



## Full wwPDB EM Validation Report ⓘ

Mar 3, 2024 – 01:17 PM EST

PDB ID : 6B6H  
EMDB ID : EMD-7059  
Title : The cryo-EM structure of a bacterial class I transcription activation complex  
Authors : Liu, B.; Hong, C.; Huang, R.; Yu, Z.; Steitz, T.A.  
Deposited on : 2017-10-02  
Resolution : 3.90 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](mailto: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:

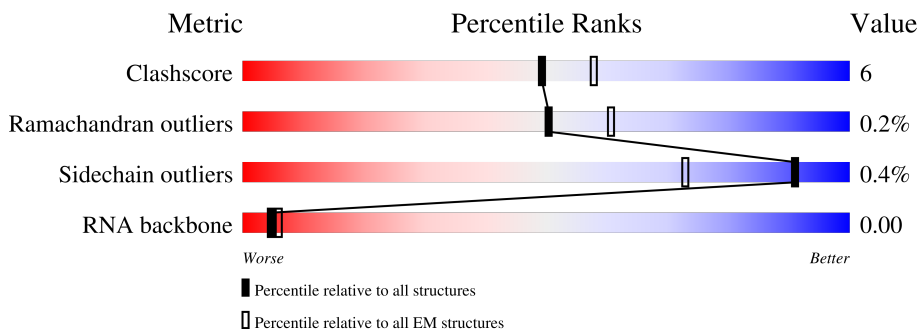
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 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 3.90 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.



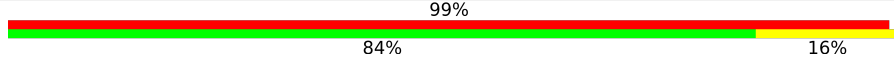
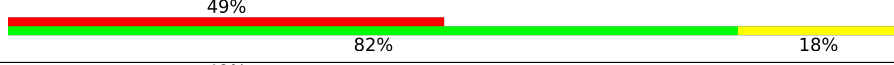
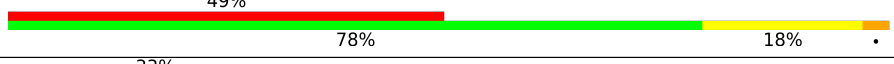
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	
1	B	329	
2	C	1342	
3	D	1407	
4	E	91	
5	F	628	
6	G	210	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
6	H	210	
7	I	75	
8	1	88	
9	2	88	
10	3	3	

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 72103 atoms, of which 35433 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	H	N	O			S
1	A	230	Total	C	H	N	O	S	0	0
			3599	1112	1813	317	351	6		
1	B	228	Total	C	H	N	O	S	0	0
			3556	1100	1789	312	349	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	C	1340	Total	C	H	N	O	S	0	0
			21152	6631	10582	1841	2055	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	D	1337	Total	C	H	N	O	S	0	0
			21010	6531	10614	1853	1962	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	E	79	Total	C	H	N	O	S	0	0
			1261	382	634	118	126	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	F	497	Total	C	H	N	O	S	0	0
			8105	2512	4083	719	768	23		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-14	MET	-	initiating methionine	UNP P00579

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-13	ARG	-	expression tag	UNP P00579
F	-12	GLY	-	expression tag	UNP P00579
F	-11	SER	-	expression tag	UNP P00579
F	-10	HIS	-	expression tag	UNP P00579
F	-9	HIS	-	expression tag	UNP P00579
F	-8	HIS	-	expression tag	UNP P00579
F	-7	HIS	-	expression tag	UNP P00579
F	-6	HIS	-	expression tag	UNP P00579
F	-5	HIS	-	expression tag	UNP P00579
F	-4	THR	-	expression tag	UNP P00579
F	-3	ASP	-	expression tag	UNP P00579
F	-2	GLN	-	expression tag	UNP P00579
F	-1	PHE	-	expression tag	UNP P00579
F	0	THR	-	expression tag	UNP P00579

- Molecule 6 is a protein called cAMP-activated global transcriptional regulator CRP.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	201	Total	C	H	N	O	S	0	0
			3219	1007	1629	279	295	9		
6	H	201	Total	C	H	N	O	S	0	0
			3223	1007	1632	280	295	9		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	75	Total	C	H	N	O	S	0	0
			1198	370	614	102	110	2		

- Molecule 8 is a DNA chain called SYNTHETIC NONTEMPLATE STRAND DNA (88-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
8	1	88	Total	C	H	N	O	P	0	0
			2796	860	992	331	525	88		

- Molecule 9 is a DNA chain called SYNTHETIC TEMPLATE STRAND DNA (88-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
9	2	88	Total	C	H	N	O	P	0	0
			2805	863	996	325	533	88		

- Molecule 10 is a RNA chain called NASCENT RNA 3-MER.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
10	3	3	110	30	33	15	27	5	0	0

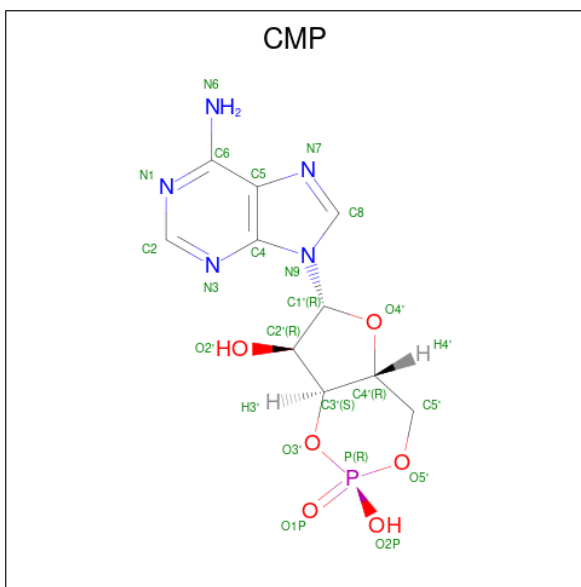
- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 13 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: C<sub>10</sub>H<sub>12</sub>N<sub>5</sub>O<sub>6</sub>P).

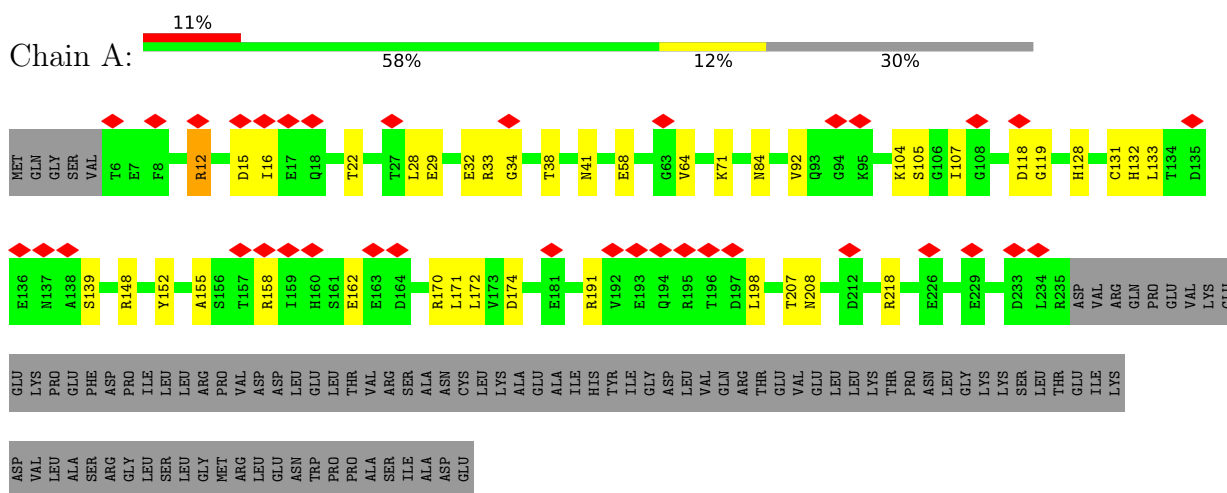


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
13	G	1	33	10	11	5	6	1	0
13	H	1	33	10	11	5	6	1	0

