Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 04:28 pm GMT

PDB ID	:	5NSR
EMDB ID	:	EMD-3695
Title	:	Cryo-EM structure of RNA polymerase-sigma54 holo enzyme with promoter DNA closed complex
Authors	:	Glyde, R.; Ye, F.Z.; Darbari, V.C.; Zhang, N.; Buck, M.; Zhang, X.D.
Deposited on	:	2017-04-26
Resolution	:	3.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

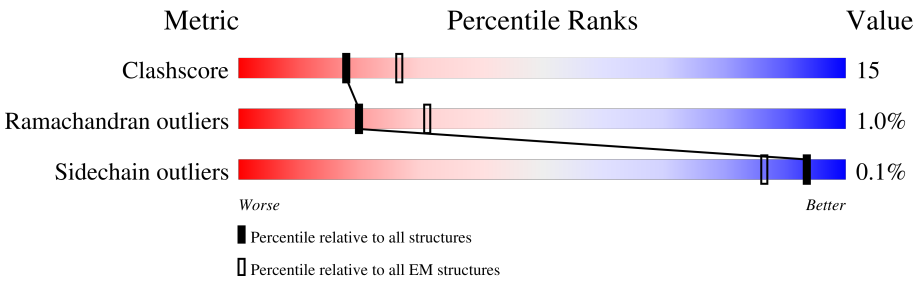
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	329	• 44% 27% 29%
1	B	329	• 49% 19% 32%
2	C	1342	• 75% 24% •
3	D	1407	7% 72% 22% 6%
4	E	91	9% 69% 12% 19%
5	M	573	9% 58% 9% • 33%
6	F	63	5% 13% 14% 13% 60%
7	G	63	• 11% 19% 16% 54%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 25363 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
			Total	C	N	O	S		
1	A	233	1694	1059	302	327	6	0	0
1	B	223	1606	1005	283	313	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	1341	9472	5946	1648	1844	34	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	1320	8969	5618	1623	1692	36	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	74	532	326	104	101	1	0	0

- Molecule 5 is a protein called RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	M	386	1983	1195	387	400	1	0	0

- Molecule 6 is a DNA chain called Non-Template promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	F	25	511	242	94	150	25	0	0

- Molecule 7 is a DNA chain called Template DNA promoter.

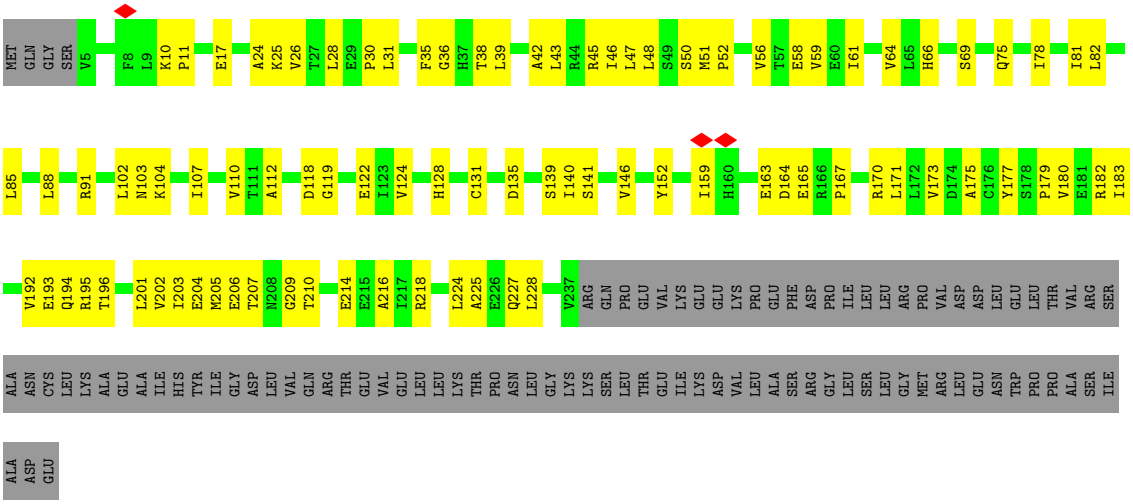
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	G	29	596	282	111	174	29	0	0

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.

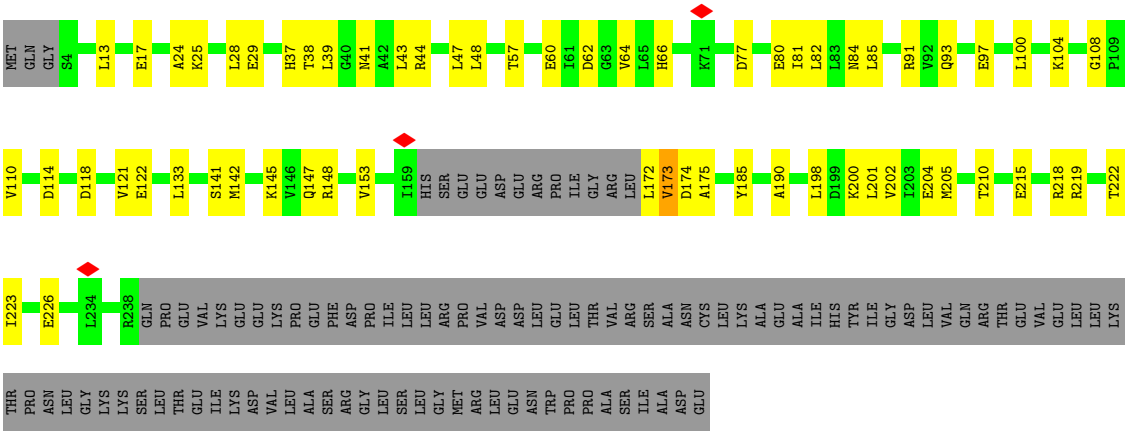
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A: 44% 27% 29%



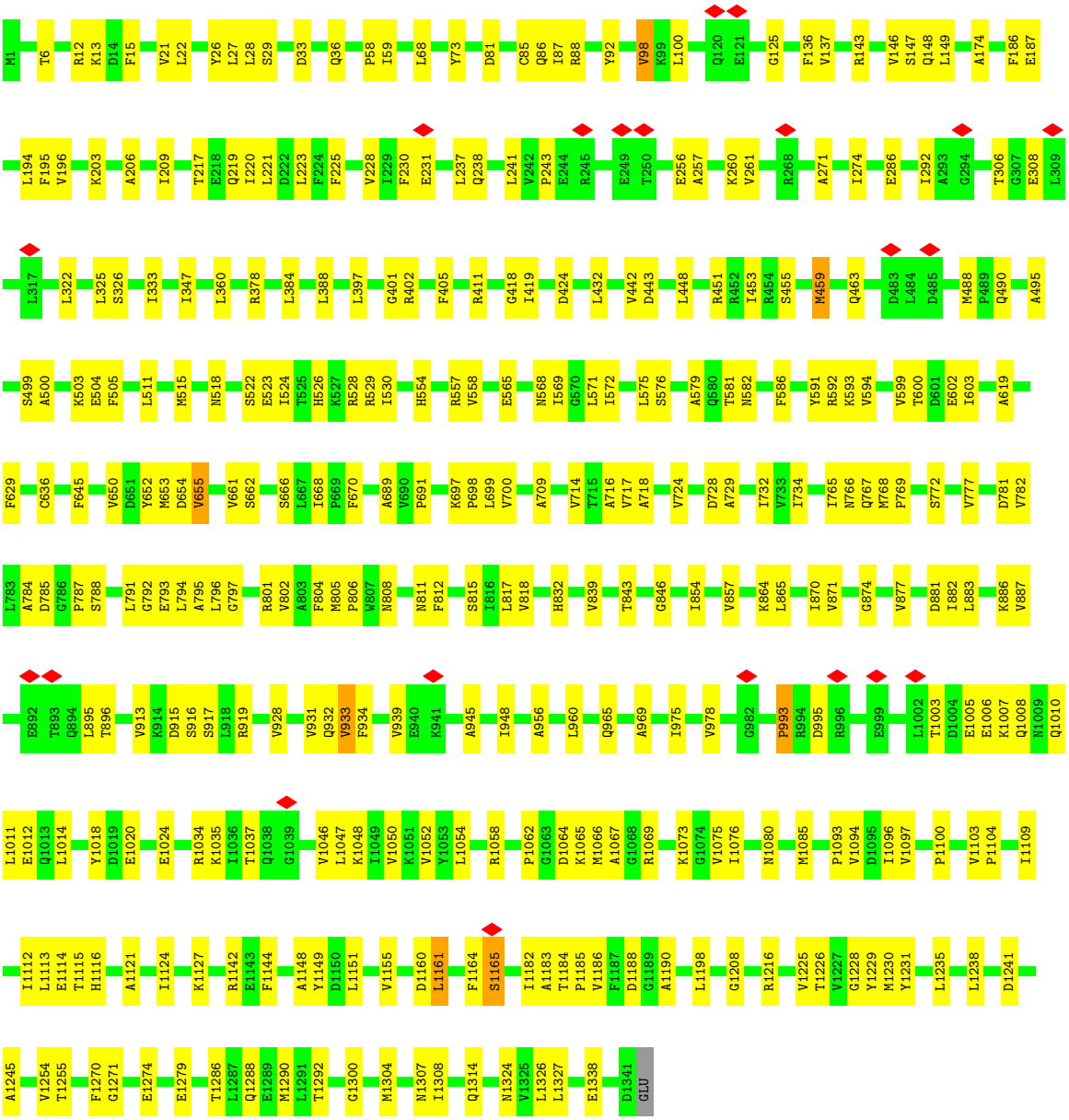
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B: 49% 19% 32%



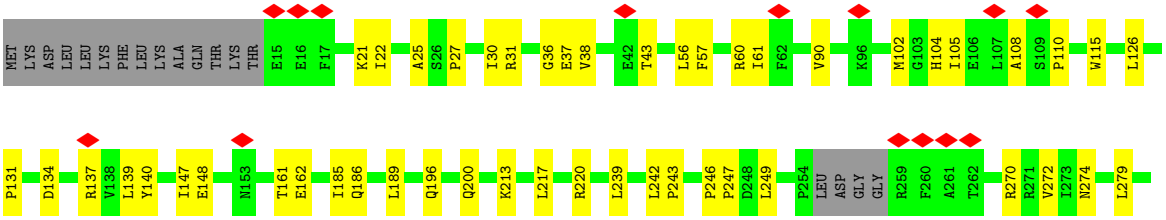
• Molecule 2: DNA-directed RNA polymerase subunit beta

