C:1194:ILE:HG12	1.87	0.55
4:C:1295:ASP:N	4:C:1295:ASP:OD1	2.40	0.55
8:F:384:LYS:O	8:F:388:VAL:HG12	2.07	0.55
4:C:188:PHE:HE2	4:C:436:ARG:HG2	1.72	0.55
4:C:1314:MET:HG3	4:C:1316:PRO:HD3	1.89	0.55
4:C:141:THR:HG21	4:C:514:PHE:CE1	2.40	0.54
4:C:176:ILE:CG2	4:C:184:LEU:HB3	2.36	0.54
8:F:387:MET:O	8:F:391:ASN:ND2	2.40	0.54
7:G:289:GLU:HA	7:G:292:LYS:HD2	1.89	0.54
4:C:360:ILE:O	4:C:364:VAL:HG13	2.08	0.54
4:C:362:ALA:O	4:C:366:ILE:HG13	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:510:LEU:HD11	5:D:624:ILE:HG23	1.90	0.54
7:A:101:ILE:HG13	7:A:145:ILE:HB	1.89	0.54
8:F:235:LYS:HZ3	8:F:260:VAL:HG23	1.72	0.54
7:G:258:VAL:O	7:G:261:LEU:HB2	2.07	0.54
9:I:42:ILE:HG21	9:I:80:ILE:HD11	1.90	0.54
1:H:46:LEU:O	1:H:50:LEU:HG	2.07	0.54
4:C:1002:LEU:HD13	4:C:1007:LEU:HB3	1.89	0.54
3:T:41:DC:H2"	3:T:42:DA:C8	2.43	0.54
4:C:255:ILE:HG21	4:C:262:TYR:CD2	2.43	0.54
4:C:1066:MET:HE2	4:C:1076:ILE:HD11	1.89	0.54
4:C:724:ILE:HD13	4:C:734:VAL:HG22	1.90	0.54
5:D:134:ASP:O	5:D:138:VAL:HG23	2.08	0.54
5:D:381:ILE:HD11	5:D:412:LEU:HD13	1.89	0.54
5:D:140:TYR:CD2	8:F:102:MET:HE1	2.44	0.53
1:H:80:GLN:OE1	2:N:-39:DA:N6	2.40	0.53
1:K:78:LEU:O	1:K:82:ILE:HG13	2.09	0.53
1:H:31:LYS:HD2	1:H:32:PRO:HD2	1.90	0.53
4:C:835:GLU:HG3	4:C:1053:TYR:CE1	2.44	0.53
8:F:553:ARG:HG2	8:F:553:ARG:HH11	1.73	0.53
7:G:303:GLU:O	7:G:307:VAL:HG23	2.08	0.53
3:T:-1:DG:H2'	3:T:0:DA:C8	2.41	0.53
7:B:91:ARG:HD3	7:B:211:THR:HG23	1.89	0.53
1:K:16:TRP:CD1	1:K:23:VAL:HG22	2.37	0.53
3:T:26:DC:H2"	3:T:27:DA:C8	2.44	0.53
4:C:59:ILE:O	4:C:67:GLU:HB2	2.09	0.53
4:C:358:ASP:OD1	4:C:359:ARG:N	2.42	0.53
1:K:40:SER:OG	1:K:41:ILE:N	2.41	0.53
1:K:101:LYS:NZ	2:N:-43:DC:O2	2.42	0.53
4:C:1259:GLY:O	4:C:1263:GLN:NE2	2.42	0.53
5:D:1145:PHE:HB3	5:D:1308:ILE:HD13	1.90	0.53
5:D:291:ILE:HD11	8:F:392:LEU:HD21	1.91	0.53
4:C:208:ILE:HD12	4:C:208:ILE:H	1.74	0.52
4:C:426:ILE:HD12	4:C:427:GLU:N	2.24	0.52
4:C:691:PRO:HD2	4:C:763:THR:HG21	1.91	0.52
5:D:885:VAL:HG12	5:D:1257:ARG:HD3	1.91	0.52
2:N:-2:DG:H2"	2:N:-1:DA:H5'	1.90	0.52
4:C:260:LYS:HZ3	4:C:282:VAL:HG13	1.75	0.52
4:C:944:ARG:O	4:C:948:ILE:HG13	2.09	0.52
8:F:603:LEU:O	8:F:607:ARG:HG3	2.10	0.52
5:D:130:MET:HE2	5:D:135:ILE:HG12	1.92	0.52
5:D:768:ASN:OD1	5:D:771:GLN:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1164:SER:HB2	5:D:1176:ILE:HG13	1.92	0.52
1:H:57:PRO:HB3	1:H:100:VAL:HG21	1.91	0.52
4:C:303:ASN:HB2	4:C:310:ILE:HD11	1.90	0.52
8:F:142:THR:HG23	8:F:277:LEU:HD13	1.91	0.52
8:F:388:VAL:HG23	8:F:420:LEU:HD22	1.92	0.52
9:I:46:LEU:HB3	9:I:107:LEU:HD13	1.91	0.52
1:H:28:ASP:HB3	1:H:29:PRO:HD2	1.92	0.52
1:H:100:VAL:HG21	1:H:106:ARG:HG3	1.91	0.52
5:D:607:GLU:HG3	5:D:611:LYS:NZ	2.25	0.52
8:F:273:GLN:O	8:F:277:LEU:HG	2.10	0.52
7:A:67:GLU:HG2	7:A:172:LEU:HD22	1.91	0.51
7:G:261:LEU:HB3	7:G:263:LEU:HG	1.92	0.51
1:H:9:GLN:OE1	1:H:111:GLN:NE2	2.34	0.51
4:C:189:ASP:OD1	4:C:193:ASN:N	2.26	0.51
8:F:235:LYS:NZ	8:F:256:ALA:O	2.42	0.51
1:K:7:ILE:HG12	1:K:17:ASN:ND2	2.25	0.51
3:T:31:DG:H8	8:F:592:ARG:HH12	1.59	0.51
5:D:1163:VAL:HG13	5:D:1175:LEU:HD21	1.91	0.51
4:C:459:MET:HE1	4:C:511:LEU:HD13	1.91	0.51
5:D:653:GLU:OE2	5:D:692:ARG:NE	2.32	0.51
4:C:411:ARG:NH1	4:C:424:ASP:OD1	2.42	0.51
4:C:1247:THR:HG21	8:F:539:PRO:HG3	1.93	0.51
4:C:70:TYR:HA	4:C:100:LEU:HD23	1.93	0.51
8:F:349:ILE:O	8:F:353:GLN:HG2	2.10	0.51
4:C:310:ILE:HD12	4:C:310:ILE:H	1.75	0.51
8:F:400:LYS:HA	8:F:400:LYS:HE2	1.93	0.51
1:H:68:TRP:CD1	1:H:73:ILE:HG13	2.46	0.51
4:C:23:ASP:N	4:C:23:ASP:OD1	2.43	0.51
5:D:805:GLN:HE21	5:D:1346:LEU:H	1.58	0.51
8:F:589:ASP:OD1	8:F:591:THR:OG1	2.28	0.51
4:C:297:SER:HA	4:C:335:VAL:HG12	1.93	0.50
7:G:300:SER:O	7:G:304:ILE:HG12	2.11	0.50
1:H:13:ASN:ND2	1:H:26:ALA:O	2.43	0.50
4:C:1058:ARG:HG2	4:C:1058:ARG:HH11	1.75	0.50
4:C:1115:VAL:HG13	4:C:1227:GLY:HA3	1.93	0.50
8:F:503:ARG:O	8:F:507:LYS:HG3	2.12	0.50
5:D:72:CYS:HB2	5:D:88:CYS:SG	2.51	0.50
5:D:844:VAL:HG13	5:D:864:LEU:HD21	1.91	0.50
9:I:16:PHE:HB2	9:I:23:LEU:HD12	1.94	0.50
5:D:919:ALA:O	5:D:923:ILE:HD12	2.10	0.50
4:C:803:ALA:HB2	4:C:1094:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:224:ILE:O	7:A:228:GLN:HG2	2.11	0.50
4:C:530:ILE:HD11	4:C:575:LEU:HD13	1.92	0.50
8:F:168:VAL:HB	8:F:266:GLU:HA	1.93	0.50
4:C:1065:LYS:HE2	4:C:1234:LEU:HD12	1.93	0.50
8:F:273:GLN:OE1	8:F:273:GLN:N	2.37	0.50
2:N:-48:DT:H2"	2:N:-47:DA:C8	2.46	0.50
4:C:575:LEU:HG	4:C:579:ALA:HB3	1.92	0.50
2:N:-27:DT:H2"	2:N:-26:DG:C8	2.47	0.50
3:T:19:DT:H2"	3:T:20:DA:C8	2.47	0.50
7:B:23:HIS:HD2	7:B:207:GLU:HG3	1.77	0.50
3:T:9:DT:H4'	4:C:496:LYS:HB3	1.94	0.49
5:D:1168:GLU:OE1	5:D:1191:LYS:NZ	2.45	0.49
7:G:261:LEU:HA	7:G:311:ARG:HH12	1.76	0.49
4:C:177:ILE:HG23	4:C:183:TRP:NE1	2.27	0.49
5:D:749:ARG:N	5:D:753:SER:O	2.43	0.49
5:D:252:LEU:HD13	5:D:262:THR:HB	1.93	0.49
7:A:4:SER:OG	7:A:5:VAL:N	2.45	0.49
8:F:487:LEU:HB3	8:F:489:GLU:OE1	2.12	0.49
8:F:528:GLY:HA2	8:F:531:ILE:HD12	1.93	0.49
1:K:10:PHE:HB3	1:K:96:LEU:HD21	1.95	0.49
4:C:184:LEU:HD13	4:C:198:ILE:HG12	1.94	0.49
3:T:65:DT:H2"	3:T:66:DA:C8	2.47	0.49
7:G:256:ARG:NH1	7:G:260:ASP:OD2	2.45	0.49
4:C:59:ILE:HG21	4:C:472:GLU:CG	2.43	0.49
5:D:770:LEU:O	5:D:774:ILE:HG12	2.12	0.49
3:T:47:DT:H2"	3:T:48:DA:C8	2.48	0.49
5:D:128:MET:HG2	5:D:192:MET:HE1	1.94	0.49
7:A:229:LEU:O	7:A:233:VAL:HG23	2.12	0.49
5:D:1258:GLN:OE1	5:D:1261:ARG:NH1	2.45	0.49
7:B:101:ILE:HD12	7:B:116:ILE:HG21	1.95	0.49