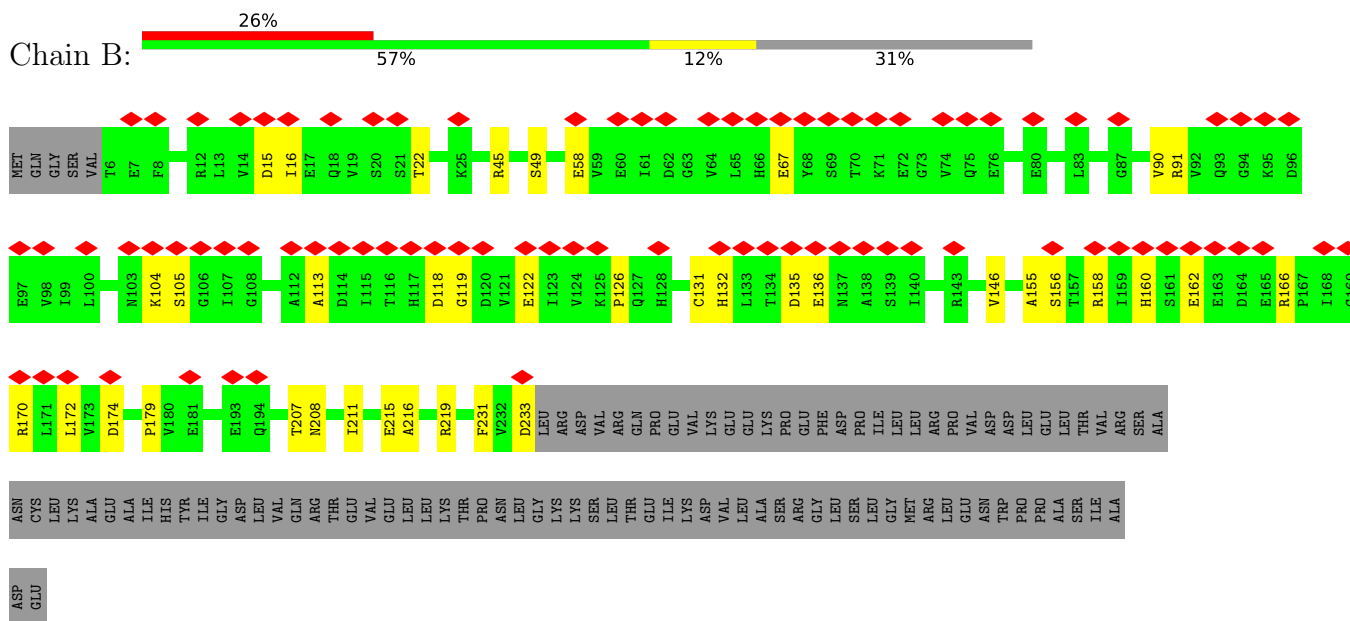
### 3 Residue-property plots [i](#)

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.

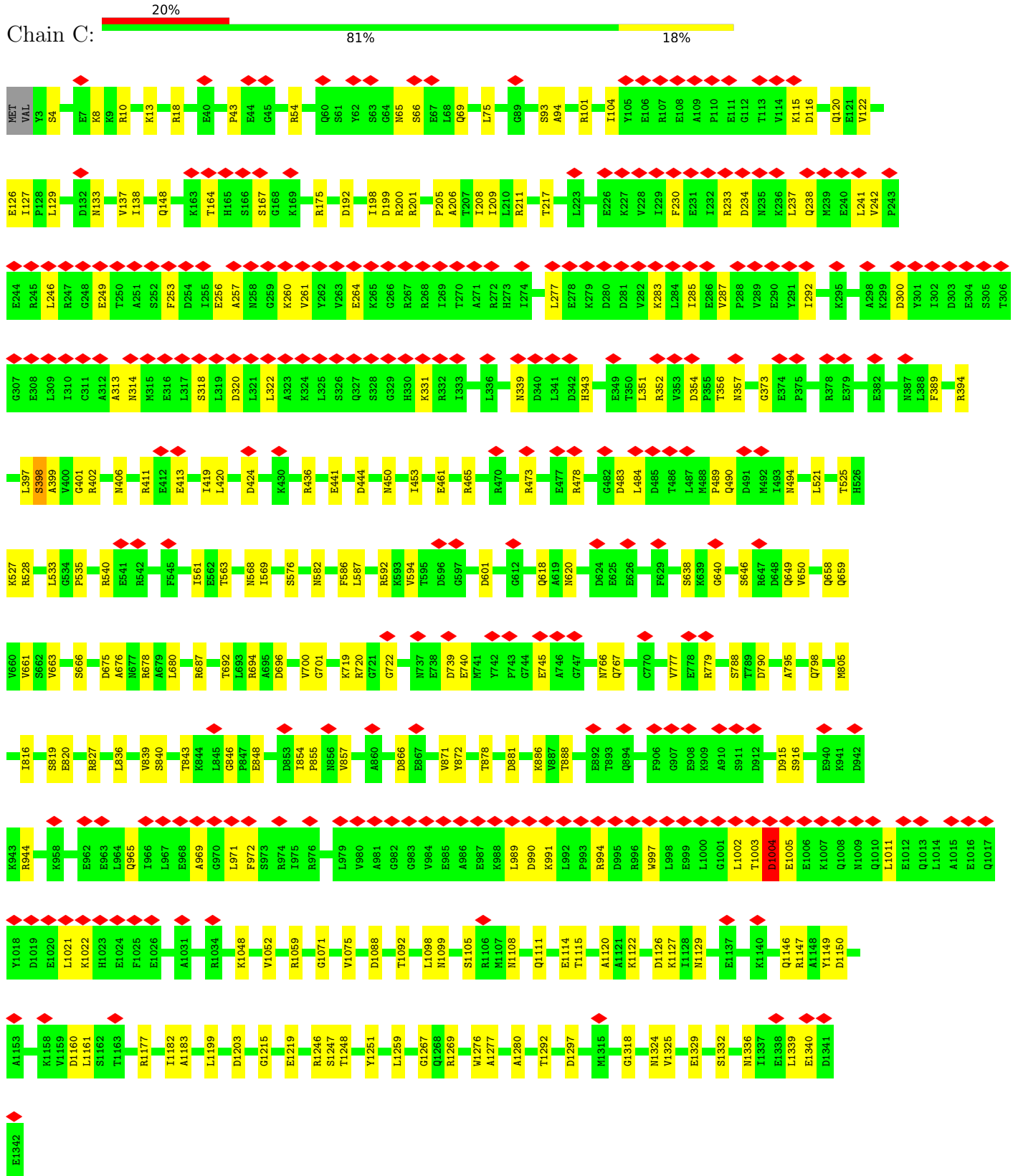
- Molecule 1: DNA-directed RNA polymerase subunit alpha



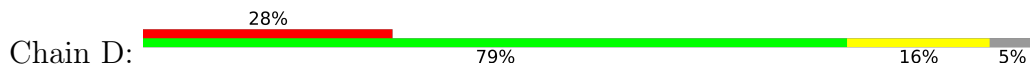
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 2: DNA-directed RNA polymerase subunit beta



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



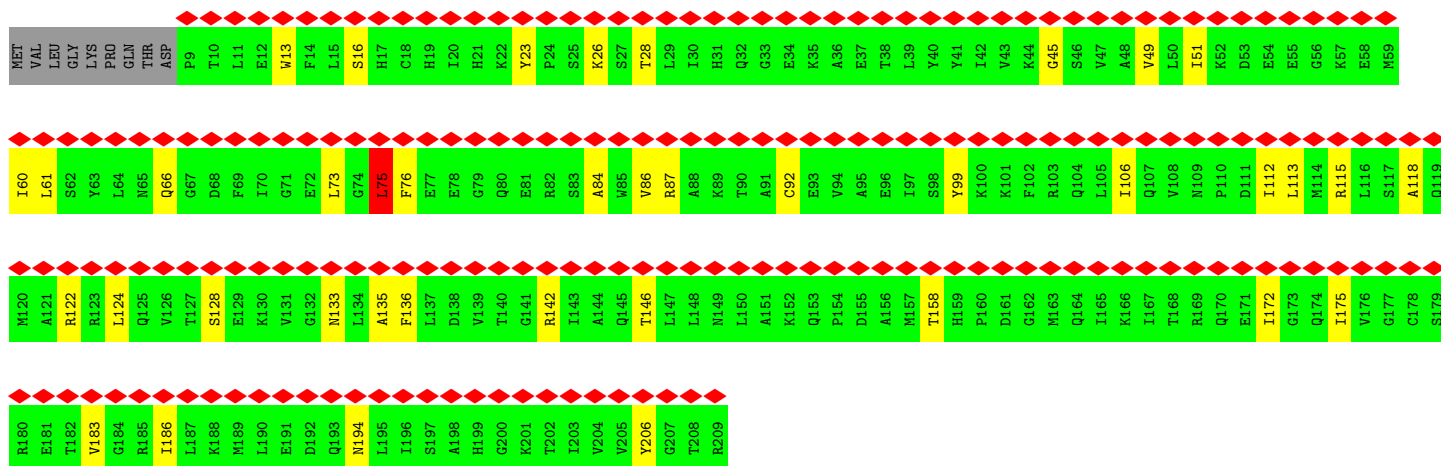
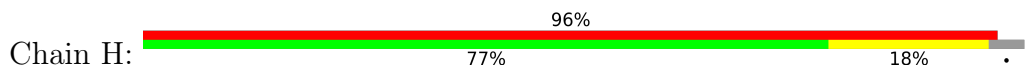




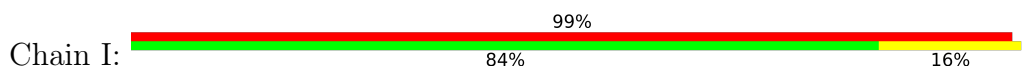




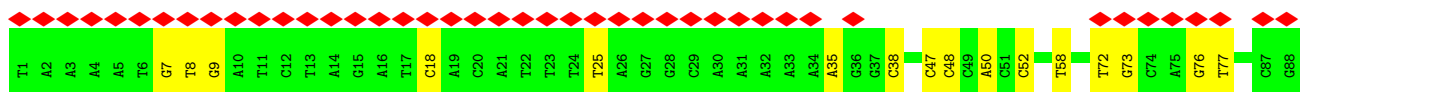
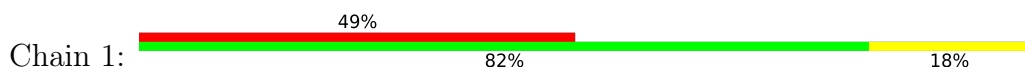
• Molecule 6: cAMP-activated global transcriptional regulator CRP