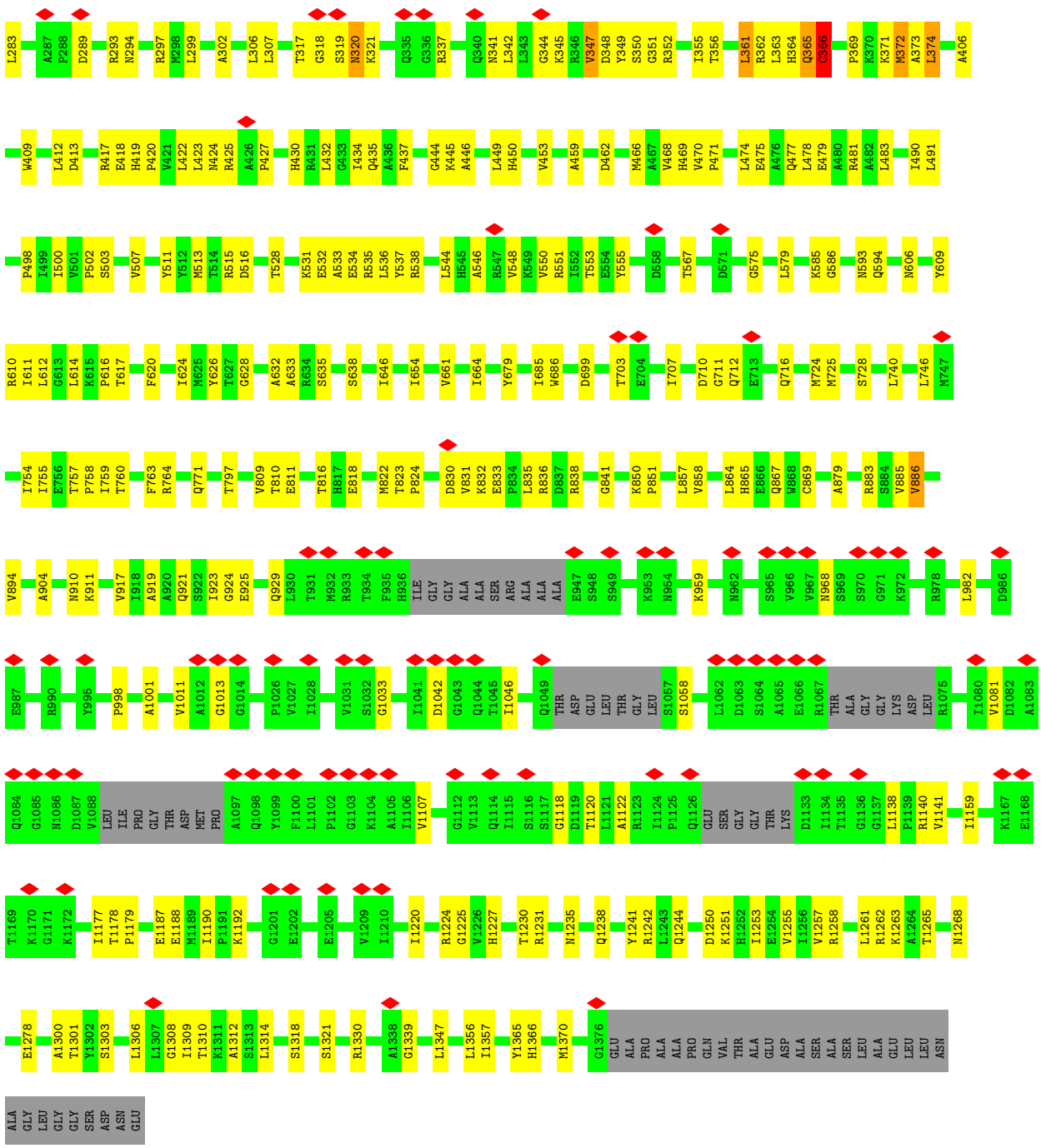
Chain C: 75% 24%



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

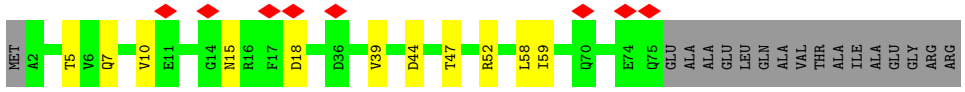
Chain D: 7% 72% 22% 6%





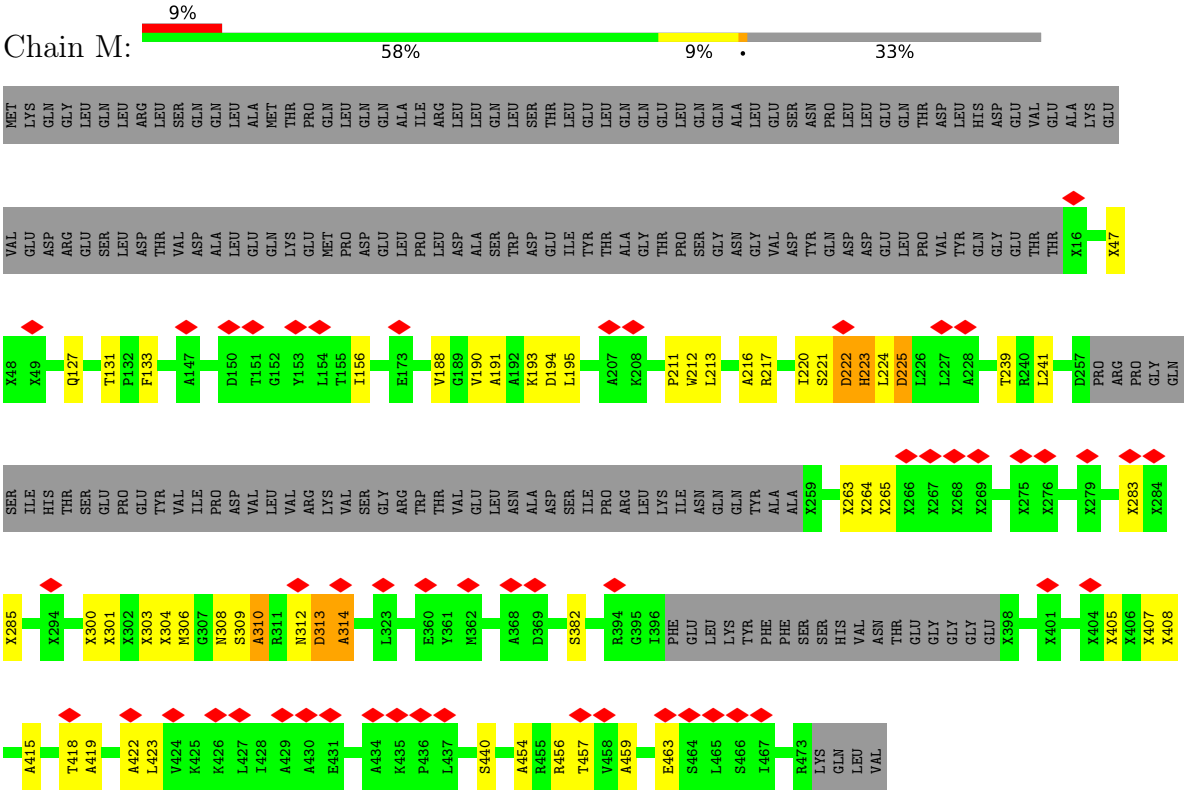
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



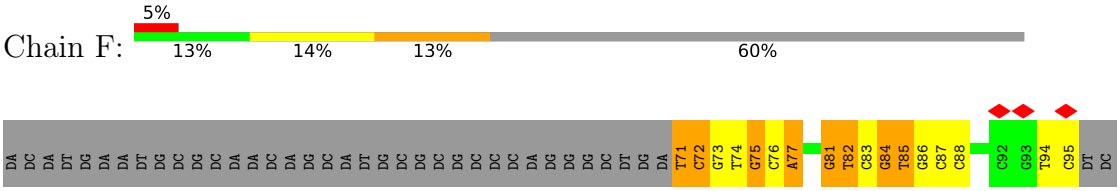
• Molecule 5: RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor

Chain M:



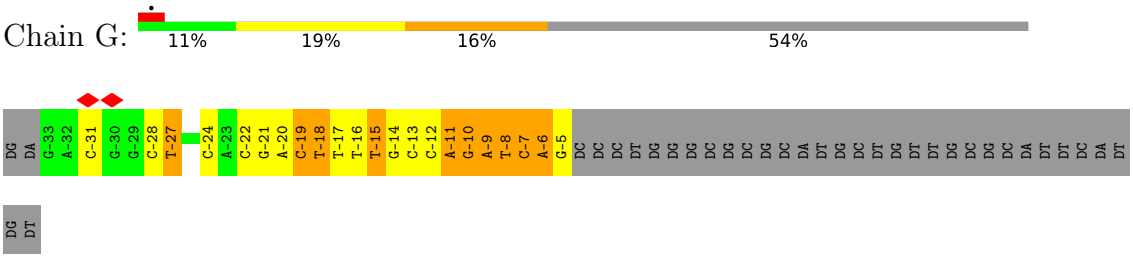
- Molecule 6: Non-Template promoter DNA

Chain F:



- Molecule 7: Template DNA promoter

Chain G:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	80810	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.080	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.23	0/1712	0.48	0/2331
1	B	0.24	0/1620	0.47	0/2206
2	C	0.24	0/9606	0.47	2/13100 (0.0%)
3	D	0.25	1/9083 (0.0%)	0.48	2/12407 (0.0%)
4	E	0.22	0/533	0.44	0/725
5	M	0.25	0/1506	0.46	0/2099
6	F	1.12	9/572 (1.6%)	1.85	7/880 (0.8%)
7	G	1.68	16/668 (2.4%)	1.61	15/1029 (1.5%)
All	All	0.40	26/25300 (0.1%)	0.61	26/34777 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	M	0	1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	-10	DG	O3'-P	-24.15	1.32	1.61
7	G	-11	DA	O3'-P	-12.20	1.46	1.61
7	G	-9	DA	O3'-P	-11.92	1.46	1.61
7	G	-7	DC	O3'-P	-11.21	1.47	1.61
6	F	77	DA	C1'-N9	-7.23	1.37	1.47
7	G	-19	DC	O3'-P	-7.17	1.52	1.61
7	G	-9	DA	C1'-N9	-6.82	1.37	1.47
7	G	-10	DG	C1'-N9	-6.59	1.38	1.47
7	G	-15	DT	O3'-P	-6.57	1.53	1.61
6	F	72	DC	O3'-P	-6.43	1.53	1.61
6	F	75	DG	C1'-N9	-6.29	1.38	1.47
3	D	858	VAL	C-N	5.77	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	84	DG	C1'-N9	-5.67	1.39	1.47
7	G	-7	DC	C1'-N1	5.31	1.56	1.49
7	G	-28	DC	C1'-N1	5.26	1.56	1.49
6	F	85	DT	C1'-N1	5.26	1.56	1.49
7	G	-18	DT	C1'-N1	5.26	1.56	1.49
6	F	95	DC	C1'-N1	5.24	1.56	1.49
6	F	87	DC	C1'-N1	5.20	1.56	1.49
7	G	-22	DC	C1'-N1	5.20	1.56	1.49
6	F	94	DT	C1'-N1	5.19	1.55	1.49
7	G	-24	DC	C1'-N1	5.16	1.55	1.49
6	F	88	DC	C1'-N1	5.13	1.55	1.49
7	G	-17	DT	C1'-N1	5.13	1.55	1.49
7	G	-31	DC	C1'-N1	5.09	1.55	1.49
7	G	-27	DT	C1'-N1	5.07	1.55	1.49

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	71	DT	P-O3'-C3'	33.12	159.44	119.70
6	F	71	DT	OP1-P-O3'	16.51	141.52	105.20
7	G	-11	DA	P-O3'-C3'	-10.50	107.10	119.70
7	G	-10	DG	P-O3'-C3'	10.04	131.75	119.70
6	F	71	DT	OP2-P-O3'	-9.60	84.09	105.20
6	F	72	DC	P-O3'-C3'	9.03	130.53	119.70
7	G	-9	DA	P-O3'-C3'	8.42	129.81	119.70
7	G	-15	DT	O5'-P-OP2	7.54	119.75	110.70
6	F	71	DT	O3'-P-O5'	-7.53	89.70	104.00
7	G	-11	DA	O4'-C4'-C3'	-7.52	101.49	106.00
7	G	-11	DA	OP2-P-O3'	7.51	121.72	105.20
7	G	-15	DT	O5'-P-OP1	-6.74	99.63	105.70
7	G	-7	DC	P-O3'-C3'	6.50	127.50	119.70
7	G	-8	DT	C1'-O4'-C4'	-6.41	103.69	110.10
7	G	-10	DG	C1'-O4'-C4'	-5.95	104.15	110.10
2	C	993	PRO	N-CA-CB	5.94	110.42	103.30
3	D	361	LEU	CA-CB-CG	5.75	128.53	115.30
7	G	-10	DG	O3'-P-O5'	5.72	114.86	104.00
7	G	-8	DT	O4'-C1'-N1	5.58	111.91	108.00
6	F	82	DT	O4'-C1'-C2'	-5.55	101.46	105.90
7	G	-8	DT	C3'-C2'-C1'	-5.41	96.00	102.50
3	D	374	LEU	CA-CB-CG	5.34	127.59	115.30
6	F	81	DG	O3'-P-O5'	-5.28	93.97	104.00
7	G	-7	DC	N1-C1'-C2'	-5.27	102.58	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	-6	DA	C5'-C4'-O4'	5.18	119.14	109.30
2	C	1161	LEU	CA-CB-CG	5.08	126.97	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	M	133	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1694	0	1681	64	0
1	B	1606	0	1579	44	0
2	C	9472	0	8776	242	0
3	D	8969	0	8154	231	0
4	E	532	0	515	9	0
5	M	1983	0	931	43	0
6	F	511	0	281	73	0
7	G	596	0	326	62	0
All	All	25363	0	22243	708	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 15.