5:D:480:ALA:HA	5:D:484:MET:HB2	1.95	0.49
8:F:382:ARG:HG3	8:F:382:ARG:HH11	1.77	0.49
1:K:32:PRO:HB3	1:K:35:LEU:HD21	1.95	0.49
8:F:273:GLN:HA	8:F:276:HIS:HB3	1.94	0.49
4:C:364:VAL:O	4:C:368:ARG:HG3	2.12	0.48
4:C:1332:LEU:HD23	5:D:307:LEU:HD22	1.95	0.48
4:C:677:ASN:ND2	5:D:779:ALA:HB1	2.28	0.48
5:D:363:LEU:O	5:D:486:SER:OG	2.26	0.48
5:D:596:LEU:HD22	5:D:600:GLN:HB3	1.96	0.48
7:B:103:LEU:HB2	7:B:116:ILE:HG12	1.96	0.48
8:F:424:VAL:HG22	8:F:435:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:84:GLU:O	4:C:88:ARG:HG3	2.13	0.48
5:D:667:GLN:HG2	5:D:672:LEU:HD12	1.95	0.48
8:F:444:ARG:HG2	8:F:444:ARG:HH11	1.78	0.48
4:C:1252:LEU:HD21	5:D:253:VAL:HG11	1.95	0.48
7:B:23:HIS:CD2	7:B:207:GLU:HG3	2.48	0.48
5:D:747:MET:HG3	5:D:759:ILE:HD12	1.96	0.48
6:E:50:ALA:O	6:E:54:ILE:HG13	2.13	0.48
1:H:100:VAL:CG2	1:H:106:ARG:HG3	2.44	0.48
4:C:59:ILE:HG12	4:C:472:GLU:CD	2.38	0.48
5:D:1286:ILE:HG22	5:D:1290:LYS:HE3	1.96	0.47
7:B:60:GLU:HB2	7:B:144:ARG:HB3	1.96	0.47
1:H:15:TRP:CD1	1:H:26:ALA:HB2	2.49	0.47
4:C:931:VAL:HG22	4:C:1052:VAL:HG22	1.96	0.47
5:D:893:GLY:O	5:D:1257:ARG:NH2	2.46	0.47
5:D:1357:PRO:HB3	5:D:1365:HIS:CD2	2.48	0.47
1:K:54:HIS:CD2	1:K:109:ILE:HB	2.50	0.47
1:K:86:ARG:HB3	1:K:91:ASP:HB3	1.95	0.47
2:N:-52:DG:H2"	2:N:-51:DT:O5'	2.13	0.47
4:C:1142:ARG:NH1	4:C:1160:ILE:O	2.48	0.47
5:D:28:ASP:OD1	5:D:28:ASP:N	2.47	0.47
9:I:34:ARG:HA	9:I:34:ARG:HD2	1.69	0.47
4:C:106:ASP:HB3	4:C:109:ALA:HB3	1.96	0.47
5:D:720:ASN:HB3	5:D:723:TYR:HB3	1.97	0.47
2:N:-40:DT:H1'	7:G:266:ARG:HH21	1.78	0.47
4:C:216:THR:HB	4:C:219:GLU:HG3	1.96	0.47
4:C:478:ARG:C	4:C:478:ARG:HD3	2.40	0.47
4:C:546:GLU:OE1	4:C:546:GLU:N	2.34	0.47
5:D:164:GLU:OE1	5:D:168:ARG:HD2	2.14	0.47
5:D:1366:GLN:HA	5:D:1369:GLN:OE1	2.15	0.47
7:B:105:LYS:HD3	7:B:111:VAL:HG22	1.97	0.47
5:D:848:ILE:HD12	5:D:858:ILE:HD12	1.96	0.47
2:N:5:DT:H2'	2:N:6:DT:H71	1.97	0.47
5:D:215:LYS:HA	5:D:218:THR:HG22	1.96	0.47
7:A:23:HIS:NE2	7:A:205:ASP:OD1	2.47	0.47
7:B:99:VAL:HG11	7:B:122:VAL:HG21	1.96	0.47
5:D:1220:LEU:HD22	5:D:1305:LEU:HB2	1.97	0.47
4:C:562:GLU:HG2	4:C:574:SER:HB2	1.97	0.46
4:C:651:ASP:N	4:C:651:ASP:OD1	2.48	0.46
4:C:949:GLU:OE1	4:C:953:LEU:HD13	2.14	0.46
5:D:859:PRO:HG2	5:D:862:THR:HG21	1.97	0.46
4:C:67:GLU:OE1	4:C:69:GLN:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:582:ASN:HD21	4:C:586:PHE:HB2	1.79	0.46
4:C:817:LEU:HD12	4:C:1078:LYS:HB3	1.97	0.46
3:T:57:DG:P	9:I:56:ARG:NH1	2.88	0.46
5:D:653:GLU:HG2	5:D:689:THR:HG23	1.97	0.46
5:D:1329:ARG:CZ	5:D:1329:ARG:HB2	2.45	0.46
7:B:46:ILE:HD11	7:B:225:LEU:HD13	1.96	0.46
2:N:-29:DT:H2"	2:N:-28:DA:C8	2.51	0.46
2:N:-20:DT:H2"	2:N:-19:DA:C8	2.50	0.46
5:D:572:THR:OG1	5:D:573:THR:N	2.44	0.46
6:E:8:ASP:HB2	6:E:55:GLU:HG2	1.96	0.46
8:F:296:MET:HE2	8:F:296:MET:HA	1.98	0.46
1:K:14:LEU:HD12	1:K:24:TYR:O	2.15	0.46
4:C:220:ILE:HG21	4:C:351:LEU:HD11	1.98	0.46
7:B:44:ARG:HA	7:B:184:ILE:HD13	1.97	0.46
3:T:6:DA:C2	5:D:259:ARG:HG3	2.51	0.46
5:D:99:ARG:HG2	5:D:248:ASP:HB3	1.97	0.46
7:B:12:ARG:HG3	7:B:13:LEU:HG	1.97	0.46
8:F:127:ASP:O	8:F:131:GLN:HG3	2.14	0.46
1:K:86:ARG:HH21	1:K:94:LYS:HB3	1.81	0.46
4:C:373:GLY:HA2	8:F:95:ARG:HE	1.81	0.46
8:F:522:ASP:OD2	8:F:524:ASP:HB2	2.16	0.46
1:H:72:PHE:O	7:G:269:ASN:ND2	2.49	0.46
4:C:540:ARG:HD2	4:C:567:PRO:HB2	1.97	0.46
4:C:694:ARG:NH2	4:C:825:ASP:O	2.49	0.46
5:D:120:LEU:HD22	5:D:120:LEU:H	1.81	0.46
5:D:370:LYS:HG2	5:D:441:LEU:HB3	1.98	0.46
2:N:-3:DT:H2"	2:N:-2:DG:C8	2.51	0.46
8:F:474:ILE:O	8:F:478:MET:HG3	2.16	0.46
3:T:-1:DG:C2	3:T:0:DA:C5	3.04	0.46
4:C:1244:ALA:HB2	5:D:372:MET:HG2	1.98	0.46
5:D:770:LEU:HD13	5:D:770:LEU:HA	1.81	0.46
4:C:1156:GLN:HG2	4:C:1158:VAL:HG23	1.98	0.45
6:E:40:PRO:O	6:E:52:ARG:NH2	2.43	0.45
7:G:261:LEU:HA	7:G:311:ARG:NH1	2.31	0.45
9:I:22:THR:HG22	9:I:34:ARG:HH12	1.80	0.45
1:K:24:TYR:HB3	1:K:35:LEU:HD23	1.98	0.45
4:C:1243:HIS:HE1	4:C:1264:PHE:HA	1.81	0.45
5:D:141:PHE:HB3	5:D:293:ARG:HD2	1.97	0.45
4:C:1119:LEU:HG	4:C:1203:LEU:HD13	1.98	0.45
5:D:1340:ARG:HG2	5:D:1340:ARG:HH11	1.81	0.45
7:A:16:ILE:HD11	7:A:214:PRO:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:225:LEU:HD23	7:B:229:LEU:HD11	1.99	0.45
5:D:111:VAL:HG11	5:D:303:VAL:HB	1.99	0.45
5:D:227:PHE:CZ	5:D:237:MET:HE2	2.52	0.45
7:B:60:GLU:OE2	7:B:60:GLU:HA	2.16	0.45
9:I:51:ASN:H	9:I:107:LEU:HD21	1.82	0.45
1:K:53:TYR:OH	1:K:62:GLN:HG2	2.17	0.45
4:C:80:PHE:HB3	4:C:84:GLU:HB2	1.98	0.45
4:C:260:LYS:HB2	4:C:260:LYS:HE2	1.77	0.45
5:D:294:ASN:O	5:D:298:MET:HG3	2.16	0.45
5:D:1183:ASP:OD1	5:D:1184:THR:N	2.48	0.45
7:A:19:ILE:HD11	7:A:25:LYS:HG3	1.97	0.45
1:K:17:ASN:OD1	1:K:20:SER:N	2.49	0.45
2:N:-1:DA:H2"	2:N:0:DA:O4'	2.17	0.45
4:C:1311:ASN:HD21	4:C:1313:ALA:HB3	1.82	0.45
5:D:519:ASN:HB2	5:D:708:ASN:HA	1.96	0.45
2:N:2:DG:H1'	2:N:3:DA:C8	2.52	0.45
4:C:217:SER:O	4:C:221:LEU:HD22	2.17	0.45
5:D:189:LEU:HD22	5:D:234:PRO:HB3	1.98	0.45
1:K:10:PHE:CE1	1:K:109:ILE:HG12	2.46	0.45
4:C:231:GLU:HG2	4:C:332:LYS:HG2	1.98	0.45
4:C:295:LYS:HB2	4:C:295:LYS:HE2	1.75	0.45
4:C:370:MET:HE2	4:C:370:MET:HA	1.99	0.45
8:F:474:ILE:HD12	8:F:495:MET:HG2	1.98	0.45
1:K:55:PRO:O	1:K:106:ARG:NH2	2.47	0.45
4:C:631:ASP:C	4:C:647:ARG:HH12	2.24	0.45
5:D:329:ASP:OD1	5:D:329:ASP:N	2.50	0.45
6:E:30:MET:HE1	6:E:49:ILE:HB	1.98	0.45
8:F:124:ARG:HB3	8:F:379:LYS:HZ2	1.82	0.45
4:C:922:ASN:OD1	4:C:922:ASN:N	2.50	0.45
8:F:353:GLN:HA	8:F:356:GLU:OE1	2.17	0.45