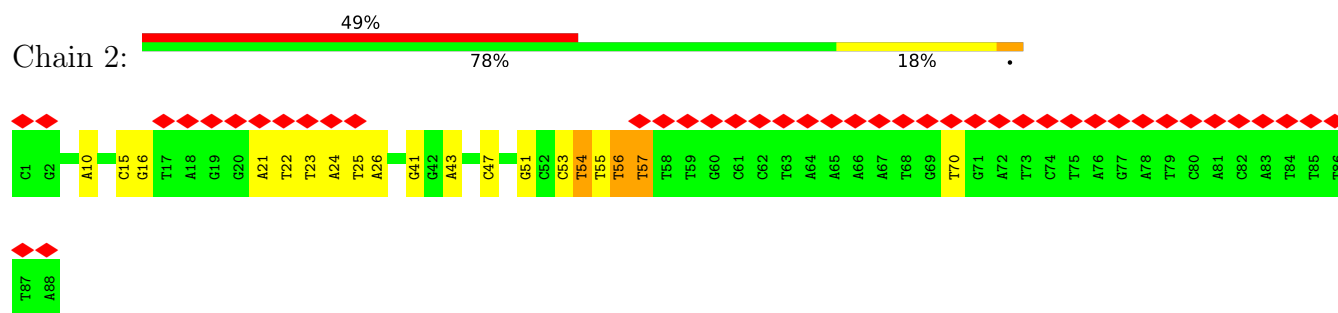
• Molecule 7: DNA-directed RNA polymerase subunit alpha



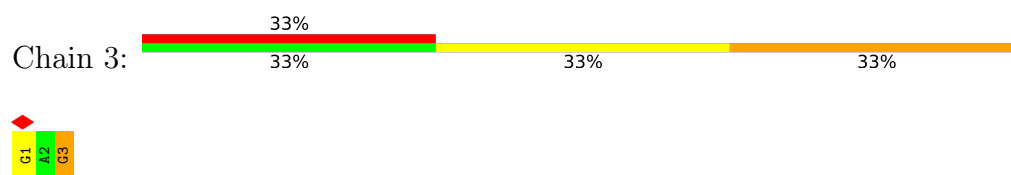
• Molecule 8: SYNTHETIC NONTEMPLATE STRAND DNA (88-MER)



- Molecule 9: SYNTHETIC TEMPLATE STRAND DNA (88-MER)



- Molecule 10: NASCENT RNA 3-MER



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	161000	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 ( $e^-/\text{\AA}^2$ )	1.37	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	37037	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.361	Depositor
Minimum map value	-0.079	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	270.0, 270.0, 270.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.40	0/1808	0.61	0/2450
1	B	0.37	0/1789	0.61	0/2425
2	C	0.44	0/10739	0.62	0/14489
3	D	0.42	0/10553	0.63	1/14248 (0.0%)
4	E	0.27	0/629	0.53	0/847
5	F	0.34	0/4076	0.60	0/5482
6	G	0.32	0/1614	0.62	1/2170 (0.0%)
6	H	0.33	0/1616	0.66	1/2174 (0.0%)
7	I	0.28	0/592	0.64	0/803
8	1	0.86	1/2024 (0.0%)	1.11	5/3121 (0.2%)
9	2	0.81	0/2028	1.06	6/3130 (0.2%)
10	3	0.52	0/50	1.28	0/76
All	All	0.47	1/37518 (0.0%)	0.70	14/51415 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	C	0	2
3	D	0	5
5	F	0	3
6	H	0	1
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	1	18	DC	C1'-N1	5.90	1.56	1.49

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	25	DT	O4'-C1'-N1	7.32	113.12	108.00
8	1	47	DC	O4'-C4'-C3'	-7.06	101.67	104.50
8	1	25	DT	C1'-O4'-C4'	-6.85	103.25	110.10
8	1	50	DA	O4'-C1'-N9	6.79	112.75	108.00
3	D	710	ASP	CB-CG-OD1	5.70	123.43	118.30
9	2	43	DA	O4'-C4'-C3'	-5.58	102.27	104.50
8	1	52	DC	O4'-C1'-N1	5.55	111.88	108.00
9	2	54	DT	N3-C4-O4	5.55	123.23	119.90
6	G	103	ARG	NE-CZ-NH1	-5.22	117.69	120.30
9	2	54	DT	C5-C4-O4	-5.20	121.26	124.90
9	2	56	DT	N3-C4-O4	5.16	122.99	119.90
9	2	57	DT	N3-C4-O4	5.08	122.95	119.90
6	H	75	LEU	CA-CB-CG	5.05	126.91	115.30
9	2	70	DT	N3-C4-O4	5.00	122.90	119.90

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191	ARG	Peptide
2	C	1004	ASP	Peptide
2	C	200	ARG	Peptide
3	D	120	LEU	Peptide
3	D	121	PRO	Peptide
3	D	174	ASP	Peptide
3	D	518	VAL	Peptide
3	D	930	LEU	Peptide
5	F	165	PHE	Peptide
5	F	322	MET	Peptide
5	F	395	THR	Peptide
6	H	75	LEU	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1786	1813	1813	24	0
1	B	1767	1789	1789	24	0
2	C	10570	10582	10582	148	0
3	D	10396	10614	10614	144	0
4	E	627	634	634	9	0
5	F	4022	4083	4083	48	0
6	G	1590	1629	1629	20	0
6	H	1591	1632	1632	26	0
7	I	584	614	614	9	0
8	1	1804	992	992	14	0
9	2	1809	996	996	19	0
10	3	77	33	33	2	0
11	D	2	0	0	0	0
12	D	1	0	0	0	0
13	G	22	11	11	2	0
13	H	22	11	11	4	0
All	All	36670	35433	35433	436	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 6.

All (436) 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)
13:G:301:CMP:H2	13:G:301:CMP:C2	0.97	1.50
13:H:301:CMP:H2	13:H:301:CMP:C2	0.97	1.49
5:F:551:LEU:HD11	5:F:598:LEU:HD21	1.55	0.86
2:C:494:ASN:ND2	9:2:24:DA:OP1	2.13	0.81
3:D:814:CYS:SG	3:D:883:ARG:NH2	2.54	0.81
3:D:1062:LEU:O	3:D:1067:ARG:NH2	2.13	0.80
2:C:398:SER:O	2:C:401:GLY:N	2.14	0.80
1:A:22:THR:OG1	1:A:207:THR:O	2.00	0.79
6:G:146:THR:HG21	6:G:175:ILE:HD13	1.65	0.79
3:D:214:ARG:NH1	3:D:218:THR:OG1	2.16	0.79
3:D:951:GLN:OE1	3:D:1016:THR:OG1	2.01	0.78
5:F:437:GLN:OE1	9:2:26:DA:N6	2.16	0.78
3:D:1025:MET:SD	3:D:1195:GLN:NE2	2.56	0.78
2:C:528:ARG:NH2	2:C:576:SER:O	2.17	0.77
6:H:172:ILE:HD13	6:H:183:VAL:HG11	1.67	0.77
2:C:234:ASP:OD1	2:C:331:LYS:NZ	2.18	0.77
6:H:133:ASN:O	6:H:142:ARG:NH1	2.18	0.76
5:F:154:GLU:OE1	5:F:157:ARG:NE	2.19	0.76