All (708) 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)
6:F:72:DC:C2'	6:F:73:DG:H5"	1.59	1.32
7:G:-12:DC:C1'	7:G:-11:DA:H5'	1.61	1.30
3:D:365:GLN:O	3:D:437:PHE:HB3	1.15	1.30
2:C:455:SER:O	2:C:459:MET:HG3	1.33	1.23
7:G:-12:DC:H1'	7:G:-11:DA:C5'	1.76	1.15
6:F:72:DC:H2"	6:F:73:DG:C5'	1.80	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:351:GLY:CA	3:D:372:MET:HE1	1.80	1.10
3:D:365:GLN:O	3:D:437:PHE:CB	2.02	1.08
6:F:83:DC:O2	7:G:-21:DG:N2	1.83	1.08
3:D:351:GLY:CA	3:D:372:MET:CE	2.33	1.06
3:D:351:GLY:HA2	3:D:372:MET:HE1	1.39	1.03
6:F:82:DT:H2"	6:F:83:DC:C4	1.93	1.03
7:G:-12:DC:H2"	7:G:-11:DA:OP2	1.53	1.03
6:F:81:DG:H1	7:G:-19:DC:N4	1.55	1.03
3:D:351:GLY:HA2	3:D:372:MET:CE	1.90	1.02
6:F:73:DG:C3'	6:F:74:DT:H5"	1.89	1.02
3:D:213:LYS:O	3:D:217:LEU:HB2	1.58	1.01
2:C:455:SER:O	2:C:459:MET:CG	2.08	1.01
5:M:220:ILE:HA	5:M:224:LEU:CB	1.90	1.00
2:C:230:PHE:HB3	2:C:333:ILE:O	1.58	0.99
6:F:73:DG:H3'	6:F:74:DT:H5"	1.41	0.99
6:F:81:DG:O6	7:G:-19:DC:N4	1.94	0.99
3:D:921:GLN:O	3:D:925:GLU:HB2	1.61	0.98
1:A:192:VAL:O	1:A:194:GLN:N	1.99	0.96
7:G:-12:DC:H1'	7:G:-11:DA:H5'	0.95	0.95
3:D:371:LYS:HE3	3:D:371:LYS:HA	1.46	0.94
6:F:71:DT:H2"	6:F:72:DC:H5'	1.48	0.94
6:F:81:DG:C6	7:G:-19:DC:N4	2.34	0.94
6:F:81:DG:N1	7:G:-19:DC:N3	2.16	0.93
6:F:72:DC:H2"	6:F:73:DG:H5"	0.95	0.92
3:D:1033:GLY:HA3	3:D:1081:VAL:O	1.71	0.91
6:F:81:DG:N1	7:G:-19:DC:N4	2.14	0.91
6:F:82:DT:N3	7:G:-20:DA:N1	2.19	0.91
1:A:103:ASN:HA	1:A:140:ILE:O	1.71	0.90
3:D:351:GLY:HA3	3:D:372:MET:HE1	1.52	0.90
2:C:1245:ALA:HB2	3:D:372:MET:HE2	1.55	0.89
6:F:74:DT:H2'	6:F:75:DG:O4'	1.73	0.89
3:D:351:GLY:HA3	3:D:372:MET:CE	2.02	0.88
3:D:350:SER:HA	3:D:468:VAL:O	1.73	0.88
3:D:1238:GLN:O	3:D:1242:ARG:HB2	1.74	0.88
1:A:17:GLU:O	1:A:25:LYS:HB2	1.74	0.87
5:M:221:SER:O	5:M:223:HIS:N	2.07	0.87
5:M:457:THR:CB	6:F:85:DT:H71	2.05	0.86
6:F:73:DG:O6	7:G:-11:DA:N6	2.09	0.86
6:F:71:DT:C2'	6:F:72:DC:H5'	2.06	0.86
3:D:369:PRO:HD3	3:D:446:ALA:O	1.74	0.85
7:G:-15:DT:H2"	7:G:-14:DG:C8	2.12	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ARG:O	1:A:196:THR:HG22	1.75	0.84
3:D:532:GLU:O	3:D:536:LEU:HB3	1.78	0.84
2:C:767:GLN:HA	2:C:785:ASP:O	1.77	0.84
5:M:216:ALA:O	5:M:220:ILE:HG13	1.78	0.83
7:G:-21:DG:H2"	7:G:-20:DA:C8	2.14	0.83
5:M:382:SER:HB2	7:G:-16:DT:OP2	1.78	0.83
7:G:-11:DA:H2"	7:G:-10:DG:H5'	1.61	0.82
1:A:24:ALA:O	1:A:204:GLU:HA	1.78	0.82
6:F:83:DC:H2'	6:F:84:DG:C8	2.14	0.82
3:D:351:GLY:CA	3:D:372:MET:HE3	2.08	0.81
5:M:457:THR:H	6:F:85:DT:H71	1.45	0.81
6:F:83:DC:H2"	6:F:84:DG:C5'	2.10	0.81
7:G:-14:DG:OP2	7:G:-14:DG:H3'	1.81	0.81
1:A:59:VAL:O	1:A:171:LEU:HB2	1.80	0.80
7:G:-11:DA:H2"	7:G:-10:DG:O4'	1.82	0.80
1:B:222:THR:O	1:B:226:GLU:HB2	1.82	0.79
7:G:-13:DC:H2"	7:G:-12:DC:H5'	1.64	0.79
1:B:190:ALA:O	1:B:198:LEU:HB2	1.83	0.78
7:G:-12:DC:C2'	7:G:-11:DA:H5'	2.12	0.78
3:D:833:GLU:HB2	3:D:1242:ARG:HH22	1.49	0.78
6:F:73:DG:C2'	6:F:74:DT:H5"	2.14	0.78
7:G:-11:DA:H2"	7:G:-10:DG:C5'	2.13	0.77
3:D:425:ARG:HG2	3:D:427:PRO:HD2	1.66	0.76
6:F:81:DG:H2"	6:F:82:DT:C7	2.15	0.76
3:D:362:ARG:HB3	3:D:365:GLN:CG	2.15	0.76
3:D:371:LYS:HG3	3:D:445:LYS:CD	2.16	0.76
6:F:82:DT:H2"	6:F:83:DC:C5	2.20	0.75
2:C:802:VAL:HG21	2:C:1230:MET:HG2	1.69	0.75
3:D:361:LEU:HD13	3:D:365:GLN:HB2	1.69	0.75
6:F:76:DC:H2'	6:F:77:DA:C8	2.21	0.75
3:D:43:THR:HG22	3:D:56:LEU:HB2	1.69	0.74
5:M:263:UNK:O	5:M:265:UNK:N	2.21	0.74
1:B:43:LEU:O	1:B:47:LEU:HB3	1.88	0.74
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.68	0.74
3:D:910:ASN:ND2	4:E:15:ASN:O	2.21	0.74
2:C:1245:ALA:CB	3:D:372:MET:HE2	2.17	0.73
4:E:5:THR:HG22	4:E:7:GLN:H	1.52	0.73
2:C:933:VAL:HG23	2:C:1050:VAL:HG22	1.71	0.73
2:C:724:VAL:HG22	2:C:734:ILE:HG12	1.70	0.72
6:F:81:DG:C2	7:G:-19:DC:N3	2.57	0.72
6:F:81:DG:C2'	6:F:82:DT:H72	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:71:DT:H3	7:G:-9:DA:N6	1.88	0.72
3:D:25:ALA:HB1	3:D:30:ILE:HD11	1.72	0.72
2:C:411:ARG:HH22	2:C:424:ASP:HA	1.55	0.71
2:C:717:VAL:HG22	2:C:782:VAL:HG12	1.72	0.71
1:A:46:ILE:HG13	1:A:224:LEU:HD12	1.72	0.71
1:B:185:TYR:HA	1:B:202:VAL:O	1.91	0.71
3:D:746:LEU:HD21	3:D:758:PRO:HA	1.73	0.71
6:F:83:DC:H2"	6:F:84:DG:H5'	1.71	0.71
7:G:-9:DA:H2"	7:G:-8:DT:O5'	1.90	0.71
1:A:195:ARG:O	1:A:196:THR:CG2	2.38	0.71
1:B:37:HIS:O	1:B:41:ASN:HB2	1.89	0.71
6:F:71:DT:H3	7:G:-9:DA:H61	1.38	0.70
2:C:802:VAL:HB	2:C:1228:GLY:O	1.92	0.70
3:D:362:ARG:HB3	3:D:365:GLN:HG3	1.72	0.70
3:D:528:THR:HG21	3:D:551:ARG:HG2	1.72	0.70
3:D:959:LYS:O	3:D:982:LEU:HA	1.92	0.70
1:B:97:GLU:HG2	1:B:147:GLN:HG2	1.73	0.70
2:C:29:SER:O	2:C:33:ASP:CB	2.40	0.70
6:F:73:DG:H2'	6:F:74:DT:H5"	1.74	0.69
3:D:369:PRO:HG2	3:D:372:MET:HG3	1.74	0.69
3:D:614:LEU:HD23	4:E:5:THR:HG21	1.75	0.69
3:D:361:LEU:HD13	3:D:365:GLN:CB	2.22	0.69
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.74	0.69
2:C:808:ASN:HD22	2:C:1216:ARG:HH12	1.41	0.68
3:D:478:LEU:HD12	4:E:47:THR:HG23	1.75	0.68
6:F:76:DC:C2'	6:F:77:DA:C8	2.77	0.68
7:G:-11:DA:C2'	7:G:-10:DG:O4'	2.42	0.68
3:D:450:HIS:HD2	3:D:453:VAL:HG23	1.59	0.67
2:C:854:ILE:HD11	2:C:865:LEU:HD22	1.75	0.67
2:C:29:SER:O	2:C:33:ASP:HB3	1.94	0.67
2:C:147:SER:HB2	2:C:529:ARG:O	1.94	0.67
6:F:81:DG:N2	7:G:-19:DC:O2	2.27	0.67
2:C:805:MET:HE3	2:C:1225:VAL:HG11	1.75	0.67
1:A:47:LEU:HD22	1:A:183:ILE:HD11	1.76	0.67
6:F:82:DT:H2"	6:F:83:DC:N4	2.10	0.67
2:C:1124:ILE:HD11	2:C:1198:LEU:HD11	1.77	0.66
3:D:616:PRO:O	3:D:620:PHE:HB3	1.95	0.66
3:D:371:LYS:HG3	3:D:445:LYS:HD3	1.78	0.66
2:C:839:VAL:HG23	2:C:1046:VAL:HG21	1.76	0.66
7:G:-11:DA:C2'	7:G:-10:DG:H5'	2.25	0.65
6:F:73:DG:H2'	6:F:74:DT:C4'	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:-21:DG:H2"	7:G:-20:DA:N7	2.11	0.65
1:B:91:ARG:HB2	1:B:122:GLU:HB2	1.76	0.65
1:B:44:ARG:O	1:B:48:LEU:HB3	1.97	0.65
1:B:57:THR:O	1:B:172:LEU:N	2.30	0.65
1:A:10:LYS:NZ	1:B:226:GLU:O	2.26	0.65
2:C:1238:LEU:HD12	2:C:1241:ASP:H	1.60	0.65
5:M:415:ALA:HB3	5:M:419:ALA:HB3	1.79	0.65
1:A:180:VAL:HG12	1:A:207:THR:HG22	1.78	0.65
1:B:222:THR:O	1:B:226:GLU:CB	2.45	0.65
7:G:-9:DA:H4'	7:G:-8:DT:OP1	1.96	0.65
3:D:104:HIS:HA	3:D:243:PRO:HA	1.79	0.65
5:M:457:THR:N	6:F:85:DT:H71	2.11	0.65
2:C:530:ILE:HD11	2:C:575:LEU:HG	1.79	0.65
5:M:457:THR:CB	6:F:85:DT:C7	2.74	0.65
3:D:185:ILE:O	3:D:189:LEU:HB3	1.96	0.64
3:D:616:PRO:O	3:D:620:PHE:CB	2.45	0.64
2:C:58:PRO:HA	2:C:68:LEU:O	1.96	0.64
2:C:241:LEU:HG	2:C:243:PRO:HD3	1.77	0.64
2:C:802:VAL:HA	2:C:1096:ILE:HG22	1.77	0.64
2:C:699:LEU:HD12	2:C:700:VAL:HG23	1.80	0.64
1:B:91:ARG:HH21	1:B:210:THR:HA	1.62	0.64
2:C:256:GLU:HA	2:C:261:VAL:HA	1.80	0.64
2:C:843:THR:OG1	2:C:846:GLY:O	2.15	0.64
3:D:1238:GLN:NE2	3:D:1250:ASP:OD1	2.30	0.64
3:D:38:VAL:HG12	3:D:105:ILE:HG21	1.79	0.64
1:A:56:VAL:HA	1:A:146:VAL:HG22	1.79	0.64
5:M:456:ARG:CB	6:F:86:DG:O6	2.46	0.64
1:A:45:ARG:NH1	1:B:38:THR:OG1	2.31	0.63
3:D:479:GLU:O	3:D:483:LEU:HB2	1.99	0.63
3:D:341:ASN:OD1	3:D:342:LEU:N	2.31	0.63
1:B:24:ALA:HB3	1:B:205:MET:O	1.99	0.63
2:C:196:VAL:O	2:C:203:LYS:HA	1.99	0.63
2:C:662:SER:O	2:C:666:SER:HB3	1.99	0.63
3:D:606:ASN:OD1	3:D:610:ARG:NH1	2.31	0.63
7:G:-12:DC:C2'	7:G:-11:DA:OP2	2.40	0.62
3:D:850:LYS:HG3	3:D:857:LEU:HD11	1.81	0.62
2:C:788:SER:HB2	2:C:796:LEU:HA	1.81	0.62
7:G:-11:DA:C2'	7:G:-10:DG:C5'	2.77	0.62
3:D:147:ILE:HG22	3:D:148:GLU:HG2	1.79	0.62
5:M:457:THR:H	6:F:85:DT:C7	2.13	0.62
2:C:1245:ALA:HB2	3:D:372:MET:CE	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1238:GLN:O	3:D:1242:ARG:CB	2.48	0.62
1:A:182:ARG:NH2	1:A:206:GLU:OE1	2.32	0.62
6:F:73:DG:C3'	6:F:74:DT:C5'	2.75	0.62
1:B:62:ASP:HB3	1:B:141:SER:HB3	1.82	0.61
3:D:612:LEU:HB3	3:D:616:PRO:HG2	1.82	0.61
3:D:475:GLU:O	3:D:479:GLU:CB	2.48	0.61
3:D:816:THR:HG22	3:D:883:ARG:HH11	1.65	0.61
2:C:13:LYS:NZ	2:C:1149:TYR:O	2.33	0.61
2:C:186:PHE:HD2	2:C:432:LEU:HD13	1.65	0.61
2:C:592:ARG:HH22	2:C:655:VAL:HG13	1.66	0.61
2:C:817:LEU:HB3	2:C:1097:VAL:HB	1.81	0.61
2:C:716:ALA:HB3	2:C:784:ALA:HB3	1.82	0.61
5:M:418:THR:O	5:M:422:ALA:HB3	2.01	0.61
2:C:1307:ASN:ND2	2:C:1314:GLN:O	2.34	0.61
3:D:885:VAL:O	3:D:886:VAL:HG12	2.01	0.61
7:G:-8:DT:H1'	7:G:-7:DC:H5"	1.83	0.61
3:D:279:LEU:O	3:D:283:LEU:HB2	2.01	0.61
6:F:72:DC:H2'	6:F:73:DG:H5"	1.76	0.61
2:C:882:ILE:HG13	2:C:919:ARG:HB3	1.81	0.60
3:D:361:LEU:O	3:D:626:TYR:OH	2.18	0.60
1:A:192:VAL:O	1:A:192:VAL:HG12	2.02	0.60
2:C:459:MET:HE1	2:C:511:LEU:HD22	1.84	0.60
6:F:83:DC:H2"	6:F:84:DG:O4'	2.00	0.60
2:C:402:ARG:NH2	2:C:419:ILE:O	2.35	0.60
1:A:31:LEU:HD13	1:A:36:GLY:HA2	1.83	0.60
3:D:531:LYS:O	3:D:535:ARG:CB	2.50	0.60
7:G:-15:DT:H2"	7:G:-14:DG:H8	1.62	0.60
2:C:463:GLN:HG2	2:C:505:PHE:HB2	1.83	0.60
3:D:347:VAL:HG12	3:D:348:ASP:H	1.65	0.60
1:A:104:LYS:O	1:A:139:SER:HA	2.02	0.60
3:D:37:GLU:HA	3:D:105:ILE:HG22	1.84	0.60
1:B:93:GLN:O	1:B:148:ARG:NH1	2.35	0.59
2:C:1226:THR:OG1	3:D:638:SER:OG	2.16	0.59
5:M:418:THR:O	5:M:422:ALA:CB	2.49	0.59
2:C:81:ASP:O	2:C:85:CYS:HB2	2.02	0.59
3:D:593:ASN:O	3:D:594:GLN:HG3	2.02	0.59
7:G:-16:DT:H2"	7:G:-15:DT:H72	1.83	0.59
2:C:13:LYS:HE3	2:C:15:PHE:HE1	1.67	0.59
7:G:-10:DG:C2'	7:G:-9:DA:H5"	2.31	0.59
6:F:81:DG:H2"	6:F:82:DT:C6	2.37	0.59
6:F:81:DG:C2'	6:F:82:DT:C7	2.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:592:ARG:HB3	2:C:653:MET:HB2	1.85	0.59
3:D:929:GLN:O	3:D:1244:GLN:NE2	2.36	0.59
5:M:440:SER:CB	7:G:-27:DT:OP2	2.50	0.59
3:D:515:ARG:HB3	3:D:544:LEU:HD22	1.84	0.59
6:F:81:DG:N2	7:G:-19:DC:C2	2.57	0.59
1:A:192:VAL:HG12	1:A:194:GLN:HB3	1.85	0.58
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.68	0.58
2:C:1338:GLU:O	3:D:21:LYS:HB3	2.03	0.58
2:C:766:ASN:OD1	2:C:767:GLN:N	2.35	0.58
2:C:797:GLY:N	2:C:1231:TYR:OH	2.35	0.58
3:D:361:LEU:HB2	3:D:365:GLN:OE1	2.03	0.58
7:G:-11:DA:H2"	7:G:-10:DG:C4'	2.33	0.58
2:C:88:ARG:NH1	2:C:1035:LYS:O	2.36	0.58
3:D:352:ARG:HA	3:D:466:MET:O	2.03	0.58
2:C:1109:ILE:HG13	3:D:763:PHE:HB3	1.85	0.58
3:D:110:PRO:O	3:D:186:GLN:NE2	2.36	0.58
5:M:312:ASN:O	5:M:313:ASP:CB	2.50	0.58
2:C:81:ASP:O	2:C:85:CYS:CB	2.52	0.58
2:C:785:ASP:OD2	2:C:791:LEU:N	2.35	0.58
2:C:808:ASN:H	3:D:633:ALA:HB2	1.69	0.58
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.84	0.58
6:F:73:DG:H2'	6:F:74:DT:C5'	2.33	0.58
2:C:174:ALA:HB3	2:C:432:LEU:HD12	1.85	0.58
3:D:371:LYS:HG3	3:D:445:LYS:HD2	1.84	0.58
3:D:1177:ILE:CB	3:D:1188:GLU:O	2.52	0.58
5:M:407:UNK:O	5:M:408:UNK:CB	2.51	0.58
7:G:-14:DG:H2"	7:G:-13:DC:O4'	2.03	0.58
3:D:968:ASN:HA	3:D:1118:GLY:HA3	1.86	0.58
3:D:534:GLU:O	3:D:538:ARG:CB	2.52	0.58