5:D:155:GLU:N	5:D:155:GLU:OE1	2.50	0.44
5:D:844:VAL:HA	5:D:882:VAL:HA	1.98	0.44
5:D:985:ILE:HG12	5:D:991:THR:HA	1.99	0.44
5:D:1005:LYS:HB3	5:D:1009:ASP:HB2	1.98	0.44
5:D:1296:LYS:HD2	5:D:1297:GLU:N	2.32	0.44
1:K:25:TYR:CE2	1:K:36:ILE:HD11	2.53	0.44
4:C:468:LEU:O	4:C:472:GLU:HB2	2.17	0.44
7:G:282:LEU:HD21	7:G:308:LEU:HD11	2.00	0.44
2:N:-11:DA:H61	8:F:428:GLU:HB2	1.83	0.44
5:D:251:PRO:HB2	5:D:253:VAL:HG13	1.99	0.44
6:E:13:ILE:HG22	6:E:15:ASN:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:152:ARG:HB3	8:F:158:LEU:HD23	2.00	0.44
8:F:478:MET:O	8:F:482:MET:HG2	2.18	0.44
4:C:83:LYS:HE3	4:C:83:LYS:HB3	1.78	0.44
5:D:368:LEU:HD23	5:D:373:ALA:HB2	2.00	0.44
1:H:25:TYR:HB2	1:H:34:ARG:HG3	1.99	0.44
8:F:445:GLN:HG3	8:F:446:ALA:N	2.31	0.44
4:C:18:ARG:O	4:C:1155:ARG:NH1	2.40	0.44
4:C:1128:ILE:O	4:C:1132:ILE:HG13	2.18	0.44
5:D:761:ALA:HB3	5:D:767:LEU:HD23	1.99	0.44
5:D:804:ALA:HA	5:D:1258:GLN:HG3	2.00	0.44
5:D:861:ASN:OD1	5:D:883:ARG:NH2	2.46	0.44
5:D:986:ASP:OD2	5:D:992:LYS:HD3	2.18	0.44
7:A:52:PRO:HB3	7:B:5:VAL:HB	1.99	0.44
8:F:145:TYR:O	8:F:148:GLU:HG3	2.18	0.44
5:D:658:GLU:HB3	5:D:662:ARG:HH22	1.82	0.44
4:C:100:LEU:HD12	4:C:122:VAL:HG21	2.00	0.44
4:C:615:VAL:HG21	4:C:645:HIS:ND1	2.33	0.44
9:I:60:HIS:ND1	9:I:60:HIS:C	2.76	0.44
9:I:94:PRO:HB3	9:I:98:LYS:HD3	1.99	0.44
2:N:1:DG:C2	4:C:538:LEU:HD21	2.53	0.44
4:C:238:MET:HE1	4:C:283:ASN:O	2.18	0.44
5:D:956:GLY:HA3	5:D:985:ILE:O	2.17	0.44
5:D:1352:VAL:HG23	5:D:1354:ARG:HG3	2.00	0.44
7:A:115:ASP:N	7:A:115:ASP:OD1	2.50	0.44
7:G:288:VAL:O	7:G:292:LYS:HG3	2.18	0.44
3:T:-1:DG:H5'	3:T:-1:DG:H8	1.83	0.43
4:C:672:GLU:HG2	4:C:673:HIS:CD2	2.53	0.43
7:B:21:THR:HG23	7:B:22:THR:HG23	2.00	0.43
8:F:287:ARG:HH11	8:F:355:ILE:HD11	1.83	0.43
4:C:295:LYS:HD2	4:C:335:VAL:HG21	2.00	0.43
5:D:298:MET:SD	8:F:410:LEU:HB3	2.57	0.43
5:D:736:GLN:O	5:D:740:LEU:HG	2.18	0.43
5:D:1146:GLU:HA	5:D:1146:GLU:OE1	2.18	0.43
9:I:67:GLN:HB3	9:I:69:PHE:CZ	2.53	0.43
2:N:-9:DT:H4'	2:N:-8:DA:OP1	2.17	0.43
4:C:323:ALA:O	4:C:327:GLN:HG3	2.18	0.43
4:C:1245:ARG:NE	5:D:348:ASP:OD1	2.47	0.43
5:D:607:GLU:HG3	5:D:611:LYS:HZ1	1.84	0.43
8:F:148:GLU:O	8:F:152:ARG:HG3	2.19	0.43
7:G:299:LYS:HB2	7:G:299:LYS:NZ	2.34	0.43
1:K:60:ASN:O	1:K:64:ILE:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:407:LEU:HA	8:F:407:LEU:HD23	1.86	0.43
8:F:593:GLU:O	8:F:597:GLN:HG2	2.17	0.43
5:D:544:LEU:HD23	5:D:544:LEU:HA	1.92	0.43
4:C:10:ARG:CZ	4:C:697:LYS:HD3	2.48	0.43
8:F:121:ILE:HG21	8:F:387:MET:HB2	2.00	0.43
1:H:23:VAL:O	1:H:36:ILE:HG22	2.18	0.43
4:C:373:GLY:O	8:F:105:ARG:HD3	2.18	0.43
5:D:794:GLY:O	5:D:797:THR:HG22	2.19	0.43
5:D:992:LYS:NZ	5:D:992:LYS:HB3	2.33	0.43
3:T:17:DC:H2"	3:T:18:DA:C8	2.53	0.43
4:C:21:VAL:HG11	4:C:592:ARG:HD2	2.00	0.43
4:C:59:ILE:O	4:C:59:ILE:HD12	2.19	0.43
4:C:1165:ASP:N	4:C:1165:ASP:OD1	2.52	0.43
5:D:826:ILE:HD13	5:D:831:VAL:HA	2.01	0.43
7:A:90:VAL:HG13	7:A:122:VAL:HG13	1.99	0.43
7:B:193:VAL:HG22	7:B:199:LEU:HD11	2.01	0.43
1:K:7:ILE:HG23	1:K:17:ASN:HD22	1.84	0.43
4:C:176:ILE:HD12	4:C:405:PHE:CE2	2.54	0.43
4:C:1024:ASP:OD1	4:C:1025:PHE:N	2.52	0.43
5:D:781:LYS:NZ	5:D:781:LYS:HB3	2.34	0.43
5:D:1160:SER:HA	5:D:1203:ILE:O	2.18	0.43
8:F:411:ASP:OD1	8:F:411:ASP:N	2.51	0.43
5:D:194:LEU:HB2	5:D:195:PRO:HD3	2.01	0.43
5:D:364:HIS:HB2	5:D:485:MET:HE2	2.01	0.43
8:F:478:MET:HB2	8:F:486:PRO:HG3	2.01	0.43
8:F:556:LEU:HB3	8:F:568:ARG:HH21	1.84	0.43
4:C:772:MET:HE3	4:C:773:PRO:HD2	2.00	0.42
5:D:149:PRO:HG3	5:D:156:ARG:HG2	2.00	0.42
5:D:955:ASN:OD1	5:D:1013:ALA:N	2.50	0.42
9:I:23:LEU:HB3	9:I:33:ILE:HB	2.01	0.42
1:K:73:ILE:HD13	1:K:73:ILE:HA	1.88	0.42
3:T:31:DG:OP2	8:F:580:THR:OG1	2.37	0.42
4:C:498:ILE:O	4:C:502:VAL:HG22	2.18	0.42
7:B:62:GLU:HA	7:B:62:GLU:OE1	2.18	0.42
4:C:258:ASP:HA	4:C:261:VAL:CG2	2.48	0.42
8:F:270:THR:H	8:F:273:GLN:HE22	1.67	0.42
4:C:142:GLU:O	4:C:515:MET:HB2	2.20	0.42
7:B:189:GLU:OE1	7:B:201:LYS:HG2	2.19	0.42
8:F:285:MET:HE3	8:F:285:MET:O	2.20	0.42
8:F:346:ARG:HA	8:F:349:ILE:HG12	2.01	0.42
8:F:581:LEU:HB3	8:F:592:ARG:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:18:ASP:OD1	5:D:18:ASP:C	2.61	0.42
5:D:93:THR:OG1	5:D:94:GLN:N	2.52	0.42
7:A:9:LEU:HD12	7:A:199:LEU:HD21	2.01	0.42
7:B:9:LEU:HD12	7:B:9:LEU:HA	1.89	0.42
4:C:633:LEU:HB3	4:C:644:LEU:HD22	2.00	0.42
4:C:943:LYS:HB3	4:C:943:LYS:HE3	1.85	0.42
5:D:102:MET:HG2	5:D:246:PRO:HD3	2.01	0.42
5:D:410:ASP:OD1	5:D:410:ASP:N	2.51	0.42
5:D:789:LYS:HD2	5:D:928:THR:O	2.19	0.42
6:E:9:ALA:HB1	6:E:19:LEU:HD21	2.00	0.42
8:F:361:LEU:HB3	8:F:365:ARG:HB2	2.01	0.42
1:K:7:ILE:HG22	1:K:15:TRP:HE3	1.85	0.42
4:C:930:ASP:OD1	4:C:931:VAL:N	2.53	0.42
5:D:645:VAL:HG22	5:D:701:LEU:HD12	2.02	0.42
5:D:1340:ARG:HG2	5:D:1340:ARG:NH1	2.34	0.42
7:G:279:ILE:O	7:G:283:VAL:HG22	2.20	0.42
5:D:1156:LEU:HD12	5:D:1156:LEU:HA	1.83	0.42
5:D:1235:GLU:O	5:D:1239:VAL:HG12	2.19	0.42
9:I:41:ARG:NH2	9:I:66:GLU:HG2	2.34	0.42
2:N:-1:DA:H2'	2:N:0:DA:C8	2.55	0.42
5:D:659:GLU:O	5:D:663:GLU:HG2	2.19	0.42
5:D:881:LYS:HB2	5:D:881:LYS:NZ	2.34	0.42
7:G:285:ARG:HD2	7:G:290:LEU:HD13	2.02	0.42
9:I:76:LEU:HD23	9:I:80:ILE:HD13	2.02	0.42
2:N:7:DT:H2"	2:N:8:DA:C8	2.55	0.42
3:T:22:DC:H2"	3:T:23:DA:C8	2.55	0.42
3:T:43:DG:H2"	3:T:44:DA:C8	2.55	0.42
4:C:342:ASP:N	4:C:342:ASP:OD1	2.53	0.42
4:C:557:ARG:NH2	4:C:611:GLU:OE1	2.48	0.42
5:D:40:LYS:HB2	5:D:40:LYS:HE3	1.85	0.42
5:D:613:GLY:O	5:D:617:THR:OG1	2.31	0.42