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:38:DC:O2	9:2:51:DG:N2	2.20	0.75
2:C:478:ARG:NH2	9:2:25:DT:OP1	2.20	0.75
3:D:278:ARG:NH2	5:F:403:ASP:OD1	2.21	0.74
3:D:464:ASP:OD1	10:3:3:G:O2'	2.05	0.74
3:D:930:LEU:HD13	3:D:1246:VAL:HG21	1.68	0.74
3:D:556:GLU:O	3:D:564:VAL:N	2.21	0.73
5:F:470:MET:SD	5:F:486:ARG:NH1	2.62	0.73
3:D:198:CYS:SG	3:D:202:ARG:NH1	2.62	0.73
3:D:1186:TYR:OH	3:D:1188:GLU:OE1	2.07	0.72
3:D:46:TYR:OH	8:1:58:DT:OP1	2.06	0.72
6:G:122:ARG:NH2	6:G:125:GLN:OE1	2.23	0.72
2:C:1088:ASP:OD2	2:C:1092:THR:OG1	2.08	0.71
1:B:179:PRO:O	1:B:207:THR:OG1	2.07	0.71
3:D:438:GLU:OE2	4:E:3:ARG:NH2	2.24	0.71
3:D:1043:GLY:O	3:D:1068:THR:OG1	2.08	0.71
2:C:1146:GLN:NE2	2:C:1150:ASP:OD2	2.24	0.71
5:F:436:ARG:O	5:F:440:THR:OG1	2.06	0.70
1:B:104:LYS:NZ	1:B:105:SER:O	2.25	0.70
2:C:300:ASP:OD1	2:C:313:ALA:N	2.25	0.69
6:G:123:ARG:NH1	13:G:301:CMP:N1	2.39	0.69
6:G:185:ARG:NH2	8:1:9:DG:N7	2.41	0.69
2:C:175:ARG:NE	8:1:77:DT:O4	2.26	0.68
3:D:1271:SER:OG	3:D:1290:ARG:NH1	2.26	0.68
2:C:43:PRO:O	2:C:54:ARG:NH2	2.28	0.67
2:C:192:ASP:OD1	2:C:436:ARG:NH2	2.26	0.67
2:C:402:ARG:NH2	2:C:419:ILE:O	2.27	0.67
2:C:798:GLN:NE2	2:C:827:ARG:O	2.27	0.67
6:H:194:ASN:O	6:H:206:TYR:OH	2.11	0.67
7:I:289:LEU:O	7:I:292:THR:OG1	2.09	0.66
5:F:87:VAL:O	5:F:91:ILE:N	2.29	0.66
2:C:411:ARG:NH2	2:C:424:ASP:OD1	2.29	0.66
3:D:844:THR:HG21	3:D:858:VAL:HG11	1.77	0.66
3:D:320:ASN:OD1	9:2:21:DA:N6	2.28	0.66
5:F:428:SER:O	5:F:432:THR:OG1	2.06	0.66
2:C:692:THR:OG1	2:C:694:ARG:O	2.13	0.66
2:C:473:ARG:NH2	8:1:73:DG:OP2	2.29	0.65
2:C:839:VAL:O	2:C:886:LYS:NZ	2.18	0.65
3:D:918:ILE:O	3:D:922:SER:OG	2.06	0.65
3:D:809:VAL:HG23	3:D:915:ILE:HD11	1.77	0.65
6:H:124:LEU:O	6:H:128:SER:OG	2.08	0.65
3:D:950:ILE:HB	3:D:1018:ALA:HB3	1.79	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLU:OE1	1:A:170:ARG:NH2	2.30	0.65
3:D:1320:ILE:O	3:D:1324:SER:OG	2.15	0.65
2:C:164:THR:O	2:C:167:SER:OG	2.12	0.64
2:C:444:ASP:O	2:C:450:ASN:ND2	2.29	0.64
3:D:85:CYS:O	3:D:89:GLY:N	2.30	0.64
3:D:955:LYS:O	3:D:992:LYS:NZ	2.31	0.64
1:A:28:LEU:HD21	1:B:231:PHE:CZ	2.32	0.64
2:C:722:GLY:O	2:C:777:VAL:N	2.30	0.64
6:H:28:THR:OG1	6:H:87:ARG:NH1	2.31	0.64
6:G:124:LEU:HD22	6:H:73:LEU:HD11	1.79	0.64
7:I:307:LEU:HD13	7:I:313:SER:HA	1.79	0.64
2:C:148:GLN:NE2	2:C:533:LEU:O	2.31	0.63
3:D:814:CYS:SG	3:D:816:THR:OG1	2.47	0.63
2:C:13:LYS:O	2:C:1183:ALA:N	2.32	0.63
2:C:989:LEU:O	2:C:997:TRP:NE1	2.31	0.63
5:F:551:LEU:HD11	5:F:598:LEU:CD2	2.26	0.63
1:A:207:THR:HG23	1:A:208:ASN:O	1.99	0.63
2:C:1329:GLU:O	2:C:1332:SER:OG	2.09	0.63
2:C:618:GLN:NE2	3:D:770:LEU:HD13	2.14	0.62
2:C:678:ARG:NH2	2:C:1071:GLY:O	2.33	0.62
3:D:1029:THR:OG1	3:D:1115:ILE:HD13	2.00	0.62
2:C:576:SER:OG	2:C:659:GLN:O	2.18	0.62
2:C:1111:GLN:O	2:C:1115:THR:OG1	2.08	0.62
3:D:70:CYS:SG	3:D:74:LYS:N	2.71	0.62
1:A:92:VAL:O	1:A:148:ARG:NH2	2.32	0.61
1:B:156:SER:O	1:B:160:HIS:ND1	2.25	0.61
2:C:1251:TYR:OH	3:D:348:ASP:OD2	2.14	0.61
2:C:1269:ARG:N	9:2:15:DC:OP1	2.33	0.61
1:A:131:CYS:SG	1:A:132:HIS:N	2.73	0.61
2:C:563:THR:OG1	2:C:569:ILE:O	2.09	0.61
2:C:13:LYS:NZ	2:C:1149:TYR:O	2.34	0.61
5:F:397:ARG:NH2	8:1:73:DG:OP1	2.33	0.60
7:I:306:VAL:O	7:I:309:SER:OG	2.12	0.60
3:D:1080:ILE:HD11	3:D:1121:LEU:HD11	1.83	0.60
5:F:114:GLU:O	5:F:118:ASP:N	2.33	0.60
2:C:318:SER:OG	2:C:320:ASP:OD1	2.15	0.60
2:C:843:THR:OG1	2:C:846:GLY:O	2.10	0.60
3:D:1040:MET:SD	3:D:1078:LEU:N	2.74	0.60
3:D:1318:SER:OG	3:D:1342:ASP:OD2	2.19	0.59
1:B:58:GLU:OE1	1:B:170:ARG:NH2	2.32	0.59
2:C:257:ALA:N	2:C:260:LYS:O	2.36	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:632:ALA:O	3:D:635:SER:OG	2.16	0.58
6:H:51:ILE:HD13	6:H:84:ALA:HA	1.84	0.58
3:D:1330:ARG:O	3:D:1333:THR:OG1	2.17	0.58
2:C:253:PHE:CZ	2:C:287:VAL:HG12	2.38	0.58
2:C:816:ILE:N	2:C:1075:VAL:O	2.35	0.58
1:A:71:LYS:NZ	1:A:139:SER:O	2.19	0.58
3:D:552:ILE:O	3:D:567:THR:OG1	2.08	0.58
6:H:13:TRP:O	6:H:16:SER:OG	2.21	0.57
2:C:93:SER:OG	2:C:126:GLU:OE1	2.20	0.57
3:D:78:LEU:O	5:F:568:ASN:ND2	2.28	0.57
1:A:38:THR:OG1	1:B:45:ARG:NE	2.35	0.57
5:F:160:ASP:O	5:F:163:THR:OG1	2.13	0.57
3:D:275:ARG:NH1	3:D:298:MET:O	2.37	0.57
8:1:38:DC:N3	9:2:51:DG:N1	2.49	0.57
2:C:1339:LEU:HD22	3:D:17:PHE:CE2	2.40	0.56
3:D:804:ALA:HB1	3:D:916:GLY:HA3	1.86	0.56
6:G:106:ILE:HD12	6:G:110:PRO:HA	1.88	0.56
1:B:131:CYS:SG	1:B:132:HIS:N	2.77	0.56
2:C:848:GLU:HG2	2:C:888:THR:HG22	1.87	0.56
2:C:658:GLN:O	2:C:661:VAL:HG22	2.05	0.56
2:C:866:ASP:OD2	2:C:944:ARG:NH1	2.37	0.56
3:D:108:ALA:HB3	3:D:279:LEU:HD23	1.87	0.56
3:D:857:LEU:HD12	3:D:858:VAL:HG13	1.87	0.56
6:G:53:ASP:OD1	6:G:56:GLY:N	2.38	0.56
1:B:215:GLU:OE2	1:B:219:ARG:NH2	2.38	0.55
2:C:394:ARG:NH2	8:1:72:DT:O2	2.39	0.55
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.88	0.55
5:F:541:ARG:O	5:F:544:THR:OG1	2.19	0.55
1:B:158:ARG:HD2	1:B:172:LEU:HD11	1.88	0.55
2:C:788:SER:OG	2:C:795:ALA:O	2.23	0.55
5:F:281:ARG:NH1	5:F:284:GLU:OE1	2.39	0.55
1:A:32:GLU:HA	1:A:198:LEU:HD23	1.88	0.55
1:A:158:ARG:O	1:A:162:GLU:N	2.39	0.55
3:D:694:SER:OG	3:D:738:ARG:NH2	2.39	0.55
5:F:88:GLU:HA	5:F:91:ILE:HD12	1.87	0.55
2:C:406:ASN:ND2	2:C:413:GLU:O	2.40	0.55
2:C:4:SER:O	2:C:8:LYS:N	2.38	0.55
2:C:10:ARG:NH2	2:C:790:ASP:O	2.40	0.55
3:D:536:LEU:O	3:D:539:SER:OG	2.17	0.55
6:G:175:ILE:HD12	6:G:176:VAL:N	2.21	0.55
1:A:104:LYS:NZ	1:A:105:SER:O	2.39	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:23:TYR:HB3	6:H:92:CYS:O	2.07	0.54
3:D:128:LEU:O	3:D:157:GLN:NE2	2.40	0.54
2:C:1276:TRP:CE2	3:D:801:VAL:HG11	2.43	0.54
3:D:631:TYR:O	3:D:635:SER:N	2.41	0.54
8:1:48:DC:H42	9:2:41:DG:H22	1.56	0.54
2:C:990:ASP:OD1	2:C:991:LYS:N	2.40	0.54
6:H:49:VAL:HG23	6:H:86:VAL:HG22	1.89	0.54
1:B:211:ILE:HG21	1:B:216:ALA:HB2	1.90	0.54
2:C:700:VAL:HG21	2:C:1114:GLU:HG3	1.89	0.54
3:D:559:ALA:O	3:D:561:GLY:N	2.40	0.54
2:C:253:PHE:HZ	2:C:287:VAL:HG12	1.72	0.54
1:A:152:TYR:OH	2:C:1059:ARG:NH2	2.41	0.53
2:C:261:VAL:HG11	2:C:264:GLU:OE2	2.07	0.53
1:A:34:GLY:O	1:A:38:THR:OG1	2.18	0.53
6:G:175:ILE:HD12	6:G:176:VAL:HG13	1.91	0.53
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.42	0.53
3:D:93:THR:HG22	3:D:94:GLN:H	1.72	0.53
3:D:968:ASN:OD1	3:D:972:LYS:N	2.42	0.53
1:B:158:ARG:O	1:B:162:GLU:N	2.42	0.53
2:C:199:ASP:O	8:1:76:DG:N2	2.42	0.53
2:C:65:ASN:OD1	2:C:66:SER:N	2.41	0.53
3:D:424:ASN:HD22	3:D:425:ARG:N	2.07	0.53
5:F:585:GLU:HG2	9:2:47:DC:H41	1.74	0.52
3:D:478:LEU:CD2	4:E:47:THR:HG23	2.40	0.52
3:D:536:LEU:O	3:D:540:GLY:N	2.38	0.52
5:F:151:VAL:HB	5:F:161:LEU:HD23	1.91	0.52