2:C:148:GLN:HB2	2:C:511:LEU:HD21	1.85	0.57
2:C:1064:ASP:HA	2:C:1238:LEU:HA	1.86	0.57
3:D:272:VAL:HG21	3:D:306:LEU:HG	1.86	0.57
6:F:81:DG:H2'	6:F:82:DT:H72	1.86	0.57
2:C:455:SER:C	2:C:459:MET:HG3	2.18	0.57
2:C:933:VAL:HA	2:C:1050:VAL:HA	1.85	0.57
3:D:724:MET:O	3:D:728:SER:CB	2.52	0.57
3:D:707:ILE:HD13	3:D:716:GLN:HB3	1.86	0.57
1:A:159:ILE:O	1:A:163:GLU:CB	2.52	0.57
2:C:801:ARG:HG3	2:C:1229:TYR:HE1	1.69	0.57
1:B:60:GLU:O	1:B:142:MET:HA	2.03	0.57
2:C:149:LEU:HD11	2:C:451:ARG:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:318:GLY:C	3:D:320:ASN:H	2.08	0.57
2:C:915:ASP:OD2	2:C:919:ARG:NH1	2.37	0.57
3:D:246:PRO:HD2	3:D:249:LEU:HD12	1.85	0.57
2:C:237:LEU:HD21	2:C:292:ILE:HD11	1.86	0.57
4:E:7:GLN:HA	4:E:10:VAL:HB	1.86	0.57
3:D:134:ASP:HA	3:D:137:ARG:HG2	1.86	0.57
1:B:37:HIS:O	1:B:41:ASN:CB	2.54	0.56
2:C:1085:MET:HB2	2:C:1093:PRO:HB3	1.86	0.56
3:D:533:ALA:O	3:D:537:TYR:HB2	2.05	0.56
6:F:74:DT:H3'	6:F:75:DG:H5"	1.86	0.56
6:F:82:DT:O2	7:G:-20:DA:C2	2.59	0.56
7:G:-12:DC:H1'	7:G:-11:DA:C4'	2.35	0.56
3:D:500:ILE:HG22	3:D:502:PRO:HD3	1.88	0.56
7:G:-8:DT:H1'	7:G:-7:DC:C5'	2.35	0.56
2:C:12:ARG:HD3	2:C:1183:ALA:HB2	1.87	0.56
2:C:1300:GLY:O	2:C:1304:MET:CB	2.53	0.56
6:F:72:DC:H2"	6:F:73:DG:C4'	2.36	0.56
2:C:1103:VAL:HB	2:C:1104:PRO:HD3	1.88	0.56
2:C:384:LEU:O	2:C:388:LEU:CB	2.54	0.56
2:C:782:VAL:HG21	2:C:792:GLY:HA3	1.87	0.56
3:D:418:GLU:HG3	4:E:44:ASP:HA	1.88	0.56
2:C:27:LEU:O	2:C:528:ARG:NH2	2.39	0.56
3:D:161:THR:HG22	3:D:162:GLU:H	1.71	0.56
5:M:300:UNK:O	5:M:301:UNK:CB	2.54	0.56
2:C:1014:LEU:O	2:C:1018:TYR:HB2	2.06	0.56
3:D:422:LEU:HA	3:D:435:GLN:O	2.05	0.56
2:C:993:PRO:C	2:C:995:ASP:H	2.09	0.55
5:M:309:SER:O	5:M:310:ALA:HB2	2.05	0.55
2:C:73:TYR:HA	2:C:98:VAL:HB	1.88	0.55
2:C:1160:ASP:OD1	2:C:1161:LEU:N	2.39	0.55
1:A:91:ARG:HB3	1:A:210:THR:HG23	1.88	0.55
5:M:224:LEU:O	5:M:225:ASP:CB	2.54	0.55
6:F:71:DT:C3'	6:F:72:DC:H5'	2.37	0.55
1:B:17:GLU:HB3	1:B:25:LYS:HB3	1.88	0.55
3:D:710:ASP:OD1	3:D:711:GLY:N	2.39	0.55
3:D:923:ILE:HD11	3:D:1253:ILE:HG12	1.88	0.55
6:F:82:DT:O2	7:G:-20:DA:H2	1.89	0.55
1:A:85:LEU:HA	1:A:88:LEU:HD13	1.88	0.55
2:C:384:LEU:O	2:C:388:LEU:HB3	2.06	0.55
2:C:928:VAL:HA	2:C:1054:LEU:HA	1.87	0.55
3:D:841:GLY:H	3:D:864:LEU:HB2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:39:VAL:HG11	4:E:52:ARG:HE	1.72	0.55
2:C:568:ASN:HB2	2:C:571:LEU:HD12	1.89	0.55
1:A:167:PRO:HD2	1:A:170:ARG:HD2	1.89	0.54
2:C:221:LEU:O	2:C:225:PHE:HB2	2.07	0.54
2:C:804:PHE:HB3	2:C:1100:PRO:HG3	1.88	0.54
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.88	0.54
6:F:73:DG:H5'	6:F:73:DG:H8	1.71	0.54
7:G:-16:DT:H2"	7:G:-15:DT:C7	2.36	0.54
3:D:364:HIS:O	3:D:364:HIS:ND1	2.41	0.54
6:F:73:DG:H3'	6:F:74:DT:C5'	2.28	0.54
4:E:58:LEU:HD12	4:E:59:ILE:HG12	1.90	0.54
6:F:73:DG:H1	7:G:-11:DA:N6	2.05	0.54
3:D:759:ILE:HG12	3:D:771:GLN:HG2	1.89	0.54
3:D:1120:THR:HG22	3:D:1122:ALA:H	1.72	0.54
2:C:714:VAL:O	2:C:767:GLN:NE2	2.41	0.54
3:D:131:PRO:HG2	3:D:134:ASP:HB2	1.90	0.54
5:M:301:UNK:O	5:M:303:UNK:N	2.41	0.54
1:B:104:LYS:NZ	1:B:114:ASP:OD2	2.41	0.53
2:C:136:PHE:HB2	2:C:143:ARG:O	2.09	0.53
1:B:100:LEU:HD11	1:B:121:VAL:HG21	1.90	0.53
1:B:44:ARG:O	1:B:48:LEU:CB	2.56	0.53
1:B:82:LEU:HD23	1:B:85:LEU:HD12	1.89	0.53
2:C:965:GLN:O	2:C:969:ALA:HB3	2.09	0.53
2:C:221:LEU:HA	2:C:225:PHE:HD2	1.74	0.53
2:C:1115:THR:HB	2:C:1228:GLY:HA3	1.89	0.53
3:D:60:ARG:H	3:D:90:VAL:HG22	1.72	0.53
3:D:406:ALA:HA	3:D:409:TRP:HD1	1.72	0.53
5:M:454:ALA:CB	6:F:85:DT:H2'	2.39	0.53
7:G:-16:DT:H2"	7:G:-15:DT:C5	2.43	0.53
1:A:152:TYR:HA	1:A:175:ALA:O	2.08	0.53
2:C:401:GLY:O	2:C:405:PHE:HB2	2.08	0.53
2:C:956:ALA:O	2:C:960:LEU:HB3	2.09	0.53
3:D:108:ALA:HB1	3:D:299:LEU:HD21	1.90	0.53
2:C:801:ARG:NH1	2:C:1229:TYR:OH	2.41	0.53
2:C:728:ASP:OD1	2:C:729:ALA:N	2.42	0.53
2:C:1254:VAL:HG12	2:C:1255:THR:HG23	1.90	0.53
2:C:125:GLY:H	2:C:495:ALA:HB1	1.73	0.53
3:D:347:VAL:HG12	3:D:348:ASP:N	2.24	0.53
5:M:405:UNK:CB	7:G:-18:DT:H4'	2.39	0.53
5:M:419:ALA:O	5:M:423:LEU:CB	2.57	0.53
3:D:850:LYS:HB3	3:D:851:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:27:LEU:HD22	2:C:524:ILE:HD11	1.91	0.52
2:C:68:LEU:HB3	2:C:100:LEU:HD13	1.90	0.52
2:C:219:GLN:O	2:C:223:LEU:HB2	2.10	0.52
2:C:965:GLN:O	2:C:969:ALA:CB	2.57	0.52
6:F:73:DG:C5'	6:F:73:DG:H8	2.23	0.52
7:G:-11:DA:C3'	7:G:-10:DG:H5'	2.39	0.52
3:D:371:LYS:CG	3:D:445:LYS:HD2	2.39	0.52
2:C:499:SER:O	2:C:503:LYS:CB	2.58	0.52
1:A:58:GLU:OE2	1:A:170:ARG:NH1	2.43	0.52
2:C:397:LEU:HB2	2:C:418:GLY:HA2	1.91	0.52
2:C:662:SER:O	2:C:666:SER:CB	2.58	0.52
2:C:22:LEU:HD12	2:C:603:ILE:HG21	1.92	0.52
2:C:219:GLN:O	2:C:223:LEU:CB	2.58	0.52
6:F:81:DG:H2"	6:F:82:DT:C5	2.45	0.52
2:C:886:LYS:HB3	2:C:917:SER:HA	1.91	0.52
3:D:60:ARG:HG2	3:D:61:ILE:HD12	1.91	0.52
3:D:364:HIS:O	3:D:365:GLN:HG2	2.10	0.52
3:D:1263:LYS:HA	3:D:1278:GLU:O	2.10	0.52
3:D:422:LEU:HD11	3:D:469:HIS:HB2	1.92	0.52
3:D:1366:HIS:O	3:D:1370:MET:CB	2.58	0.52
6:F:74:DT:H2'	6:F:75:DG:C4'	2.40	0.52
1:A:78:ILE:HD13	1:A:81:ILE:HD12	1.92	0.51
2:C:697:LYS:HA	2:C:795:ALA:HB2	1.92	0.51
2:C:271:ALA:HA	2:C:274:ILE:HB	1.92	0.51
1:B:104:LYS:HE2	1:B:110:VAL:HG22	1.93	0.51
5:M:313:ASP:O	5:M:314:ALA:HB3	2.10	0.51
7:G:-10:DG:H2"	7:G:-9:DA:C5'	2.40	0.51
3:D:1220:ILE:O	3:D:1224:ARG:HB2	2.10	0.51
3:D:679:TYR:OH	3:D:754:ILE:O	2.24	0.51
2:C:196:VAL:HG21	2:C:209:ILE:HG21	1.93	0.51
2:C:1064:ASP:CG	2:C:1065:LYS:H	2.14	0.51
3:D:362:ARG:HB3	3:D:365:GLN:HG2	1.93	0.51
2:C:1080:ASN:HB2	2:C:1085:MET:HE1	1.91	0.51
3:D:1230:THR:HG22	3:D:1257:VAL:HG11	1.93	0.51
7:G:-12:DC:C1'	7:G:-11:DA:C5'	2.54	0.51
2:C:933:VAL:HG22	2:C:934:PHE:H	1.76	0.51
3:D:363:LEU:HA	3:D:450:HIS:CE1	2.45	0.51
3:D:424:ASN:HB2	3:D:434:ILE:HG12	1.93	0.51
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.93	0.51
1:A:102:LEU:O	1:A:141:SER:HA	2.10	0.51
2:C:29:SER:O	2:C:33:ASP:HB2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:146:VAL:HG13	2:C:529:ARG:HB2	1.93	0.51
2:C:864:LYS:NZ	2:C:881:ASP:OD2	2.45	0.50
3:D:490:ILE:HD12	3:D:614:LEU:HD11	1.93	0.50
3:D:1262:ARG:NH2	3:D:1312:ALA:O	2.44	0.50
2:C:1007:LYS:O	2:C:1011:LEU:CB	2.59	0.50
2:C:1014:LEU:O	2:C:1018:TYR:CB	2.59	0.50
3:D:474:LEU:O	3:D:478:LEU:HB3	2.10	0.50
2:C:217:THR:HA	2:C:220:ILE:HD12	1.92	0.50
3:D:1314:LEU:HD22	3:D:1330:ARG:HH22	1.77	0.50
6:F:73:DG:H1	7:G:-11:DA:H61	1.53	0.50
7:G:-16:DT:C2'	7:G:-15:DT:H72	2.41	0.50
3:D:270:ARG:O	3:D:274:ASN:HB2	2.12	0.50
5:M:239:THR:HG23	5:M:241:LEU:H	1.77	0.50
2:C:360:LEU:HD13	2:C:378:ARG:HH21	1.75	0.50
3:D:351:GLY:C	3:D:372:MET:HE3	2.32	0.50
2:C:1286:THR:O	2:C:1290:MET:CB	2.60	0.50
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.94	0.50
5:M:47:UNK:O	5:M:300:UNK:N	2.45	0.50
2:C:717:VAL:HG12	2:C:718:ALA:H	1.77	0.50
3:D:185:ILE:O	3:D:189:LEU:CB	2.60	0.50
2:C:594:VAL:HG22	2:C:599:VAL:HG13	1.94	0.50
3:D:272:VAL:HG22	3:D:302:ALA:HB1	1.92	0.50
3:D:362:ARG:H	3:D:365:GLN:HG3	1.77	0.49
3:D:628:GLY:O	3:D:632:ALA:HB2	2.13	0.49
3:D:1011:VAL:HG22	3:D:1013:GLY:H	1.77	0.49
1:A:39:LEU:O	1:A:43:LEU:HB2	2.13	0.49
1:A:110:VAL:HG11	1:A:140:ILE:HD11	1.94	0.49
2:C:1288:GLN:O	2:C:1292:THR:OG1	2.21	0.49
3:D:548:VAL:HG12	3:D:550:VAL:H	1.78	0.49
2:C:530:ILE:O	2:C:572:ILE:HA	2.12	0.49
2:C:557:ARG:O	2:C:576:SER:N	2.46	0.49
3:D:609:TYR:HB2	3:D:617:THR:HG21	1.94	0.49
2:C:691:PRO:HB3	2:C:788:SER:HB3	1.95	0.49
2:C:500:ALA:O	2:C:504:GLU:CB	2.61	0.49
3:D:365:GLN:O	3:D:366:CYS:HB2	2.12	0.49
2:C:629:PHE:HE2	2:C:650:VAL:HG11	1.78	0.49
3:D:886:VAL:HG23	3:D:1258:ARG:HA	1.95	0.49
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.95	0.48
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.48	0.48
1:A:195:ARG:C	1:A:196:THR:HG22	2.33	0.48
2:C:592:ARG:HH12	2:C:655:VAL:HA	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:698:PRO:HD3	2:C:795:ALA:HB2	1.94	0.48
2:C:956:ALA:O	2:C:960:LEU:CB	2.61	0.48
3:D:528:THR:HG22	3:D:550:VAL:HA	1.95	0.48
3:D:740:LEU:HD23	3:D:763:PHE:HD2	1.77	0.48
1:A:75:GLN:NE2	2:C:772:SER:O	2.46	0.48
3:D:36:GLY:HA2	3:D:61:ILE:HD13	1.95	0.48
6:F:76:DC:H2"	6:F:77:DA:C8	2.47	0.48
2:C:801:ARG:HD3	2:C:1094:VAL:HA	1.95	0.48
2:C:975:ILE:HA	2:C:978:VAL:HG12	1.94	0.48
6:F:72:DC:H2"	6:F:73:DG:O4'	2.13	0.48
7:G:-6:DA:H2'	7:G:-5:DG:C8	2.49	0.48
1:B:43:LEU:O	1:B:47:LEU:CB	2.59	0.48
1:B:77:ASP:O	1:B:81:ILE:HD12	2.14	0.48
2:C:322:LEU:HA	2:C:325:LEU:HG	1.94	0.48
2:C:765:ILE:HG22	2:C:787:PRO:HG3	1.95	0.48
3:D:102:MET:HG2	3:D:246:PRO:HD3	1.96	0.48
3:D:1042:ASP:HA	3:D:1046:ILE:HB	1.94	0.48
1:A:48:LEU:HG	1:A:183:ILE:HD12	1.95	0.48
2:C:1006:GLU:O	2:C:1010:GLN:CB	2.61	0.48
2:C:12:ARG:NH2	2:C:793:GLU:OE1	2.46	0.48
3:D:755:ILE:HG22	3:D:757:THR:H	1.79	0.48
2:C:1279:GLU:HB2	3:D:917:VAL:HG11	1.95	0.48
2:C:1290:MET:HG3	3:D:347:VAL:HG11	1.96	0.48
4:E:15:ASN:HD22	4:E:18:ASP:HB2	1.79	0.48
5:M:304:UNK:C	5:M:306:MET:N	2.76	0.48
1:A:104:LYS:HE2	1:A:110:VAL:HG12	1.96	0.47
2:C:306:THR:OG1	2:C:308:GLU:OE1	2.25	0.47
2:C:709:ALA:HB2	2:C:794:LEU:HB2	1.96	0.47
2:C:939:VAL:HG21	2:C:1048:LYS:HD3	1.97	0.47
3:D:161:THR:HG22	3:D:162:GLU:N	2.29	0.47
3:D:503:SER:HA	3:D:507:VAL:HG23	1.95	0.47
5:M:454:ALA:HB2	6:F:85:DT:H2'	1.95	0.47
1:B:173:VAL:HG12	1:B:174:ASP:H	1.80	0.47
2:C:92:TYR:HB3	2:C:137:VAL:HB	1.95	0.47
3:D:661:VAL:HG21	3:D:686:TRP:NE1	2.29	0.47
1:A:28:LEU:HD13	1:A:201:LEU:HD11	1.96	0.47
2:C:895:LEU:HD12	2:C:896:THR:N	2.28	0.47
1:A:25:LYS:HA	1:A:203:ILE:O	2.14	0.47
2:C:21:VAL:HB	2:C:592:ARG:HH21	1.78	0.47
2:C:231:GLU:CB	2:C:238:GLN:O	2.63	0.47
6:F:73:DG:C2'	6:F:74:DT:C5'	2.91	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1008:GLN:O	2:C:1012:GLU:CB	2.63	0.47
2:C:717:VAL:HA	2:C:782:VAL:HA	1.97	0.47
2:C:832:HIS:CD2	2:C:1058:ARG:HD2	2.50	0.47
3:D:369:PRO:HB2	3:D:444:GLY:O	2.15	0.47
3:D:373:ALA:O	3:D:374:LEU:HG	2.14	0.47
3:D:450:HIS:CD2	3:D:453:VAL:HG23	2.45	0.47
3:D:294:ASN:HA	3:D:297:ARG:HG2	1.96	0.47
7:G:-11:DA:OP2	7:G:-11:DA:H3'	2.15	0.47
1:A:82:LEU:HB3	1:A:173:VAL:HG11	1.96	0.47
2:C:591:TYR:HB3	2:C:652:TYR:HB3	1.97	0.47
5:M:127:GLN:O	5:M:131:THR:CB	2.63	0.47
3:D:369:PRO:CB	3:D:444:GLY:O	2.63	0.46
3:D:1265:THR:OG1	3:D:1303:SER:HB3	2.15	0.46
3:D:374:LEU:HB3	3:D:412:LEU:HD22	1.97	0.46
3:D:616:PRO:O	3:D:620:PHE:HB2	2.16	0.46
3:D:646:ILE:HD11	3:D:764:ARG:HD3	1.96	0.46
2:C:1003:THR:O	2:C:1005:GLU:N	2.43	0.46
3:D:1220:ILE:O	3:D:1225:GLY:N	2.39	0.46
2:C:777:VAL:HG13	2:C:781:ASP:HB3	1.97	0.46
2:C:1075:VAL:HG21	3:D:355:ILE:O	2.15	0.46
3:D:818:GLU:OE2	3:D:1227:HIS:NE2	2.49	0.46