5:D:805:GLN:NE2	5:D:1346:LEU:H	2.17	0.42
2:N:-41:DG:N2	7:G:266:ARG:HH22	2.11	0.41
3:T:9:DT:H2"	3:T:10:DA:C8	2.54	0.41
7:B:126:ASN:OD1	7:B:126:ASN:N	2.52	0.41
2:N:-23:DT:H2"	2:N:-22:DG:C8	2.55	0.41
4:C:1275:TRP:CE2	5:D:801:VAL:HG11	2.55	0.41
5:D:735:ALA:O	5:D:739:GLN:HG3	2.19	0.41
5:D:749:ARG:HG2	5:D:750:PRO:HD3	2.01	0.41
8:F:290:THR:O	8:F:293:ARG:HG2	2.20	0.41
2:N:-64:DT:H2"	2:N:-63:DG:C8	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:58:DA:H2"	3:T:59:DA:C8	2.54	0.41
4:C:55:SER:OG	4:C:465:ARG:NH1	2.53	0.41
4:C:178:PRO:HG3	4:C:395:TYR:CE1	2.55	0.41
7:B:205:ASP:OD1	7:B:205:ASP:C	2.63	0.41
7:B:215:GLU:O	7:B:219:ARG:HG3	2.20	0.41
8:F:400:LYS:O	8:F:400:LYS:HD3	2.21	0.41
8:F:405:ARG:HB2	8:F:451:ILE:HD12	2.02	0.41
8:F:434:LYS:HB3	8:F:434:LYS:HE2	1.61	0.41
4:C:261:VAL:HG12	4:C:262:TYR:O	2.21	0.41
4:C:265:LYS:HE3	4:C:265:LYS:HB3	1.88	0.41
5:D:34:SER:OG	5:D:36:GLY:O	2.37	0.41
2:N:9:DA:H2"	2:N:10:DG:C8	2.55	0.41
4:C:471:VAL:HG21	4:C:498:ILE:HD11	2.02	0.41
4:C:954:LYS:HD2	4:C:954:LYS:O	2.19	0.41
5:D:278:ARG:NE	8:F:415:GLU:OE2	2.53	0.41
7:A:79:LEU:HD12	7:A:79:LEU:HA	1.81	0.41
7:A:82:LEU:O	7:A:86:LYS:HG3	2.21	0.41
8:F:575:MET:HB3	8:F:575:MET:HE2	1.73	0.41
8:F:605:LYS:HE2	8:F:605:LYS:HB3	1.81	0.41
4:C:24:ILE:HG12	4:C:578:PHE:CZ	2.55	0.41
4:C:39:ILE:HG13	4:C:75:LEU:HD11	2.02	0.41
4:C:129:LEU:HD23	4:C:129:LEU:HA	1.91	0.41
4:C:204:LEU:HD21	4:C:369:MET:HG3	2.02	0.41
4:C:382:GLU:OE1	4:C:382:GLU:C	2.64	0.41
4:C:1021:LEU:HA	4:C:1024:ASP:OD2	2.20	0.41
1:H:46:LEU:HD12	1:H:47:LEU:N	2.36	0.41
1:K:100:VAL:HG23	1:K:103:GLN:HB2	2.02	0.41
4:C:727:VAL:HG11	7:A:75:GLN:HE21	1.84	0.41
4:C:820:GLU:O	4:C:824:GLN:HG3	2.21	0.41
5:D:585:LYS:NZ	5:D:585:LYS:HB2	2.36	0.41
7:A:126:ASN:OD1	7:A:126:ASN:N	2.53	0.41
7:B:90:VAL:HG23	7:B:122:VAL:HG13	2.02	0.41
7:B:229:LEU:O	7:B:233:VAL:HG23	2.21	0.41
9:I:107:LEU:H	9:I:107:LEU:HD23	1.86	0.41
4:C:39:ILE:HD11	4:C:127:ILE:HG21	2.02	0.41
4:C:96:LEU:HD23	4:C:124:MET:HB3	2.02	0.41
3:T:8:DA:H4'	3:T:9:DT:OP2	2.20	0.41
4:C:74:ARG:NH2	4:C:97[A]:ARG:HD3	2.36	0.41
4:C:172:TYR:CD2	4:C:435:ILE:HG22	2.56	0.41
4:C:729:ALA:HA	4:C:769:PRO:HG2	2.03	0.41
5:D:51:PRO:HB3	5:D:57:PHE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1265:ILE:HD13	5:D:1265:ILE:HA	1.94	0.41
5:D:1348:GLU:O	5:D:1352:VAL:HG22	2.21	0.41
7:A:15:ASP:OD1	7:A:16:ILE:N	2.54	0.41
7:B:15:ASP:OD1	7:B:15:ASP:C	2.63	0.41
7:B:208:THR:HG23	7:B:214:PRO:HG3	2.02	0.41
7:B:220:ARG:O	7:B:224:ILE:HG13	2.21	0.41
8:F:420:LEU:C	8:F:420:LEU:HD23	2.46	0.41
7:G:290:LEU:HD12	7:G:290:LEU:HA	1.90	0.41
9:I:41:ARG:HH22	9:I:66:GLU:HG2	1.86	0.41
2:N:-18:DT:H2"	2:N:-17:DG:C8	2.56	0.41
3:T:10:DA:H5"	8:F:476:ARG:NH2	2.36	0.41
5:D:1223:ARG:HE	5:D:1223:ARG:HB2	1.51	0.41
5:D:1274:LEU:O	5:D:1277:GLU:HB2	2.21	0.41
1:K:91:ASP:CG	1:K:96:LEU:H	2.28	0.40
3:T:20:DA:H2"	3:T:21:DA:H8	1.85	0.40
4:C:533:LEU:HD21	4:C:571:LEU:HD13	2.02	0.40
5:D:127:LEU:HD12	5:D:127:LEU:HA	1.94	0.40
5:D:312:ARG:HA	5:D:312:ARG:HD2	1.87	0.40
5:D:912:GLY:O	5:D:1359:GLY:N	2.52	0.40
7:A:232:PHE:HE1	7:B:39:LEU:HD13	1.86	0.40
7:B:216:GLU:O	7:B:220:ARG:HG3	2.21	0.40
8:F:335:VAL:HG12	8:F:339:ARG:HE	1.86	0.40
9:I:22:THR:HG22	9:I:34:ARG:NH1	2.36	0.40
3:T:15:DT:H2"	3:T:16:DA:C8	2.56	0.40
4:C:42:ASP:OD2	4:C:46:GLN:NE2	2.54	0.40
4:C:1339:GLU:OE1	5:D:21:LYS:HD2	2.21	0.40
5:D:29:MET:HE2	5:D:29:MET:HB2	1.84	0.40
5:D:126:LEU:HD21	5:D:223:LEU:HD22	2.03	0.40
5:D:482:THR:O	5:D:488:ASN:ND2	2.53	0.40
5:D:681:LYS:HB3	5:D:681:LYS:HE3	1.79	0.40
5:D:858:ILE:HG12	5:D:868:TRP:CZ3	2.56	0.40
5:D:1346:LEU:HD22	5:D:1356:ILE:HB	2.04	0.40
3:T:1:DA:H3'	3:T:2:DG:H8	1.87	0.40
1:H:42:MET:HE2	1:H:42:MET:HB3	1.94	0.40
2:N:-55:DT:H2"	2:N:-54:DA:C8	2.56	0.40
4:C:127:ILE:HD13	4:C:127:ILE:HA	1.89	0.40
4:C:472:GLU:OE1	4:C:472:GLU:HA	2.21	0.40
4:C:618:GLN:NE2	5:D:770:LEU:HD23	2.36	0.40
5:D:434:ILE:HG12	5:D:484:MET:HE1	2.03	0.40
5:D:493:PRO:HB3	5:D:904:ALA:HB2	2.04	0.40
5:D:1148:ARG:HG2	5:D:1148:ARG:HH11	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1269:PHE:CZ	4:C:1273:GLU:HB3	2.57	0.40
5:D:1197:VAL:HG11	5:D:1203:ILE:HG21	2.04	0.40
8:F:424:VAL:HG22	8:F:435:PHE:HZ	1.86	0.40
8:F:470:LYS:NZ	8:F:495:MET:HE3	2.37	0.40
8:F:553:ARG:HG2	8:F:553:ARG:NH1	2.36	0.40
8:F:612:SER:O	8:F:612:SER:OG	2.34	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	H	110/115 (96%)	103 (94%)	7 (6%)	0	100	100
1	K	107/115 (93%)	101 (94%)	6 (6%)	0	100	100
4	C	1323/1341 (99%)	1305 (99%)	18 (1%)	0	100	100
5	D	1192/1401 (85%)	1169 (98%)	23 (2%)	0	100	100
6	E	67/90 (74%)	66 (98%)	1 (2%)	0	100	100
7	A	227/330 (69%)	223 (98%)	4 (2%)	0	100	100
7	B	218/330 (66%)	216 (99%)	2 (1%)	0	100	100
7	G	68/330 (21%)	65 (96%)	3 (4%)	0	100	100
8	F	462/621 (74%)	456 (99%)	6 (1%)	0	100	100
9	I	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
All	All	3882/4783 (81%)	3808 (98%)	74 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	H	104/106 (98%)	101 (97%)	3 (3%)	37 71
1	K	101/106 (95%)	100 (99%)	1 (1%)	68 89
4	C	1135/1144 (99%)	1128 (99%)	7 (1%)	78 93
5	D	1012/1168 (87%)	1000 (99%)	12 (1%)	63 86
6	E	58/74 (78%)	58 (100%)	0	100 100
7	A	195/283 (69%)	194 (100%)	1 (0%)	81 93
7	B	186/283 (66%)	185 (100%)	1 (0%)	81 93
7	G	62/283 (22%)	59 (95%)	3 (5%)	23 55
8	F	417/544 (77%)	414 (99%)	3 (1%)	76 92
9	I	103/103 (100%)	100 (97%)	3 (3%)	37 71
All	All	3373/4094 (82%)	3339 (99%)	34 (1%)	65 89