2:C:1146:GLN:HB2	2:C:1161:LEU:HD12	1.90	0.52
2:C:483:ASP:OD1	2:C:484:LEU:N	2.42	0.52
1:B:118:ASP:OD1	1:B:119:GLY:N	2.42	0.52
1:A:15:ASP:OD1	1:A:16:ILE:N	2.43	0.52
6:H:45:GLY:N	6:H:66:GLN:OE1	2.43	0.52
3:D:576:ARG:NH1	3:D:593:ASN:O	2.42	0.52
7:I:298:LYS:NZ	9:2:56:DT:OP1	2.40	0.51
1:A:118:ASP:OD1	1:A:119:GLY:N	2.42	0.51
3:D:527:LEU:HD22	3:D:533:ALA:HB2	1.92	0.51
2:C:1259:LEU:O	2:C:1267:GLY:N	2.44	0.51
3:D:319:SER:OG	9:2:21:DA:N6	2.43	0.51
1:A:12:ARG:N	1:A:29:GLU:O	2.40	0.51
2:C:397:LEU:O	2:C:398:SER:OG	2.12	0.51
6:H:60:ILE:HB	6:H:175:ILE:HD13	1.93	0.51
2:C:104:ILE:HD12	2:C:116:ASP:HB3	1.91	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1045:THR:O	3:D:1067:ARG:NE	2.40	0.51
3:D:1164:SER:O	3:D:1176:VAL:N	2.44	0.51
5:F:505:ILE:HG22	5:F:505:ILE:O	2.11	0.51
1:B:15:ASP:OD1	1:B:16:ILE:N	2.43	0.51
2:C:675:ASP:OD1	2:C:676:ALA:N	2.44	0.51
2:C:1088:ASP:OD1	2:C:1092:THR:N	2.44	0.51
3:D:848:VAL:HG22	3:D:858:VAL:HG22	1.92	0.51
6:G:39:LEU:HD23	6:G:102:PHE:CZ	2.46	0.51
2:C:719:LYS:O	2:C:779:ARG:NE	2.43	0.51
3:D:530:PRO:O	3:D:533:ALA:HB3	2.11	0.51
7:I:304:LYS:HD2	7:I:307:LEU:HD11	1.93	0.51
2:C:18:ARG:NH2	2:C:620:ASN:O	2.45	0.50
5:F:551:LEU:CD1	5:F:598:LEU:HD21	2.36	0.50
2:C:1129:ASN:OD1	2:C:1177:ARG:NH2	2.44	0.50
2:C:246:LEU:HD23	2:C:249:GLU:OE1	2.11	0.50
3:D:1080:ILE:HD12	3:D:1115:ILE:HD11	1.93	0.50
6:H:183:VAL:HA	6:H:186:ILE:HG22	1.94	0.50
3:D:1089:LEU:HD22	3:D:1094:ASP:O	2.11	0.50
2:C:594:VAL:HG11	2:C:650:VAL:HB	1.94	0.50
1:B:155:ALA:N	1:B:174:ASP:OD1	2.41	0.50
2:C:720:ARG:NH1	2:C:745:GLU:OE2	2.44	0.50
3:D:24:LEU:HD12	3:D:232:ASN:HB3	1.93	0.50
6:H:135:ALA:HB3	6:H:136:PHE:CD2	2.47	0.50
2:C:389:PHE:HB3	2:C:420:LEU:HD12	1.94	0.49
3:D:140:TYR:O	3:D:297:ARG:NE	2.38	0.49
3:D:1229:VAL:O	3:D:1233:ILE:HD12	2.12	0.49
1:B:67:GLU:OE1	1:B:67:GLU:N	2.40	0.49
3:D:342:LEU:HD21	3:D:1352:ILE:HG23	1.94	0.49
1:B:135:ASP:OD1	1:B:136:GLU:N	2.45	0.49
5:F:573:LEU:HD11	5:F:584:ARG:O	2.12	0.49
2:C:211:ARG:NH1	2:C:357:ASN:O	2.46	0.49
3:D:353:SER:OG	3:D:354:VAL:N	2.44	0.49
2:C:205:PRO:O	2:C:208:ILE:HG22	2.12	0.49
2:C:540:ARG:NH2	2:C:568:ASN:HD21	2.10	0.49
1:A:155:ALA:N	1:A:174:ASP:OD1	2.40	0.49
1:B:207:THR:OG1	1:B:208:ASN:N	2.46	0.49
2:C:701:GLY:N	2:C:1182:ILE:O	2.44	0.49
3:D:1029:THR:O	3:D:1118:GLY:N	2.43	0.49
2:C:69:GLN:OE1	2:C:101:ARG:NH2	2.45	0.49
2:C:242:VAL:HG22	2:C:283:LYS:NZ	2.28	0.49
3:D:1063:ASP:O	3:D:1067:ARG:NH1	2.45	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:256:ASP:OD1	3:D:257:GLY:N	2.45	0.48
3:D:267:ASP:OD1	3:D:270:ARG:NH2	2.44	0.48
3:D:1327:GLU:N	9:2:10:DA:OP1	2.44	0.48
4:E:10:VAL:HG21	4:E:16:ARG:HH11	1.78	0.48
5:F:311:THR:O	5:F:345:GLN:NE2	2.46	0.48
6:G:120:MET:CE	6:H:124:LEU:HD13	2.43	0.48
2:C:354:ASP:OD2	2:C:356:THR:OG1	2.23	0.48
3:D:22:ILE:HD11	3:D:1319:PHE:CE2	2.48	0.48
3:D:661:VAL:HG12	3:D:682:VAL:HG13	1.95	0.48
3:D:1162:ILE:HG23	3:D:1178:THR:HB	1.94	0.48
3:D:1319:PHE:O	3:D:1323:ALA:N	2.44	0.48
4:E:42:GLU:OE1	4:E:52:ARG:NH1	2.45	0.48
3:D:975:ILE:O	3:D:1000:GLY:N	2.45	0.48
3:D:1002:VAL:O	3:D:1019:ASN:N	2.46	0.48
2:C:840:SER:OG	2:C:1048:LYS:N	2.47	0.48
3:D:1368:ASP:OD1	3:D:1371:ARG:NH1	2.46	0.48
5:F:316:PHE:HZ	5:F:330:LEU:HD22	1.77	0.48
5:F:511:ILE:HG21	5:F:519:LEU:HD13	1.95	0.48
2:C:971:LEU:HD13	2:C:1021:LEU:HD21	1.96	0.48
2:C:854:ILE:HB	2:C:857:VAL:HG21	1.95	0.48
3:D:29:MET:SD	3:D:33:TRP:NE1	2.87	0.48
2:C:582:ASN:N	2:C:586:PHE:O	2.40	0.48
2:C:1219:GLU:OE2	3:D:634:ARG:NE	2.47	0.48
5:F:387:VAL:HG21	5:F:412:LEU:HD22	1.96	0.48
5:F:551:LEU:HD21	5:F:598:LEU:HD11	1.96	0.48
2:C:525:THR:HG21	2:C:687:ARG:CD	2.44	0.48
3:D:527:LEU:CD2	3:D:533:ALA:HB2	2.43	0.48
3:D:960:LEU:N	3:D:1007:ASP:OD1	2.46	0.47
5:F:407:GLU:HA	5:F:410:ILE:HD12	1.96	0.47
3:D:702:GLN:O	3:D:718:SER:N	2.47	0.47
3:D:1019:ASN:OD1	3:D:1020:TRP:N	2.48	0.47
5:F:387:VAL:CG2	5:F:412:LEU:HD22	2.44	0.47
1:A:64:VAL:HG11	1:A:171:LEU:HD11	1.97	0.47
1:B:90:VAL:HG11	1:B:146:VAL:HG11	1.96	0.47
3:D:816:THR:OG1	3:D:883:ARG:NH2	2.45	0.47
4:E:6:VAL:HG12	4:E:6:VAL:O	2.15	0.47
2:C:561:ILE:O	2:C:680:LEU:HD12	2.14	0.47
3:D:1111:ASP:OD1	3:D:1112:GLY:N	2.48	0.47
5:F:86:SER:O	5:F:89:SER:OG	2.18	0.47
2:C:292:ILE:HD13	2:C:322:LEU:HD13	1.96	0.47
3:D:262:THR:O	5:F:507:MET:N	2.41	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:48:DC:N4	9:2:41:DG:H22	2.13	0.47
1:A:107:ILE:HG23	1:A:133:LEU:O	2.14	0.47
5:F:330:LEU:O	5:F:330:LEU:HD23	2.15	0.47
6:G:137:LEU:O	6:G:142:ARG:NH2	2.44	0.47
3:D:38:VAL:HG13	3:D:55:GLY:O	2.15	0.47
3:D:865:HIS:ND1	3:D:867:GLN:OE1	2.46	0.47
5:F:124:GLU:OE1	5:F:128:ASN:ND2	2.48	0.47
5:F:337:VAL:O	5:F:340:ALA:HB3	2.14	0.47
6:H:115:ARG:O	6:H:118:ALA:HB3	2.15	0.47
3:D:1342:ASP:OD1	3:D:1343:GLU:N	2.44	0.47
3:D:968:ASN:OD1	3:D:971:GLY:N	2.48	0.47
5:F:242:HIS:O	5:F:246:GLN:N	2.43	0.47
1:B:113:ALA:N	1:B:126:PRO:O	2.48	0.47
3:D:519:ASN:OD1	3:D:520:ALA:N	2.48	0.47
3:D:960:LEU:HD11	3:D:982:LEU:HD12	1.97	0.47
3:D:1040:MET:HE3	3:D:1046:ILE:HG21	1.97	0.46
6:G:121:ALA:HB2	6:H:76:PHE:CD2	2.50	0.46
2:C:217:THR:HG23	2:C:351:LEU:HD13	1.97	0.46
2:C:972:PHE:O	2:C:994:ARG:NH2	2.48	0.46
1:B:22:THR:OG1	1:B:207:THR:O	2.33	0.46
2:C:206:ALA:O	2:C:209:ILE:HG22	2.15	0.46
5:F:278:ASP:O	5:F:282:THR:OG1	2.16	0.46
6:H:113:LEU:HD23	6:H:113:LEU:H	1.80	0.46
2:C:1160:ASP:OD1	2:C:1161:LEU:N	2.49	0.46
3:D:70:CYS:SG	3:D:73:GLY:N	2.89	0.46
3:D:623:GLN:O	3:D:627:THR:HG22	2.15	0.46
2:C:461:GLU:OE2	2:C:465:ARG:NH2	2.49	0.46
3:D:824:PRO:HB2	3:D:826:ILE:HG23	1.98	0.46
3:D:1215:GLU:N	3:D:1215:GLU:OE1	2.48	0.46
2:C:521:LEU:O	2:C:525:THR:HG22	2.16	0.46
2:C:739:ASP:OD1	2:C:740:GLU:N	2.45	0.46
6:G:139:VAL:O	6:G:143:ILE:HG22	2.16	0.46
2:C:373:GLY:O	5:F:87:VAL:HG13	2.16	0.46
3:D:1288:ALA:O	3:D:1292:LEU:HD22	2.16	0.46
7:I:275:ILE:CG2	7:I:281:LEU:HD22	2.46	0.46
2:C:133:ASN:O	2:C:527:LYS:NZ	2.47	0.45
3:D:986:ASP:OD1	3:D:990:ARG:N	2.49	0.45
2:C:148:GLN:NE2	2:C:535:PRO:O	2.47	0.45
2:C:339:ASN:O	2:C:343:HIS:N	2.46	0.45
6:G:42:ILE:HA	6:G:94:VAL:HG22	1.97	0.45
2:C:441:GLU:OE1	2:C:441:GLU:N	2.49	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:453:ILE:CD1	2:C:587:LEU:HD21	2.47	0.45
2:C:1324:ASN:OD1	2:C:1325:VAL:N	2.50	0.45
2:C:561:ILE:O	2:C:561:ILE:HG22	2.16	0.45
5:F:526:THR:HG23	5:F:526:THR:O	2.17	0.45
8:1:72:DT:OP1	8:1:73:DG:N2	2.48	0.45
2:C:1247:SER:OG	2:C:1248:THR:N	2.49	0.45
3:D:809:VAL:HG22	3:D:894:VAL:HG23	1.98	0.45
4:E:10:VAL:HG21	4:E:16:ARG:NH1	2.32	0.45
3:D:740:LEU:O	3:D:762:ASN:ND2	2.50	0.45
9:2:54:DT:H2'	9:2:55:DT:H72	1.99	0.45