6:F:83:DC:C2'	6:F:84:DG:C8	2.93	0.46
1:A:47:LEU:HD11	1:A:216:ALA:HB1	1.96	0.46
2:C:801:ARG:HA	2:C:1229:TYR:CD1	2.51	0.46
2:C:1065:LYS:NZ	3:D:462:ASP:O	2.30	0.46
2:C:1148:ALA:HA	2:C:1151:LEU:HD23	1.97	0.46
5:M:283:UNK:C	5:M:285:UNK:H	2.28	0.46
2:C:636:CYS:HB2	2:C:645:PHE:HD2	1.80	0.46
2:C:1067:ALA:HB2	2:C:1235:LEU:HD11	1.98	0.46
5:M:193:LYS:C	5:M:195:LEU:H	2.17	0.46
2:C:1121:ALA:HB2	2:C:1182:ILE:HD12	1.98	0.46
2:C:1142:ARG:NH2	2:C:1165:SER:O	2.49	0.46
3:D:511:TYR:OH	3:D:515:ARG:NH2	2.48	0.46
2:C:593:LYS:HA	2:C:652:TYR:HD1	1.80	0.46
2:C:668:ILE:HD12	2:C:1069:ARG:HB3	1.98	0.46
2:C:717:VAL:HG12	2:C:718:ALA:N	2.31	0.46
3:D:998:PRO:HG2	3:D:1001:ALA:HB2	1.97	0.46
7:G:-13:DC:C5'	7:G:-13:DC:H6	2.29	0.46
2:C:442:VAL:HG12	2:C:443:ASP:H	1.81	0.46
2:C:854:ILE:HG22	2:C:857:VAL:HB	1.97	0.46
3:D:810:THR:O	3:D:911:LYS:NZ	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1304:MET:O	2:C:1308:ILE:HG12	2.16	0.46
3:D:363:LEU:HG	3:D:450:HIS:NE2	2.31	0.46
2:C:442:VAL:HG12	2:C:443:ASP:N	2.32	0.45
3:D:474:LEU:O	3:D:478:LEU:CB	2.64	0.45
3:D:654:ILE:HD13	3:D:760:THR:HB	1.98	0.45
2:C:125:GLY:HA2	2:C:499:SER:HB3	1.97	0.45
3:D:699:ASP:O	3:D:703:THR:HG22	2.16	0.45
1:A:91:ARG:HE	1:A:122:GLU:HG2	1.82	0.45
2:C:238:GLN:HA	2:C:286:GLU:HA	1.98	0.45
2:C:411:ARG:NH2	2:C:424:ASP:HA	2.29	0.45
2:C:453:ILE:HD11	2:C:581:THR:HG21	1.99	0.45
2:C:1160:ASP:O	2:C:1161:LEU:HG	2.15	0.45
3:D:1261:LEU:HD23	3:D:1306:LEU:HB3	1.97	0.45
1:A:39:LEU:O	1:A:43:LEU:CB	2.64	0.45
2:C:230:PHE:HD2	2:C:333:ILE:HB	1.80	0.45
2:C:325:LEU:HD12	2:C:326:SER:N	2.31	0.45
2:C:1149:TYR:HD2	2:C:1160:ASP:HB2	1.82	0.45
3:D:423:LEU:O	3:D:434:ILE:HA	2.16	0.45
3:D:430:HIS:CE1	3:D:432:LEU:HB2	2.52	0.45
3:D:516:ASP:HB2	3:D:546:ALA:HB2	1.97	0.45
3:D:196:GLN:O	3:D:200:GLN:CB	2.65	0.45
1:A:46:ILE:O	1:A:50:SER:OG	2.32	0.45
2:C:221:LEU:HA	2:C:225:PHE:CD2	2.52	0.45
3:D:115:TRP:HE1	3:D:307:LEU:HD22	1.82	0.45
3:D:126:LEU:O	3:D:220:ARG:NH1	2.48	0.45
3:D:425:ARG:NH1	3:D:459:ALA:HA	2.32	0.45
2:C:33:ASP:HA	2:C:36:GLN:HG2	1.98	0.45
2:C:661:VAL:HG12	2:C:662:SER:N	2.31	0.45
3:D:1268:ASN:HB3	3:D:1301:THR:H	1.81	0.45
3:D:1347:LEU:HD22	3:D:1357:ILE:HG23	1.99	0.45
5:M:221:SER:C	5:M:223:HIS:N	2.70	0.45
6:F:82:DT:C2	7:G:-20:DA:N1	2.82	0.45
2:C:874:GLY:H	2:C:928:VAL:HG23	1.80	0.45
2:C:931:VAL:HG22	2:C:1052:VAL:HG22	1.99	0.45
3:D:824:PRO:HD3	3:D:835:LEU:HD13	1.98	0.45
1:A:227:GLN:HG2	1:B:39:LEU:HD11	1.98	0.45
2:C:812:PHE:H	2:C:815:SER:HG	1.62	0.45
2:C:1020:GLU:O	2:C:1024:GLU:HB2	2.17	0.45
3:D:632:ALA:O	3:D:635:SER:OG	2.25	0.45
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.51	0.45
1:A:28:LEU:HB2	1:A:201:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:HIS:CE1	1:A:69:SER:HB2	2.52	0.45
1:B:108:GLY:O	1:B:133:LEU:HB3	2.17	0.45
2:C:1254:VAL:O	2:C:1255:THR:OG1	2.30	0.45
2:C:1279:GLU:HG2	3:D:1357:ILE:HD13	1.98	0.45
3:D:355:ILE:HD11	3:D:466:MET:SD	2.57	0.45
3:D:419:HIS:HE1	3:D:470:VAL:HG13	1.82	0.45
3:D:711:GLY:O	3:D:712:GLN:HG2	2.16	0.45
3:D:823:THR:O	3:D:838:ARG:NH2	2.50	0.45
2:C:455:SER:O	2:C:459:MET:HG2	2.09	0.44
3:D:369:PRO:O	3:D:372:MET:N	2.50	0.44
3:D:361:LEU:CD1	3:D:365:GLN:HB2	2.43	0.44
7:G:-16:DT:H2"	7:G:-15:DT:C6	2.52	0.44
1:A:31:LEU:HD11	1:A:201:LEU:HD23	1.99	0.44
2:C:518:ASN:HB3	2:C:689:ALA:O	2.17	0.44
2:C:1020:GLU:O	2:C:1024:GLU:CB	2.66	0.44
2:C:1034:ARG:HA	2:C:1037:THR:HG22	1.99	0.44
6:F:81:DG:C8	6:F:82:DT:H72	2.52	0.44
2:C:1103:VAL:HG11	2:C:1112:ILE:HD11	2.00	0.44
3:D:362:ARG:CB	3:D:365:GLN:HG3	2.45	0.44
3:D:832:LYS:HB3	3:D:1242:ARG:HD3	1.98	0.44
2:C:448:LEU:HD11	2:C:554:HIS:HD2	1.83	0.44
1:A:35:PHE:HB3	1:A:39:LEU:HD13	2.00	0.44
2:C:515:MET:SD	2:C:523:GLU:HG3	2.57	0.44
2:C:1058:ARG:HH11	2:C:1238:LEU:HD11	1.83	0.44
2:C:1270:PHE:O	3:D:344:GLY:HA3	2.17	0.44
3:D:239:LEU:HD13	3:D:242:LEU:HB2	1.98	0.44
5:M:304:UNK:O	5:M:308:ASN:N	2.50	0.44
2:C:194:LEU:HD22	2:C:206:ALA:HB2	2.00	0.44
2:C:1271:GLY:N	2:C:1274:GLU:OE1	2.50	0.44
2:C:15:PHE:HD2	2:C:1184:THR:HG22	1.82	0.44
5:M:193:LYS:O	5:M:195:LEU:N	2.50	0.44
1:B:219:ARG:O	1:B:223:ILE:HD12	2.18	0.43
2:C:732:ILE:HD11	2:C:769:PRO:HG3	1.99	0.43
3:D:349:TYR:O	3:D:469:HIS:HA	2.18	0.43
3:D:1318:SER:OG	3:D:1321:SER:OG	2.27	0.43
2:C:1066:MET:O	2:C:1073:LYS:HA	2.17	0.43
2:C:488:MET:O	2:C:490:GLN:N	2.49	0.43
2:C:945:ALA:O	2:C:948:ILE:HG13	2.18	0.43
2:C:1271:GLY:HA2	3:D:344:GLY:HA3	1.99	0.43
3:D:279:LEU:HD13	3:D:299:LEU:HD13	2.00	0.43
3:D:471:PRO:O	3:D:477:GLN:NE2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:VAL:O	1:A:202:VAL:HA	2.19	0.43
3:D:57:PHE:CD1	3:D:247:PRO:HB3	2.54	0.43
3:D:1268:ASN:HB3	3:D:1300:ALA:HB1	1.99	0.43
2:C:576:SER:HB3	2:C:579:ALA:HB2	2.00	0.43
2:C:1062:PRO:O	2:C:1076:ILE:HB	2.19	0.43
2:C:1104:PRO:HG2	3:D:725:MET:SD	2.58	0.43
2:C:1116:HIS:HD2	2:C:1208:GLY:HA3	1.83	0.43
3:D:1190:ILE:HG22	3:D:1192:LYS:H	1.82	0.43
1:A:61:ILE:HG23	1:A:64:VAL:HB	2.01	0.43
5:M:217:ARG:HA	5:M:220:ILE:HD12	2.01	0.43
5:M:457:THR:CA	6:F:85:DT:H71	2.48	0.43
2:C:187:GLU:O	2:C:195:PHE:HB2	2.19	0.43
2:C:522:SER:O	2:C:526:HIS:CB	2.67	0.43
2:C:1286:THR:O	2:C:1290:MET:HB2	2.18	0.43
3:D:27:PRO:O	3:D:31:ARG:CB	2.67	0.43
3:D:356:THR:O	3:D:449:LEU:N	2.37	0.43
3:D:1177:ILE:O	3:D:1187:GLU:HA	2.19	0.43
2:C:87:ILE:O	2:C:932:GLN:NE2	2.34	0.43
2:C:600:THR:HG22	2:C:602:GLU:H	1.84	0.43
1:A:107:ILE:HG22	1:A:135:ASP:HA	2.00	0.43
2:C:592:ARG:NH2	2:C:655:VAL:HG13	2.30	0.43
2:C:1274:GLU:HG3	3:D:434:ILE:HD11	2.01	0.43
3:D:513:MET:O	3:D:575:GLY:HA3	2.18	0.43
3:D:822:MET:O	3:D:879:ALA:HA	2.19	0.43
2:C:6:THR:OG1	2:C:781:ASP:OD1	2.34	0.42
2:C:877:VAL:HG21	2:C:883:LEU:HD12	2.00	0.42
3:D:22:ILE:HG23	3:D:1339:GLY:HA2	2.01	0.42
2:C:1326:LEU:HD13	3:D:337:ARG:HD2	2.01	0.42
3:D:366:CYS:SG	3:D:423:LEU:HD11	2.59	0.42
2:C:557:ARG:HG3	2:C:558:VAL:H	1.85	0.42
2:C:1047:LEU:HG	2:C:1048:LYS:HG2	2.00	0.42
3:D:1138:LEU:O	3:D:1140:ARG:N	2.48	0.42
7:G:-14:DG:H3'	7:G:-14:DG:P	2.58	0.42
2:C:500:ALA:O	2:C:504:GLU:HB2	2.20	0.42
2:C:582:ASN:HD22	2:C:586:PHE:HB2	1.84	0.42
2:C:661:VAL:HG12	2:C:662:SER:H	1.85	0.42
2:C:870:ILE:HD13	2:C:931:VAL:HG21	2.01	0.42
3:D:413:ASP:O	3:D:417:ARG:HG3	2.19	0.42
3:D:830:ASP:OD1	3:D:831:VAL:N	2.52	0.42
1:B:108:GLY:O	1:B:133:LEU:HA	2.19	0.42
3:D:289:ASP:O	3:D:293:ARG:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:345:LYS:O	3:D:347:VAL:HG23	2.20	0.42
3:D:686:TRP:CE2	3:D:758:PRO:HG3	2.53	0.42
7:G:-10:DG:H4'	7:G:-9:DA:OP1	2.19	0.42
1:A:177:TYR:O	1:A:179:PRO:HD3	2.19	0.42
2:C:59:ILE:HB	2:C:68:LEU:HD12	2.01	0.42
3:D:664:ILE:HD11	3:D:685:ILE:HD13	2.01	0.42
1:B:215:GLU:HA	1:B:218:ARG:HG2	2.00	0.42
2:C:565:GLU:HA	2:C:569:ILE:HD13	2.01	0.42
1:A:124:VAL:HG21	1:A:209:GLY:HA3	2.02	0.42
3:D:1251:LYS:O	3:D:1255:VAL:HG23	2.20	0.42
1:A:81:ILE:HG12	1:A:131:CYS:HB3	2.02	0.42
5:M:211:PRO:C	5:M:213:LEU:H	2.22	0.42
1:B:118:ASP:HB2	1:B:121:VAL:HB	2.02	0.42
2:C:1069:ARG:HH21	2:C:1114:GLU:CD	2.23	0.42
3:D:836:ARG:HG3	3:D:869:CYS:SG	2.60	0.42
3:D:1178:THR:N	3:D:1179:PRO:HD2	2.35	0.42
1:B:145:LYS:HE2	1:B:147:GLN:HE21	1.85	0.41
2:C:832:HIS:HD2	2:C:1058:ARG:HD2	1.84	0.41
5:M:222:ASP:O	5:M:223:HIS:CB	2.68	0.41
6:F:84:DG:H2"	6:F:85:DT:C6	2.54	0.41
1:A:118:ASP:OD1	1:A:119:GLY:N	2.48	0.41
2:C:257:ALA:N	2:C:260:LYS:O	2.48	0.41
2:C:522:SER:O	2:C:526:HIS:HB2	2.20	0.41
1:A:51:MET:SD	1:A:52:PRO:HD2	2.60	0.41
1:A:214:GLU:O	1:A:218:ARG:HB2	2.20	0.41
2:C:768:MET:O	2:C:784:ALA:HA	2.21	0.41
2:C:1326:LEU:HB2	3:D:337:ARG:CZ	2.50	0.41
5:M:191:ALA:C	5:M:193:LYS:H	2.23	0.41
6:F:75:DG:H2'	6:F:76:DC:C1'	2.50	0.41
1:B:24:ALA:O	1:B:204:GLU:HA	2.20	0.41
2:C:86:GLN:HE21	2:C:137:VAL:HG22	1.85	0.41
3:D:318:GLY:C	3:D:320:ASN:N	2.73	0.41
3:D:585:LYS:HB2	3:D:612:LEU:HD21	2.02	0.41
3:D:810:THR:HG23	3:D:811:GLU:N	2.36	0.41
2:C:870:ILE:HD12	2:C:871:VAL:O	2.21	0.41
3:D:1058:SER:HA	3:D:1107:VAL:O	2.21	0.41
5:M:459:ALA:O	5:M:463:GLU:CB	2.69	0.41
2:C:15:PHE:CD2	2:C:1190:ALA:HB2	2.55	0.41
2:C:619:ALA:HA	2:C:654:ASP:HB2	2.02	0.41
2:C:916:SER:HB3	5:M:264:UNK:C	2.50	0.41
1:A:11:PRO:HA	1:A:30:PRO:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:GLU:O	1:A:25:LYS:CB	2.59	0.41
2:C:993:PRO:C	2:C:995:ASP:N	2.73	0.41
3:D:491:LEU:HA	3:D:498:PRO:HA	2.03	0.41
1:A:66:HIS:HB3	2:C:874:GLY:HA3	2.02	0.41
1:A:192:VAL:C	1:A:194:GLN:N	2.72	0.41
1:B:215:GLU:O	1:B:219:ARG:HG3	2.21	0.41
3:D:919:ALA:C	3:D:921:GLN:H	2.24	0.41
1:A:38:THR:O	1:A:42:ALA:HB3	2.20	0.41
1:A:112:ALA:HB2	1:A:128:HIS:HB3	2.03	0.41
2:C:887:VAL:HB	2:C:913:VAL:CG1	2.51	0.41
3:D:420:PRO:HD3	3:D:481:ARG:HH22	1.86	0.41
3:D:553:THR:HA	3:D:567:THR:HA	2.01	0.41
7:G:-7:DC:H2"	7:G:-6:DA:OP2	2.20	0.41
1:A:10:LYS:NZ	1:B:226:GLU:HG2	2.36	0.41
2:C:1324:ASN:HA	2:C:1327:LEU:HD12	2.03	0.41
3:D:513:MET:SD	3:D:579:LEU:HB2	2.61	0.41
3:D:1356:LEU:HD21	3:D:1365:TYR:CD2	2.56	0.41
1:A:42:ALA:HB1	1:B:38:THR:HG23	2.03	0.40
2:C:59:ILE:HB	2:C:68:LEU:HB2	2.03	0.40
2:C:895:LEU:O	2:C:896:THR:OG1	2.29	0.40
3:D:139:LEU:HD12	3:D:140:TYR:CD2	2.57	0.40
3:D:555:TYR:HB2	3:D:586:GLY:HA2	2.03	0.40
3:D:628:GLY:O	3:D:632:ALA:CB	2.70	0.40
5:M:221:SER:C	5:M:223:HIS:H	2.23	0.40
1:A:225:ALA:HA	1:A:228:LEU:HD12	2.04	0.40
1:B:13:LEU:HB3	1:B:28:LEU:HD23	2.03	0.40
1:B:64:VAL:HG12	1:B:66:HIS:H	1.86	0.40
3:D:810:THR:HG23	3:D:811:GLU:H	1.85	0.40
3:D:1231:ARG:O	3:D:1235:ASN:HB2	2.21	0.40
1:B:28:LEU:HD12	1:B:201:LEU:HD23	2.03	0.40
1:B:80:GLU:O	1:B:84:ASN:ND2	2.53	0.40
2:C:818:VAL:HG23	2:C:1076:ILE:HG12	2.03	0.40
2:C:1127:LYS:HD2	2:C:1144:PHE:CZ	2.56	0.40
3:D:369:PRO:O	3:D:372:MET:HB2	2.21	0.40
3:D:620:PHE:CZ	3:D:624:ILE:HD11	2.57	0.40
3:D:1308:GLY:C	3:D:1310:THR:H	2.24	0.40
6:F:75:DG:C2'	6:F:76:DC:O4'	2.68	0.40
6:F:75:DG:C3'	6:F:76:DC:O4'	2.70	0.40
2:C:230:PHE:CB	2:C:333:ILE:O	2.48	0.40
3:D:1141:VAL:HG11	3:D:1241:TYR:HE2	1.85	0.40
7:G:-10:DG:H2"	7:G:-9:DA:C4'	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ALA:HB3	1:A:205:MET:HB3	2.02	0.40
1:A:164:ASP:OD1	1:A:165:GLU:N	2.49	0.40
2:C:670:PHE:CE2	2:C:1113:LEU:HB3	2.57	0.40
3:D:511:TYR:HE2	3:D:724:MET:HG2	1.85	0.40
6:F:72:DC:C3'	6:F:73:DG:H5"	2.39	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	231/329 (70%)	211 (91%)	19 (8%)	1 (0%)	34	70
1	B	219/329 (67%)	203 (93%)	15 (7%)	1 (0%)	29	66
2	C	1339/1342 (100%)	1227 (92%)	103 (8%)	9 (1%)	22	60
3	D	1306/1407 (93%)	1163 (89%)	132 (10%)	11 (1%)	19	57
4	E	72/91 (79%)	68 (94%)	4 (6%)	0	100	100
5	M	284/573 (50%)	243 (86%)	30 (11%)	11 (4%)	3	28
All	All	3451/4071 (85%)	3115 (90%)	303 (9%)	33 (1%)	20	52