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	35	LEU
1	H	88	PHE
1	H	109	ILE
1	K	30	MET
4	C	39	ILE
4	C	221	LEU
4	C	370	MET
4	C	403	MET
4	C	984	TYR
4	C	1000	GLN
4	C	1060	ILE
5	D	248	ASP
5	D	421	VAL
5	D	499	ILE
5	D	553	THR
5	D	749	ARG

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Mol	Chain	Res	Type
5	D	770	LEU
5	D	822	MET
5	D	1158	GLU
5	D	1159	HIS
5	D	1192	HIS
5	D	1195	LEU
5	D	1313	LEU
7	A	177	THR
7	B	58	GLU
8	F	102	MET
8	F	522	ASP
8	F	560	THR
7	G	278	TYR
7	G	285	ARG
7	G	300	SER
9	I	54	ILE
9	I	60	HIS
9	I	82	THR

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

Mol	Chain	Res	Type
1	H	70	HIS
1	K	62	GLN
1	K	70	HIS
4	C	65	ASN
4	C	494	ASN
4	C	510	GLN
4	C	513	GLN
4	C	596	ASN
4	C	618	GLN
4	C	673	HIS
4	C	677	ASN
4	C	737	ASN
4	C	808	ASN
4	C	1136	GLN
4	C	1208	GLN
4	C	1235	ASN
4	C	1236	HIS
4	C	1311	ASN
5	D	200	GLN
5	D	266	ASN

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Mol	Chain	Res	Type
5	D	277	ASN
5	D	469	HIS
5	D	488	ASN
5	D	581	GLN
5	D	665	GLN
5	D	705	GLN
5	D	720	ASN
5	D	805	GLN
5	D	825	HIS
6	E	31	GLN
7	A	66	HIS
7	A	75	GLN
7	B	23	HIS
7	B	37	HIS
8	F	463	HIS
8	F	526	HIS
8	F	579	HIS
7	G	277	HIS
7	G	321	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

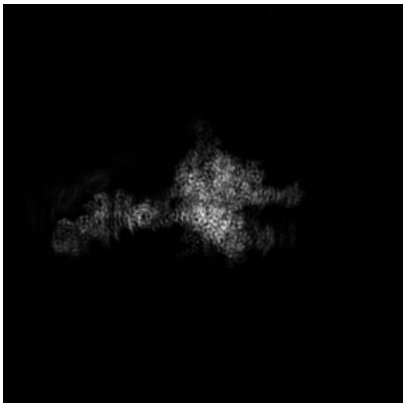
This section contains visualisations of the EMDB entry EMD-51277. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