3:D:825:VAL:HG22	3:D:833:GLU:HB3	1.99	0.44
6:H:61:LEU:HD21	13:H:301:CMP:C6	2.52	0.44
2:C:104:ILE:HD12	2:C:116:ASP:CB	2.46	0.44
2:C:314:ASN:OD1	2:C:352:ARG:NH2	2.51	0.44
2:C:1122:LYS:NZ	2:C:1126:ASP:OD1	2.49	0.44
5:F:600:HIS:O	5:F:602:SER:N	2.40	0.44
6:G:124:LEU:HD21	13:H:301:CMP:C5	2.52	0.44
4:E:60:ASN:OD1	4:E:61:ASN:N	2.50	0.44
6:G:120:MET:HE1	6:H:124:LEU:HD13	1.99	0.44
1:A:58:GLU:HG2	1:A:172:LEU:HD12	2.00	0.44
3:D:1109:LEU:HD23	3:D:1113:VAL:HG11	2.00	0.44
6:H:158:THR:O	7:I:287:VAL:HG23	2.18	0.44
2:C:1292:THR:O	2:C:1297:ASP:N	2.44	0.44
3:D:418:GLU:OE2	4:E:3:ARG:NE	2.50	0.44
3:D:1004:ALA:N	3:D:1017:VAL:O	2.44	0.44
6:G:39:LEU:HD12	6:G:70:ILE:O	2.18	0.44
6:H:75:LEU:HD23	6:H:99:TYR:CE1	2.53	0.44
3:D:661:VAL:CG1	3:D:682:VAL:HG13	2.48	0.44
3:D:1032:SER:OG	3:D:1117:SER:N	2.51	0.44
5:F:399:LEU:HD12	5:F:447:ALA:HB2	2.00	0.44
2:C:241:LEU:HD23	2:C:277:LEU:HD21	2.00	0.43
3:D:139:LEU:HD21	3:D:185:ILE:HD12	1.99	0.43
3:D:502:PRO:HB3	3:D:506:VAL:HG11	1.99	0.43
2:C:915:ASP:OD1	2:C:916:SER:N	2.50	0.43
5:F:396:ASN:O	5:F:398:GLY:N	2.45	0.43
3:D:478:LEU:CB	4:E:20:VAL:HG13	2.49	0.43
2:C:840:SER:HG	2:C:1048:LYS:H	1.67	0.43
3:D:1208:ASP:OD1	3:D:1209:VAL:N	2.51	0.43
3:D:572:THR:HG21	3:D:589:TYR:OH	2.18	0.43
2:C:766:ASN:OD1	2:C:767:GLN:N	2.49	0.43
1:B:166:ARG:CZ	1:B:172:LEU:HD22	2.48	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1115:ILE:HG21	3:D:1121:LEU:HD23	2.01	0.43
5:F:309:ASN:ND2	5:F:314:THR:OG1	2.51	0.43
2:C:94:ALA:HB2	2:C:129:LEU:HD11	2.00	0.43
2:C:525:THR:HG21	2:C:687:ARG:HD3	1.99	0.43
2:C:836:LEU:O	2:C:1052:VAL:N	2.47	0.43
3:D:973:LEU:HB3	3:D:1003:LEU:HD12	2.01	0.43
3:D:948:SER:O	3:D:949:SER:OG	2.28	0.43
3:D:552:ILE:HD12	3:D:553:THR:N	2.33	0.42
3:D:1027:VAL:HG12	3:D:1027:VAL:O	2.19	0.42
6:H:146:THR:HG21	6:H:175:ILE:HG21	2.00	0.42
2:C:819:SER:OG	2:C:820:GLU:N	2.52	0.42
3:D:97:VAL:HG21	3:D:101:ARG:CZ	2.49	0.42
3:D:1058:SER:OG	3:D:1109:LEU:O	2.33	0.42
5:F:399:LEU:HD23	5:F:400:GLN:HB3	2.01	0.42
2:C:104:ILE:HD13	2:C:484:LEU:HB3	2.02	0.42
1:A:218:ARG:NE	1:B:233:ASP:O	2.53	0.42
2:C:198:ILE:O	2:C:201:ARG:N	2.51	0.42
2:C:1277:ALA:O	2:C:1280:ALA:HB3	2.19	0.42
2:C:646:SER:OG	2:C:649:GLN:OE1	2.21	0.42
2:C:855:PRO:O	2:C:857:VAL:HG23	2.20	0.42
2:C:1120:ALA:HB2	2:C:1199:LEU:CD2	2.50	0.42
2:C:122:VAL:HG13	2:C:490:GLN:CD	2.40	0.42
3:D:517:CYS:SG	3:D:518:VAL:N	2.93	0.42
3:D:591:ILE:HG23	3:D:592:VAL:HG13	2.02	0.42
5:F:443:ILE:O	5:F:447:ALA:HB3	2.19	0.42
7:I:275:ILE:HG22	7:I:281:LEU:HD22	2.00	0.42
2:C:164:THR:OG1	2:C:167:SER:OG	2.28	0.42
2:C:568:ASN:ND2	10:3:1:GTP:O2B	2.53	0.42
3:D:885:VAL:HG11	3:D:1255:VAL:HB	2.02	0.42
3:D:1252:HIS:O	3:D:1255:VAL:HG12	2.20	0.42
6:H:135:ALA:HB3	6:H:136:PHE:CE2	2.55	0.42
2:C:871:VAL:HG12	2:C:872:TYR:O	2.20	0.42
3:D:956:GLY:N	3:D:1010:GLN:OE1	2.52	0.42
1:A:33:ARG:NH1	1:B:49:SER:O	2.51	0.41
2:C:104:ILE:HG22	2:C:115:LYS:HD3	2.02	0.41
2:C:663:VAL:O	2:C:666:SER:OG	2.20	0.41
2:C:805:MET:N	2:C:1098:LEU:O	2.52	0.41
3:D:1046:ILE:HG22	3:D:1061:VAL:HA	2.02	0.41
3:D:1175:LEU:HB2	3:D:1190:ILE:HD12	2.02	0.41
5:F:85:SER:OG	5:F:86:SER:N	2.53	0.41
6:G:76:PHE:CE2	6:H:118:ALA:HB2	2.55	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:106:ILE:CG2	6:H:112:ILE:HD11	2.50	0.41
3:D:48:THR:O	3:D:50:LYS:N	2.53	0.41
2:C:75:LEU:HD22	2:C:127:ILE:HD11	2.00	0.41
2:C:638:SER:O	2:C:640:GLY:N	2.53	0.41
2:C:1127:LYS:NZ	2:C:1203:ASP:OD2	2.47	0.41
3:D:93:THR:HG22	3:D:94:GLN:N	2.35	0.41
3:D:568:SER:OG	3:D:569:LEU:N	2.52	0.41
7:I:294:ASN:HD21	8:1:35:DA:H5''	1.85	0.41
9:2:56:DT:H2'	9:2:57:DT:H71	2.02	0.41
3:D:1040:MET:CE	3:D:1046:ILE:HG21	2.50	0.41
5:F:385:ARG:HA	5:F:388:ILE:HG22	2.02	0.41
9:2:15:DC:N4	9:2:16:DG:O6	2.54	0.41
2:C:137:VAL:O	2:C:138:ILE:HD13	2.21	0.41
2:C:1002:LEU:CD1	2:C:1011:LEU:HD11	2.50	0.41
1:A:41:ASN:ND2	2:C:1215:GLY:O	2.49	0.41
2:C:233:ARG:NH1	2:C:238:GLN:OE1	2.53	0.41
2:C:1105:SER:OG	3:D:731:ARG:NH2	2.53	0.41
3:D:450:HIS:O	3:D:453:VAL:HG22	2.20	0.41
5:F:436:ARG:O	5:F:440:THR:CB	2.68	0.41
2:C:230:PHE:HB3	2:C:237:LEU:HD11	2.03	0.41
2:C:700:VAL:O	2:C:700:VAL:HG23	2.21	0.41
2:C:1002:LEU:HD13	2:C:1011:LEU:HD11	2.02	0.41
2:C:1340:GLU:OE1	3:D:1341:ARG:NH2	2.49	0.41
9:2:53:DC:H2''	9:2:54:DT:H71	2.02	0.41
2:C:878:THR:N	2:C:881:ASP:OD2	2.51	0.41
2:C:1099:ASN:ND2	3:D:505:ASP:OD2	2.54	0.41
3:D:165:TYR:O	3:D:169:LEU:N	2.53	0.41
3:D:528:THR:HG22	3:D:532:GLU:OE2	2.21	0.41
3:D:804:ALA:HB1	3:D:916:GLY:CA	2.51	0.41
3:D:822:MET:SD	3:D:838:ARG:NH2	2.94	0.41
3:D:1173:ARG:O	3:D:1190:ILE:N	2.47	0.41
5:F:124:GLU:O	5:F:128:ASN:ND2	2.53	0.41
5:F:585:GLU:CG	9:2:47:DC:H41	2.34	0.41
6:G:124:LEU:HD21	13:H:301:CMP:C6	2.56	0.41
8:1:7:DG:H2''	8:1:8:DT:H71	2.02	0.41
2:C:965:GLN:O	2:C:969:ALA:HB2	2.21	0.41
2:C:256:GLU:O	2:C:285:ILE:HG23	2.21	0.40
2:C:592:ARG:NH2	2:C:601:ASP:OD1	2.53	0.40
2:C:1003:THR:HG22	2:C:1004:ASP:H	1.86	0.40
2:C:1336:ASN:N	3:D:23:ALA:O	2.54	0.40
3:D:965:SER:OG	3:D:973:LEU:HD11	2.21	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ASN:O	1:A:128:HIS:NE2	2.53	0.40
3:D:1371:ARG:O	3:D:1375:ALA:N	2.40	0.40
9:2:22:DT:C2	9:2:23:DT:H73	2.57	0.40
1:B:91:ARG:NH1	1:B:122:GLU:OE1	2.51	0.40
2:C:120:GLN:HE21	2:C:489:PRO:HG2	1.87	0.40
2:C:696:ASP:OD2	2:C:827:ARG:NH2	2.54	0.40
2:C:1297:ASP:OD2	2:C:1318:GLY:N	2.55	0.40
3:D:828:GLY:O	3:D:995:TYR:OH	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	A	228/329 (69%)	203 (89%)	25 (11%)	0	100	100
1	B	226/329 (69%)	208 (92%)	18 (8%)	0	100	100
2	C	1338/1342 (100%)	1219 (91%)	115 (9%)	4 (0%)	41	75
3	D	1331/1407 (95%)	1190 (89%)	140 (10%)	1 (0%)	51	84
4	E	77/91 (85%)	76 (99%)	1 (1%)	0	100	100
5	F	493/628 (78%)	438 (89%)	53 (11%)	2 (0%)	34	71
6	G	199/210 (95%)	193 (97%)	6 (3%)	0	100	100
6	H	199/210 (95%)	190 (96%)	9 (4%)	0	100	100
7	I	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
All	All	4164/4621 (90%)	3788 (91%)	369 (9%)	7 (0%)	50	79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	399	ALA
2	C	1004	ASP
2	C	1005	GLU
5	F	156	ALA
2	C	398	SER
3	D	121	PRO
5	F	166	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	198/286 (69%)	197 (100%)	1 (0%)	88	93
1	B	196/286 (68%)	196 (100%)	0	100	100
2	C	1155/1157 (100%)	1152 (100%)	3 (0%)	92	95
3	D	1120/1168 (96%)	1116 (100%)	4 (0%)	91	94
4	E	67/75 (89%)	67 (100%)	0	100	100
5	F	439/554 (79%)	435 (99%)	4 (1%)	78	87
6	G	172/181 (95%)	171 (99%)	1 (1%)	86	91
6	H	173/181 (96%)	171 (99%)	2 (1%)	71	83
7	I	66/66 (100%)	66 (100%)	0	100	100
All	All	3586/3954 (91%)	3571 (100%)	15 (0%)	91	94