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	GLU
2	C	347	ILE
3	D	886	VAL
3	D	1309	ILE
5	M	188	VAL
5	M	222	ASP
5	M	223	HIS

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Mol	Chain	Res	Type
5	M	225	ASP
5	M	310	ALA
5	M	313	ASP
3	D	317	THR
2	C	228	VAL
2	C	933	VAL
3	D	319	SER
3	D	347	VAL
3	D	366	CYS
5	M	156	ILE
5	M	314	ALA
1	B	173	VAL
2	C	655	VAL
3	D	320	ASN
3	D	321	LYS
3	D	1159	ILE
5	M	194	ASP
2	C	1164	PHE
2	C	1165	SER
3	D	365	GLN
5	M	212	TRP
5	M	190	VAL
2	C	1155	VAL
2	C	1186	VAL
2	C	98	VAL
3	D	809	VAL

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	A	175/286 (61%)	175 (100%)	0	100 100
1	B	162/286 (57%)	162 (100%)	0	100 100
2	C	892/1157 (77%)	891 (100%)	1 (0%)	93 97
3	D	761/1168 (65%)	759 (100%)	2 (0%)	92 96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	50/75 (67%)	50 (100%)	0	100	100
5	M	29/423 (7%)	29 (100%)	0	100	100
All	All	2069/3395 (61%)	2066 (100%)	3 (0%)	93	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	459	MET
3	D	366	CYS
3	D	372	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	B	147	GLN
2	C	86	GLN
2	C	139	ASN
2	C	604	HIS
2	C	808	ASN
2	C	832	HIS
2	C	1256	GLN
2	C	1288	GLN
3	D	805	GLN
3	D	897	HIS
3	D	1350	ASN
4	E	15	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	M	3
7	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	49:UNK	C	118:GLN	N	38.56
1	M	413:UNK	C	415:ALA	N	3.49
1	M	304:UNK	C	306:MET	N	2.76
1	G	-10:DG	O3'	-9:DA	P	1.32