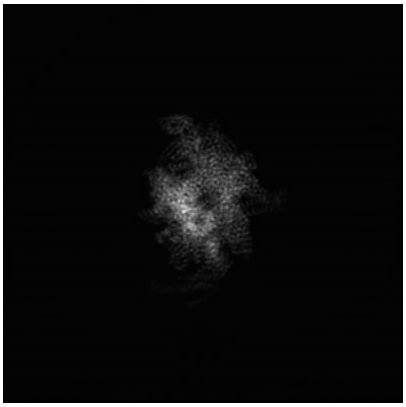
6.1 Orthogonal projections

6.1.1 Primary map

X



Y



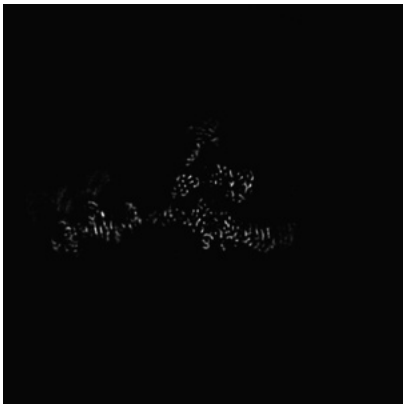
Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 256



Y Index: 256

Z Index: 256

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: 232

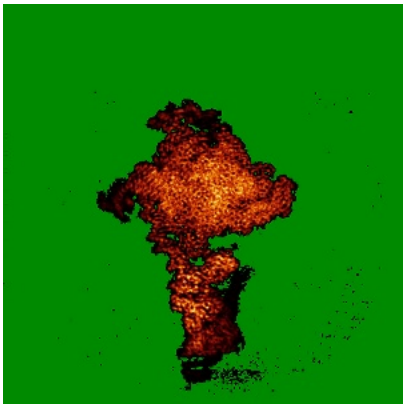
Y Index: 274

Z Index: 275

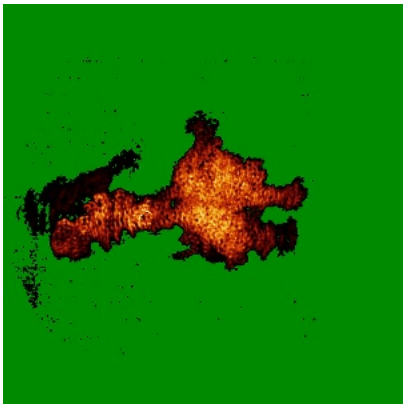
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

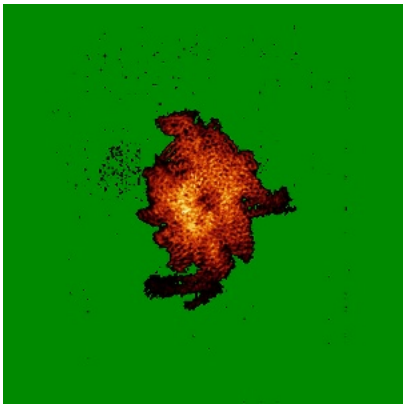
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.84. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

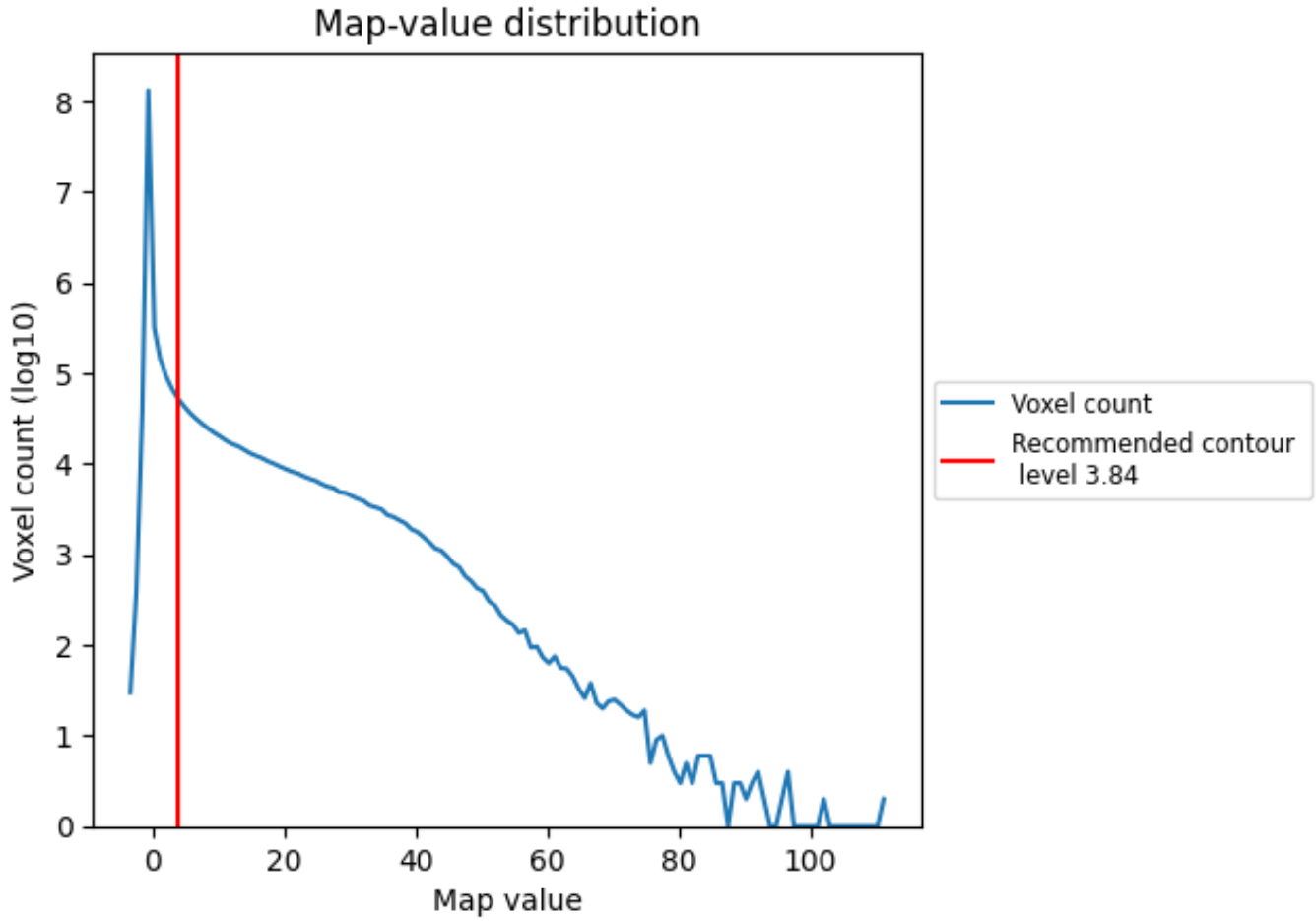
6.6 Mask visualisation (i)