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
2	C	1022	LYS
2	C	1147	ARG
2	C	1246	ARG
3	D	214	ARG
3	D	424	ASN
3	D	700	ASN
3	D	798	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	F	93	ARG
5	F	105	MET
5	F	554	ARG
5	F	557	LYS
6	G	142	ARG
6	H	26	LYS
6	H	122	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	341	ASN
3	D	805	GLN
3	D	1195	GLN
5	F	128	ASN
5	F	309	ASN
6	G	80	GLN
6	H	125	GLN
7	I	268	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	3	1/3 (33%)	1 (100%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	3	3	G

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	CMP	H	301	-	22,25,25	1.41	5 (22%)	24,39,39	1.66	5 (20%)
13	CMP	G	301	-	22,25,25	1.41	4 (18%)	24,39,39	1.77	8 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CMP	H	301	-	-	0/0/31/31	0/4/4/4
13	CMP	G	301	-	-	0/0/31/31	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	301	CMP	P-O3'	3.09	1.62	1.57
13	G	301	CMP	P-O5'	3.04	1.61	1.57
13	H	301	CMP	P-O3'	3.03	1.62	1.57
13	H	301	CMP	P-O5'	2.83	1.60	1.57
13	G	301	CMP	C5-C4	2.32	1.47	1.40
13	H	301	CMP	O5'-C5'	-2.28	1.42	1.46
13	H	301	CMP	C5-C4	2.21	1.46	1.40
13	G	301	CMP	O5'-C5'	-2.19	1.43	1.46
13	H	301	CMP	O3'-C3'	-2.11	1.41	1.44