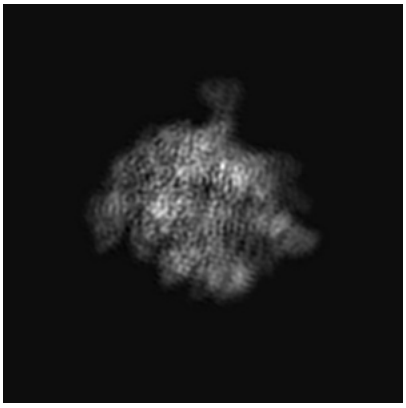
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3695. These allow visual inspection of the internal detail of the map and identification of artifacts.

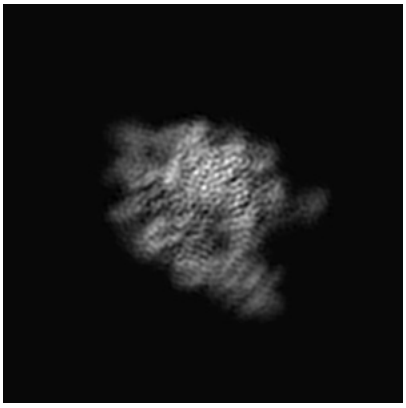
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

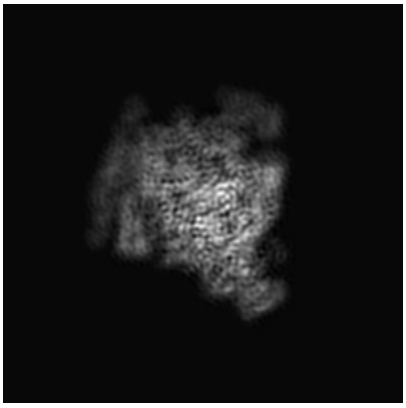
6.1.1 Primary map



X



Y

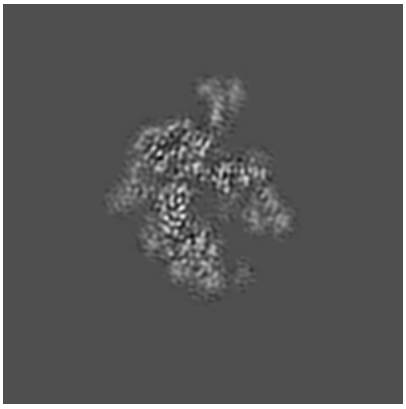


Z

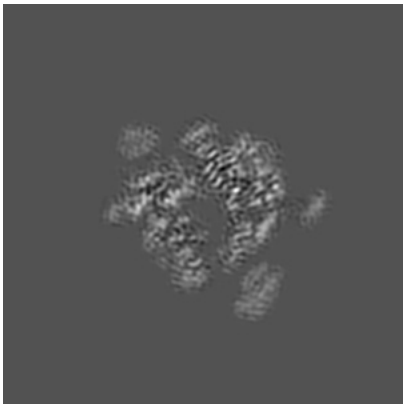
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

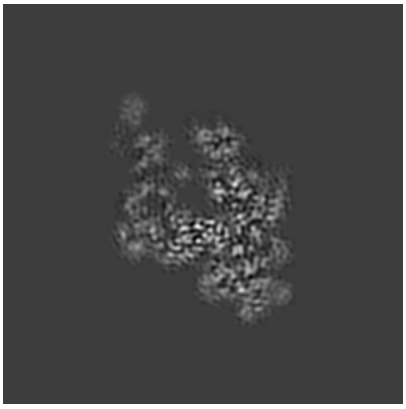
6.2.1 Primary map



X Index: 128



Y Index: 128

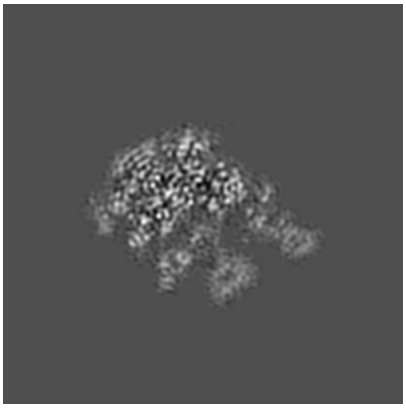


Z Index: 128

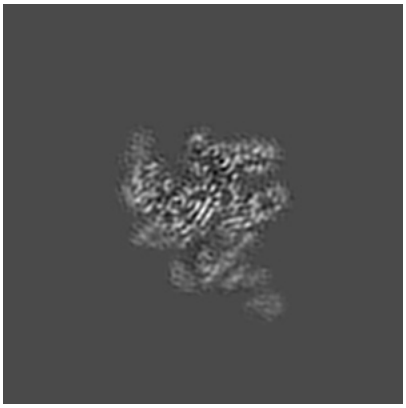
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

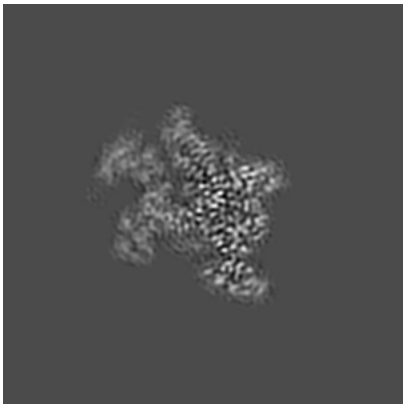
6.3.1 Primary map



X Index: 151



Y Index: 113



Z Index: 146

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

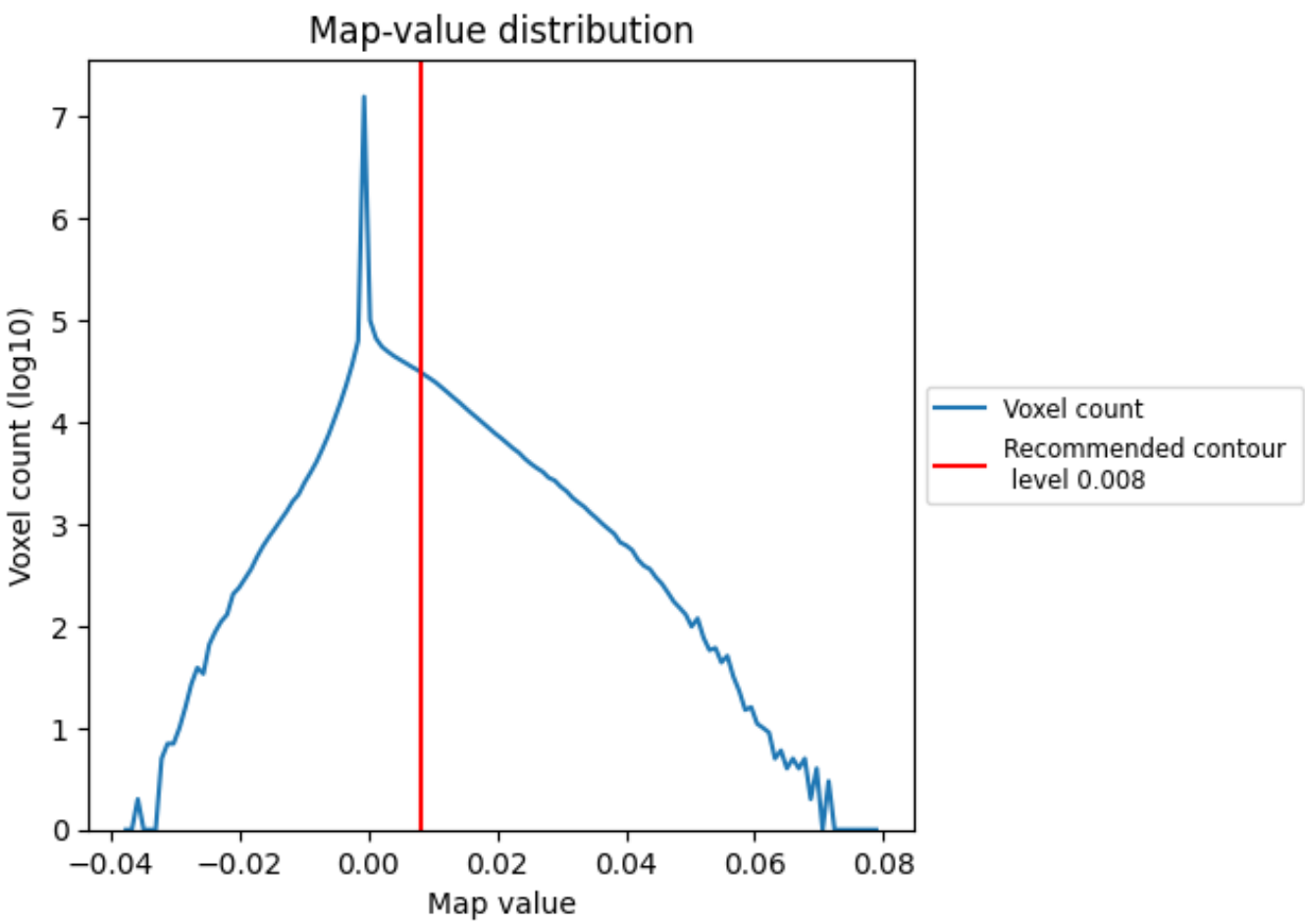
6.5 Mask visualisation (i)

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

7 Map analysis (i)

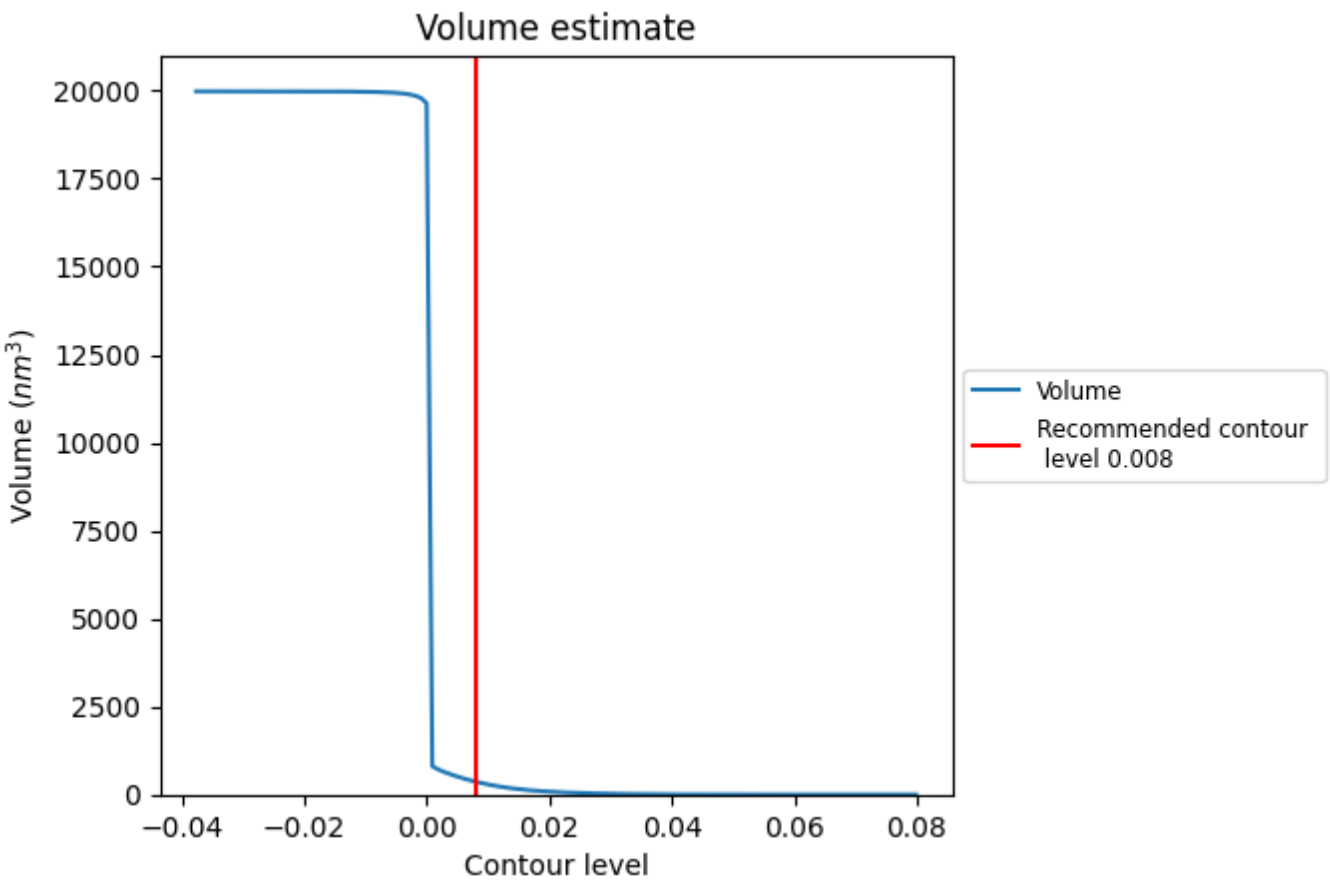
This section contains the results of statistical analysis of the map.