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

7 Map analysis

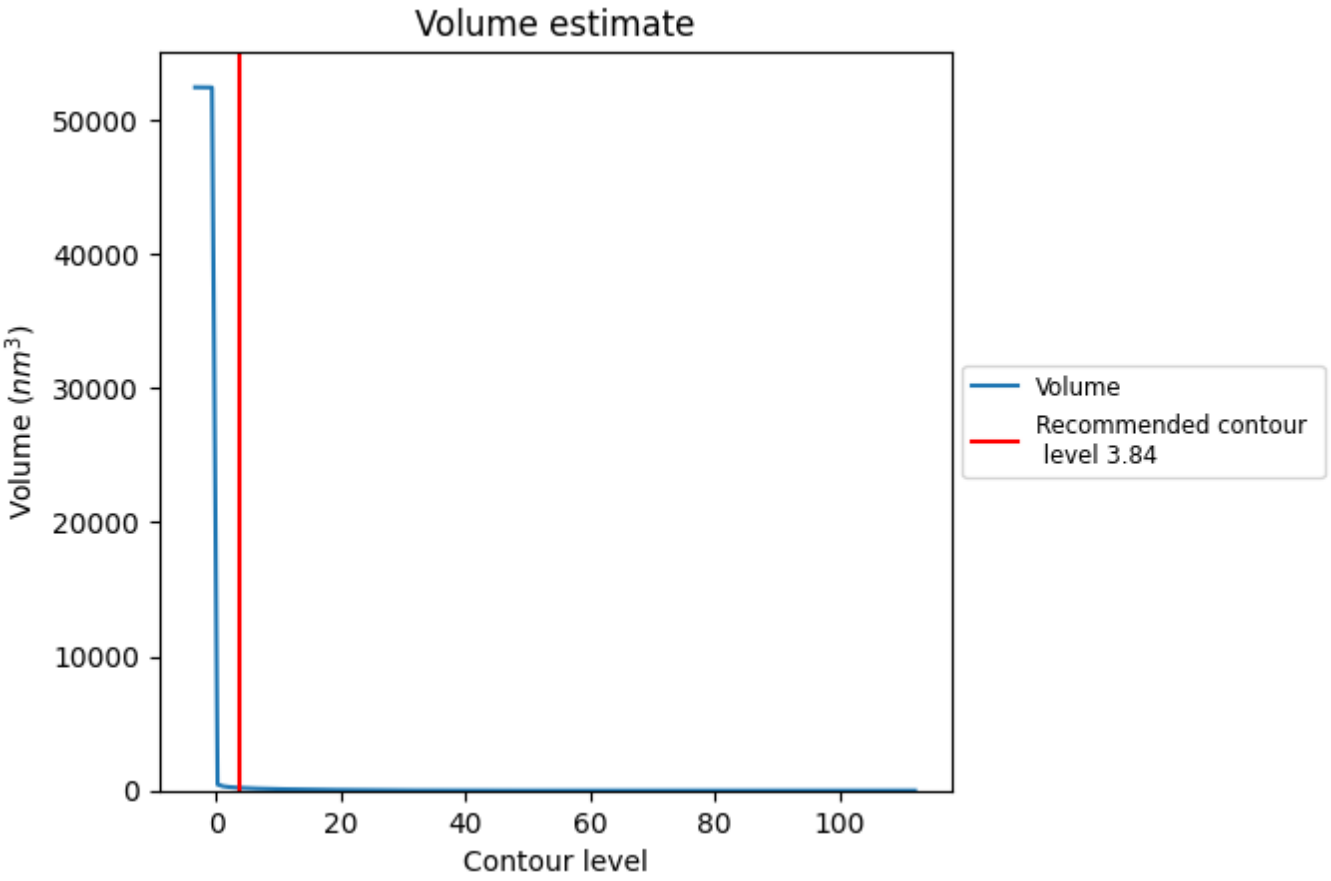
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

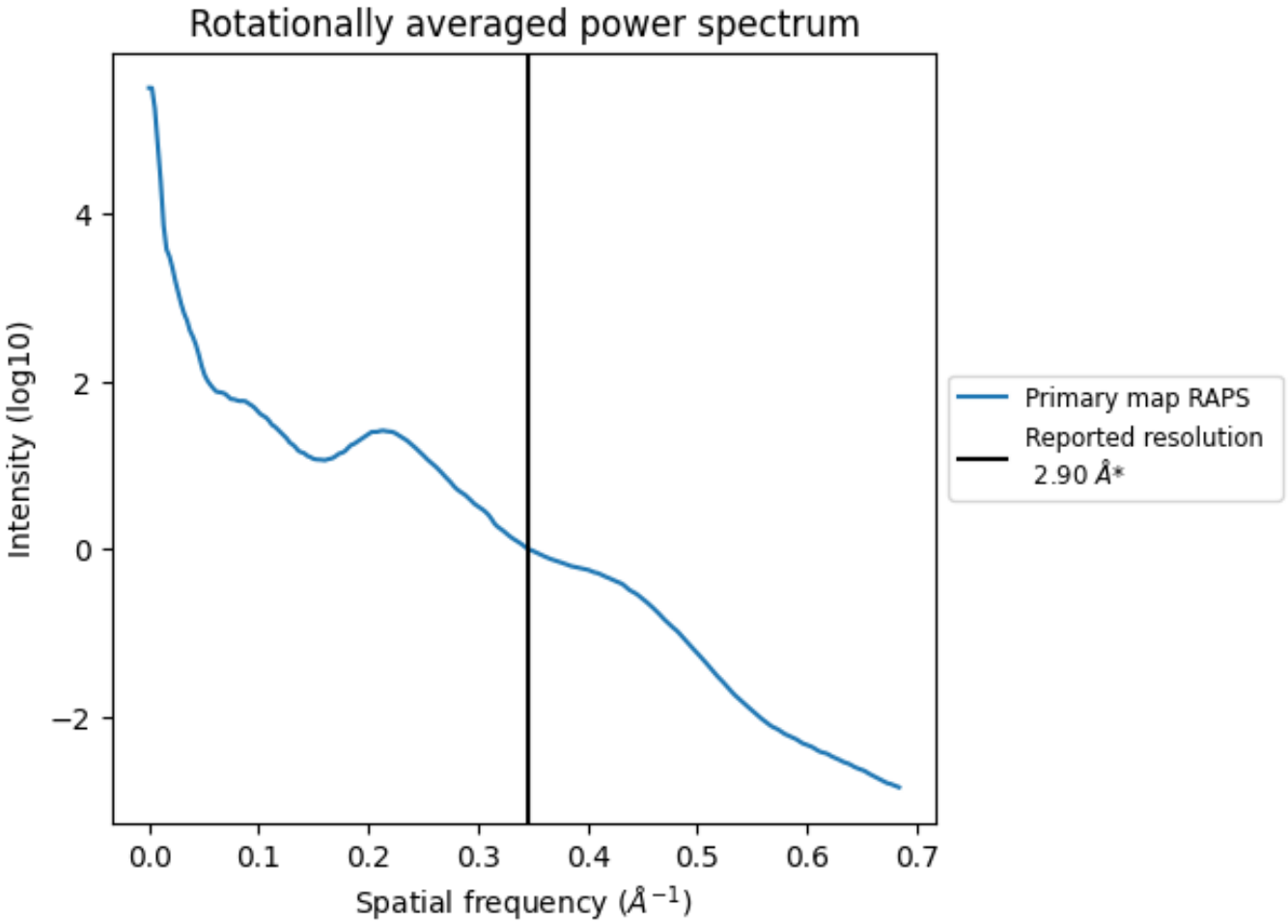
7.2 Volume estimate



The volume at the recommended contour level is 203 nm^3; this corresponds to an approximate mass of 184 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 (i)

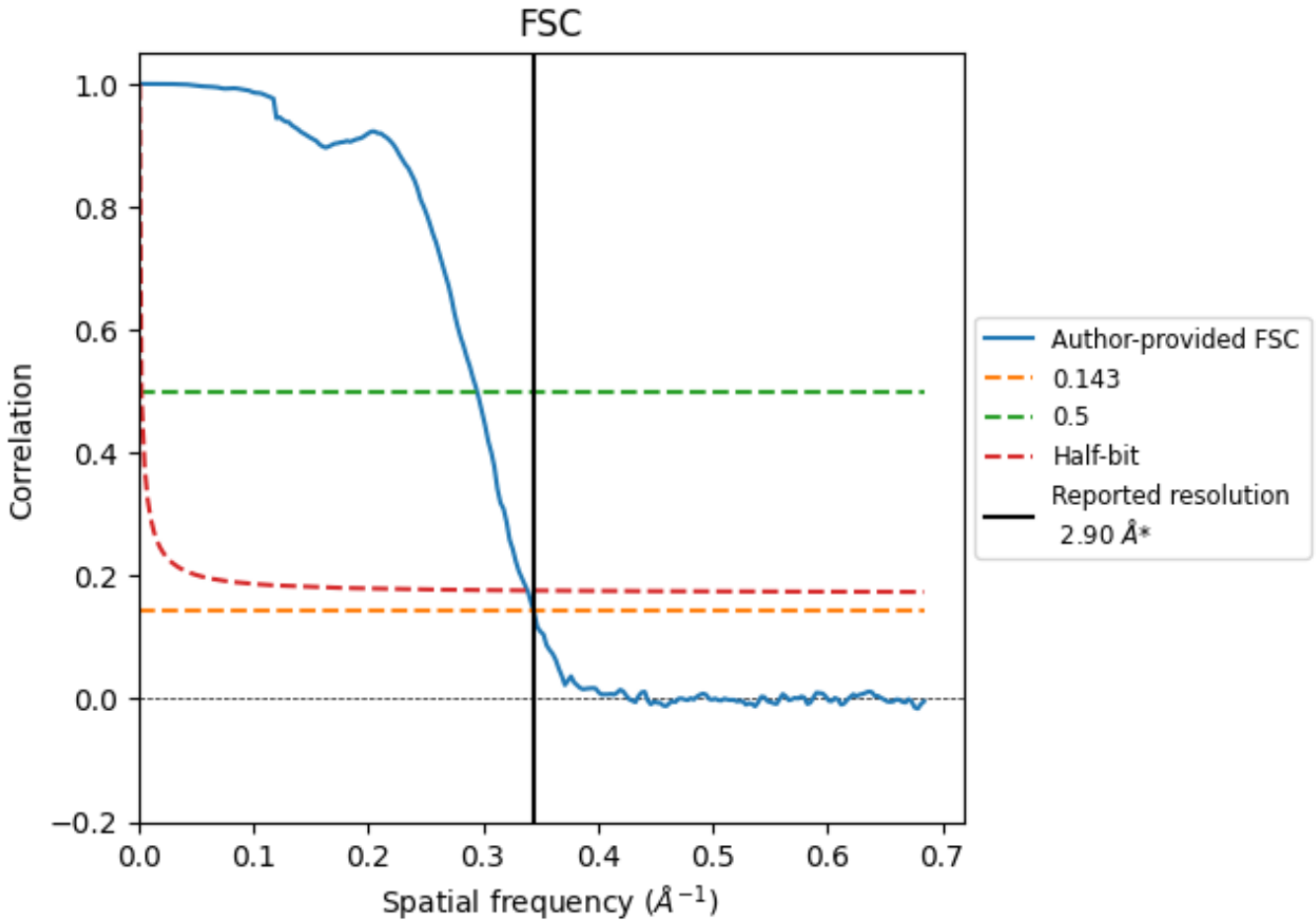


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

8.2 Resolution estimates (i)

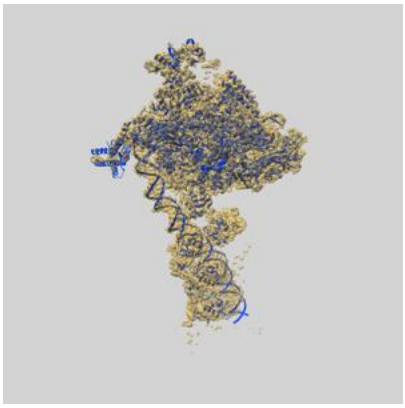
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.91	3.39	2.95
Unmasked-calculated*	-	-	-

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

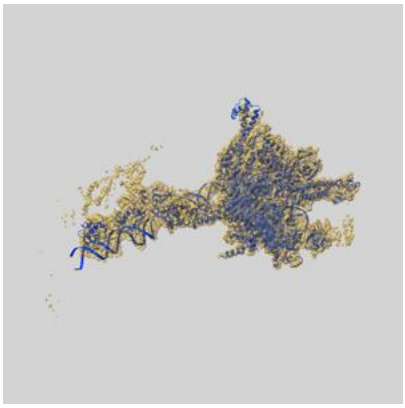
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51277 and PDB model 9GDS. Per-residue inclusion information can be found in section 3 on page 7.

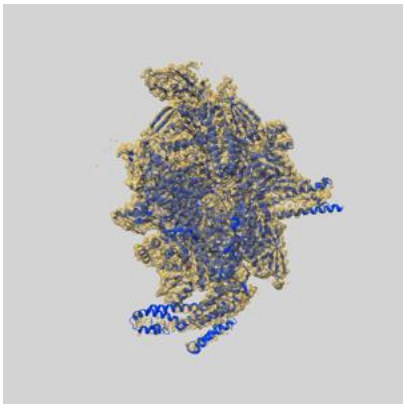
9.1 Map-model overlay



X



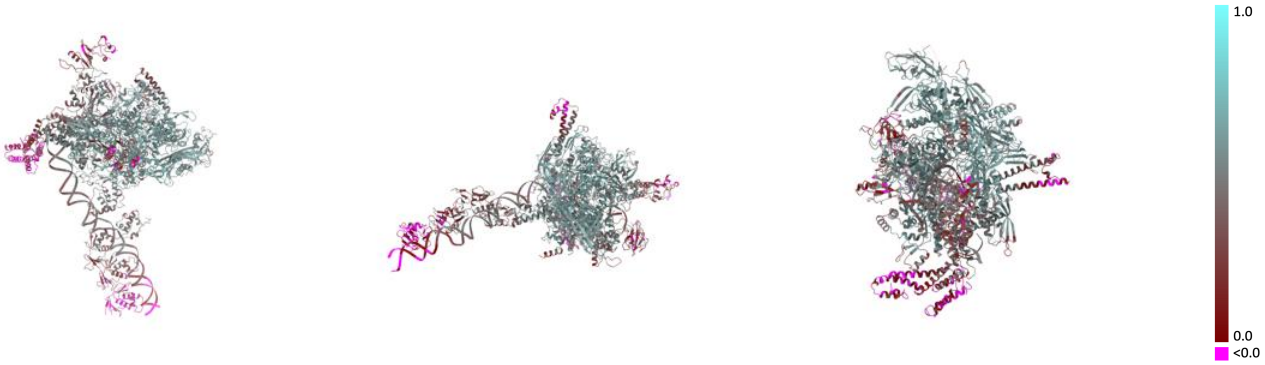
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.84 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)



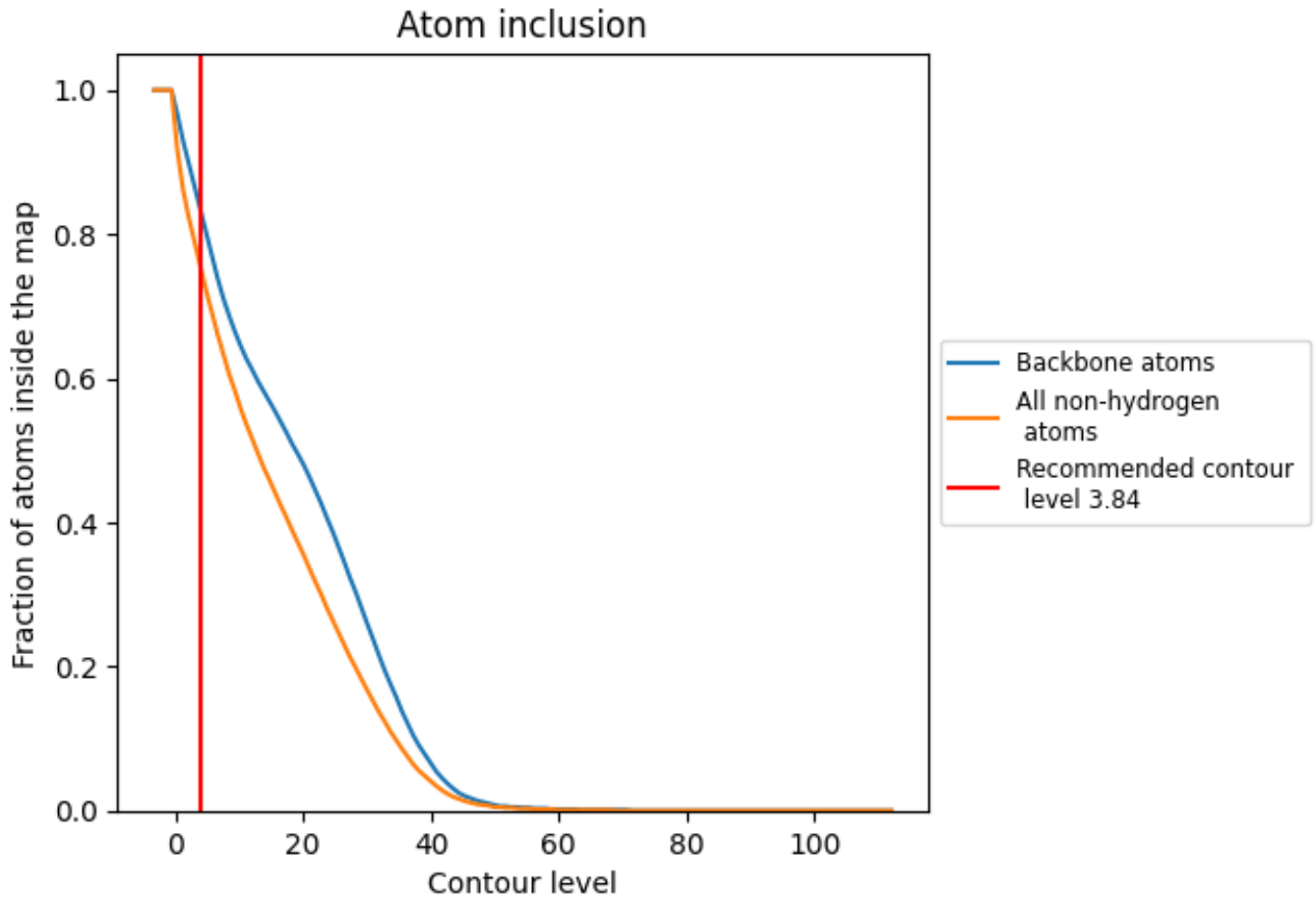
X Y Z

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

9.3 Atom inclusion mapped to coordinate model (i)

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3.84) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7590	0.4420
A	0.8700	0.5650
B	0.8660	0.5490
C	0.8140	0.5000
D	0.8370	0.5090
E	0.6420	0.4460
F	0.5000	0.2750
G	0.8380	0.3800
H	0.8040	0.3340
I	0.3440	0.0010
K	0.6890	0.2530
N	0.6800	0.3390
T	0.6580	0.3480