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.

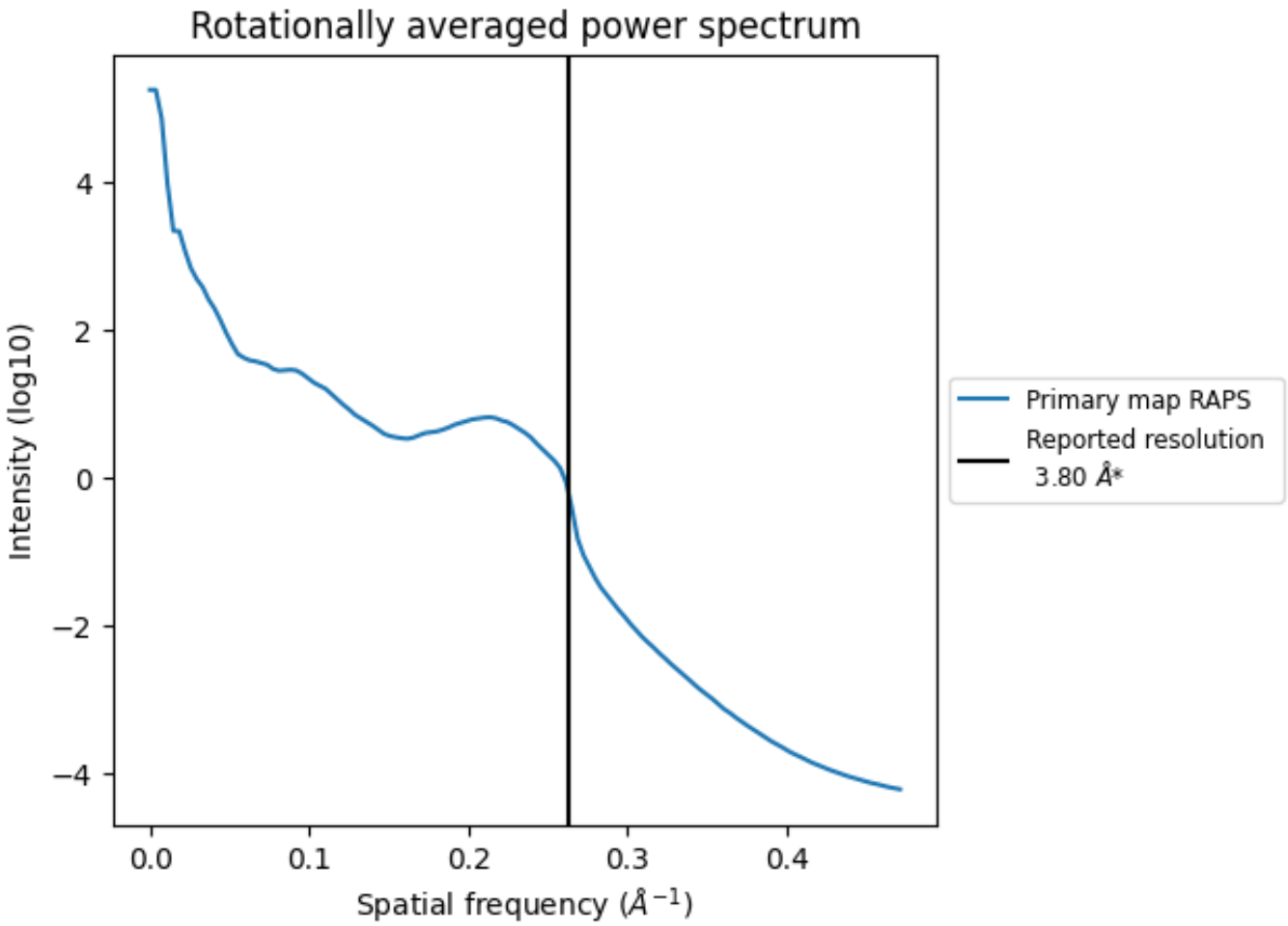
7.2 Volume estimate (i)



The volume at the recommended contour level is 363 nm^3; this corresponds to an approximate mass of 328 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 0.263 Å^{-1}

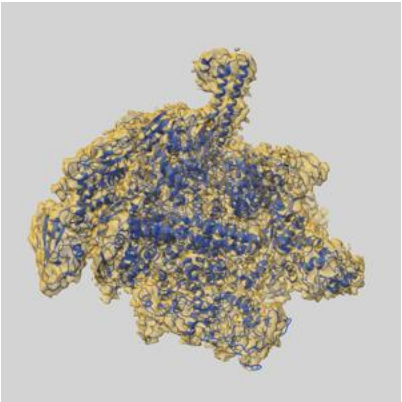
8 Fourier-Shell correlation (i)

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

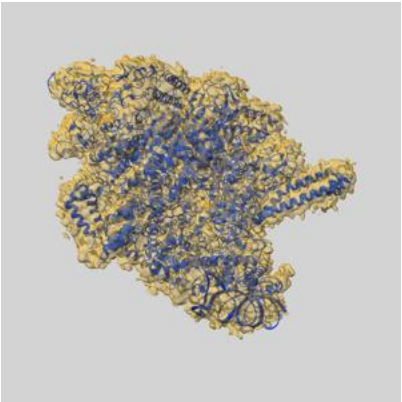
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3695 and PDB model 5NSR. Per-residue inclusion information can be found in section 3 on page 5.

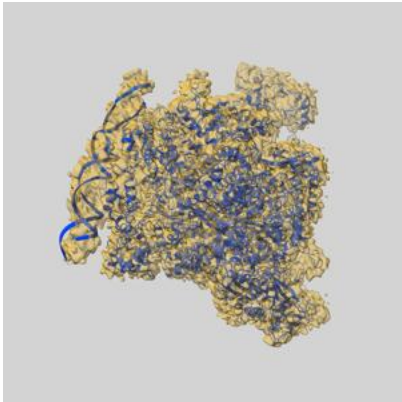
9.1 Map-model overlay (i)



X



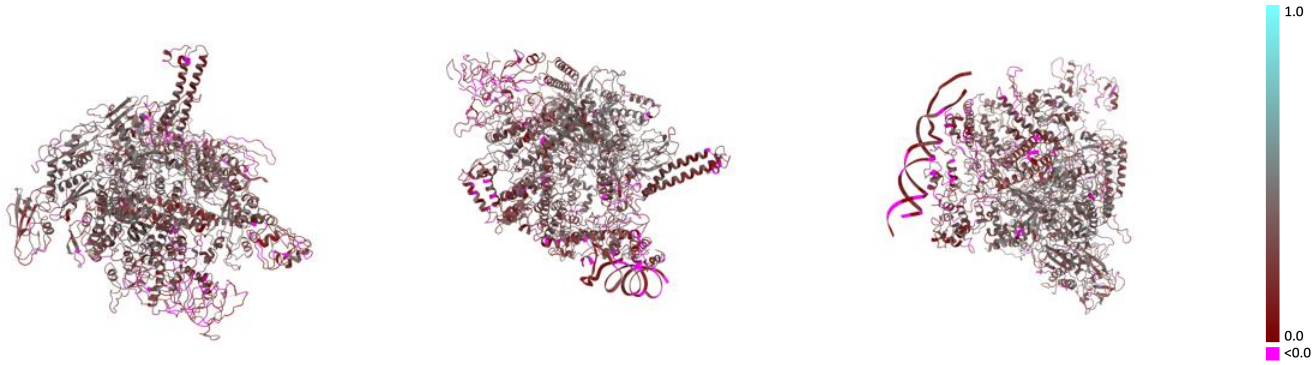
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 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.

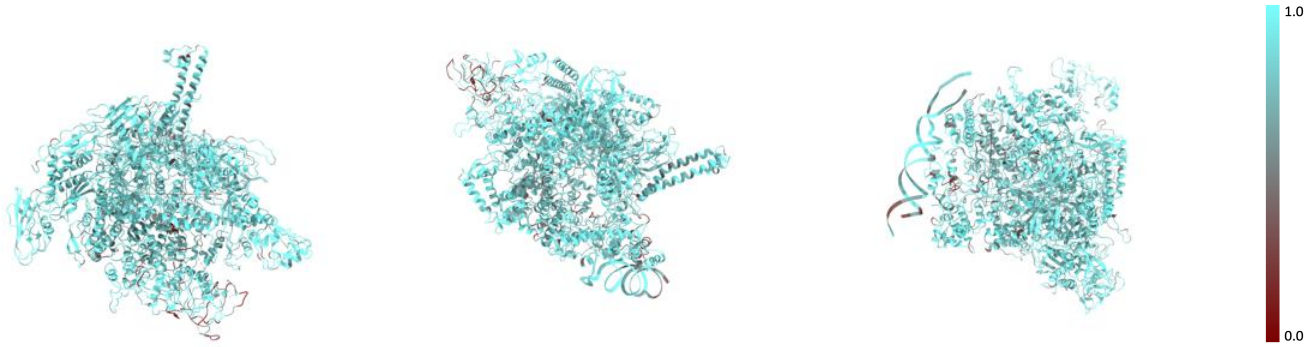
9.2 Q-score mapped to coordinate model (i)



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.

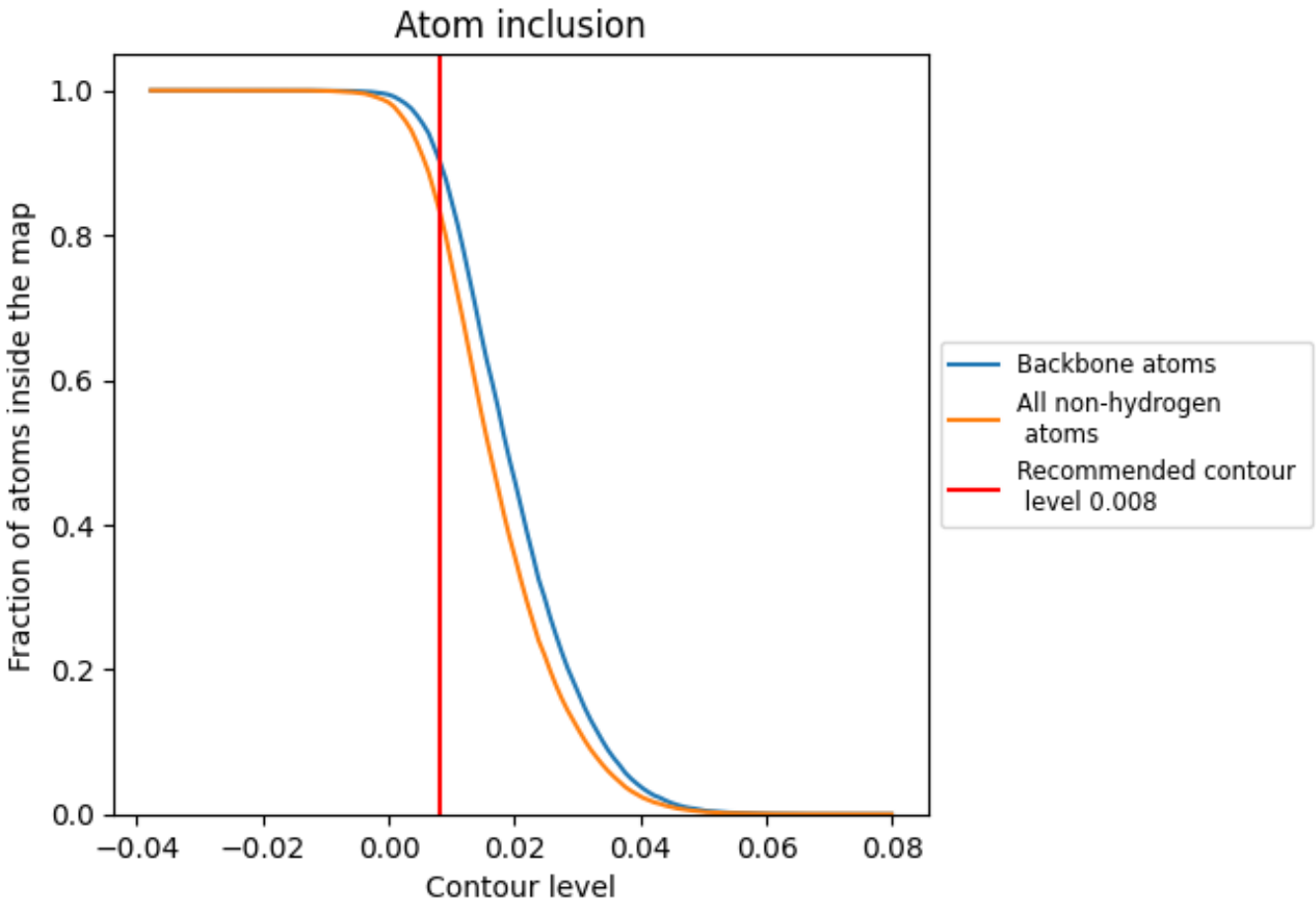
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.008).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8375	0.2890
A	0.8627	0.3480
B	0.8702	0.3090
C	0.8678	0.3230
D	0.8200	0.2810
E	0.7645	0.3090
F	0.7162	0.1270
G	0.7567	0.1070
M	0.8003	0.1910