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G	301	CMP	N3-C2-N1	-3.93	122.53	128.68
13	H	301	CMP	N3-C2-N1	-3.62	123.02	128.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	H	301	CMP	O2P-P-O1P	3.35	119.24	108.73
13	G	301	CMP	O3'-C3'-C2'	3.21	118.76	115.61
13	H	301	CMP	O5'-P-O1P	-3.20	103.06	110.44
13	G	301	CMP	C4-C5-N7	-2.62	106.67	109.40
13	H	301	CMP	O3'-C3'-C2'	2.56	118.11	115.61
13	G	301	CMP	O2P-P-O1P	2.54	116.69	108.73
13	G	301	CMP	C2-N1-C6	2.53	123.08	118.75
13	H	301	CMP	C4-C5-N7	-2.40	106.90	109.40
13	G	301	CMP	O2P-P-O3'	2.40	112.63	107.04
13	G	301	CMP	C1'-N9-C4	-2.16	122.84	126.64
13	G	301	CMP	O5'-P-O1P	-2.03	105.76	110.44

There are no chirality outliers.

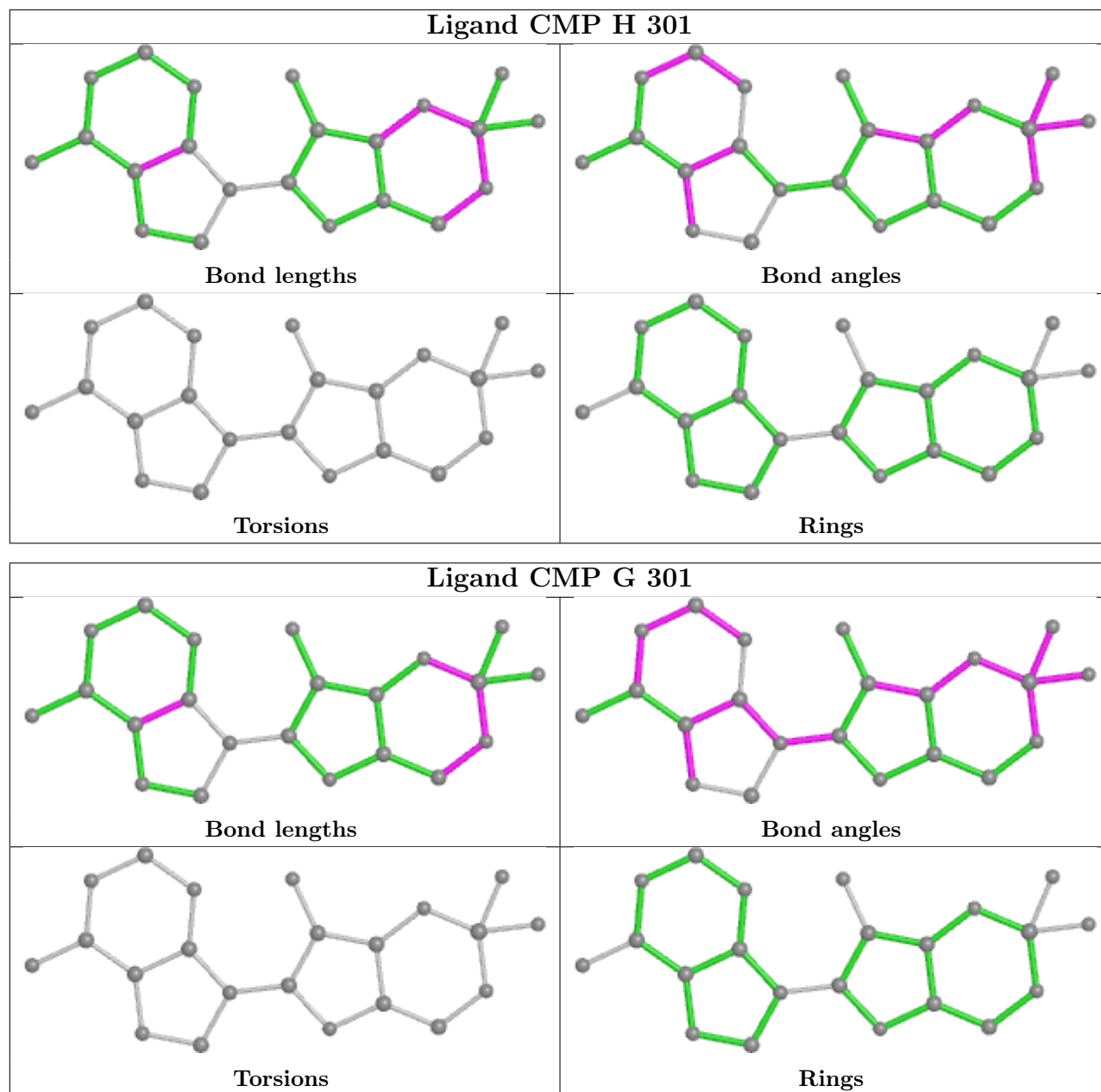
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	H	301	CMP	4	0
13	G	301	CMP	2	0

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



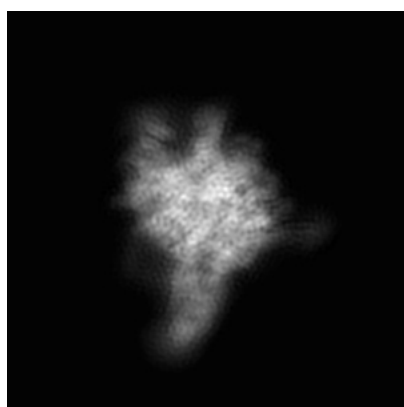
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7059. These allow visual inspection of the internal detail of the map and identification of artifacts.

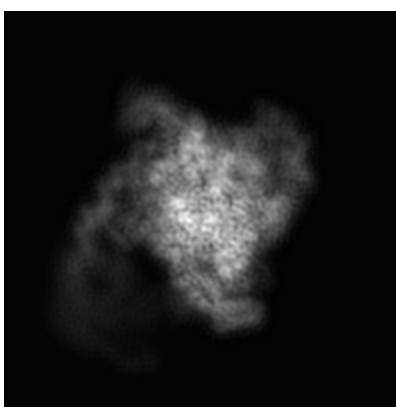
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

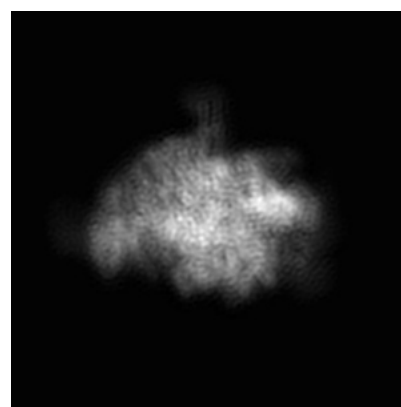
#### 6.1.1 Primary map



X



Y

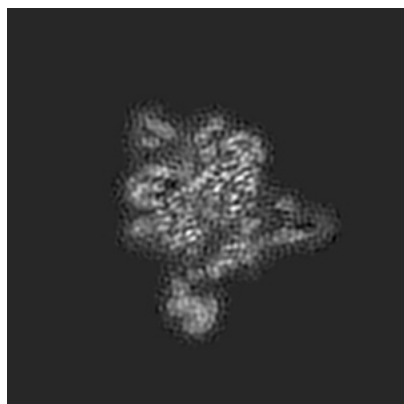


Z

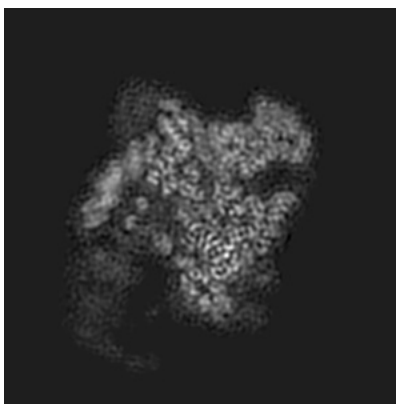
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

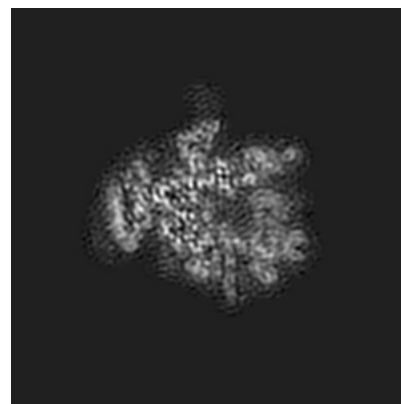
#### 6.2.1 Primary map



X Index: 100



Y Index: 100

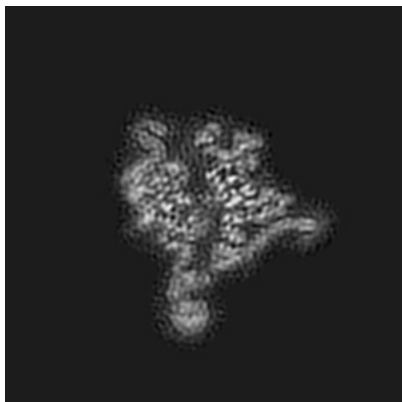


Z Index: 100

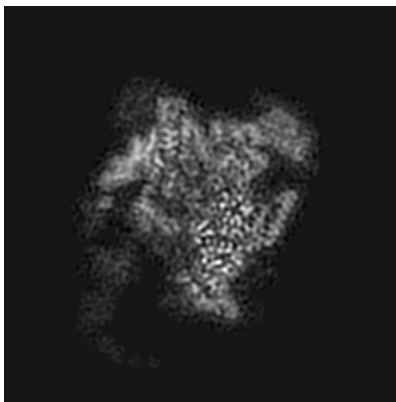
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

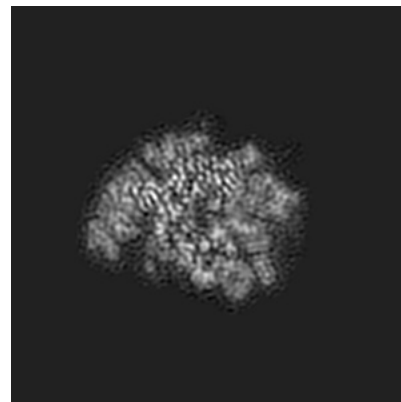
### 6.3.1 Primary map



X Index: 94



Y Index: 104



Z Index: 107

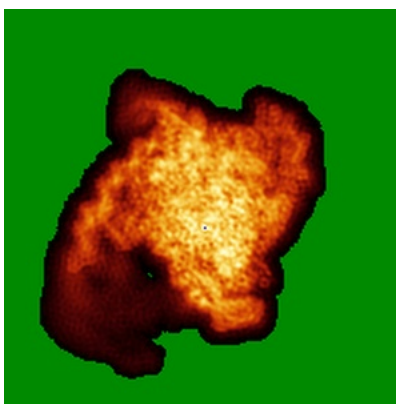
The images above show the largest variance slices of the map in three orthogonal directions.

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

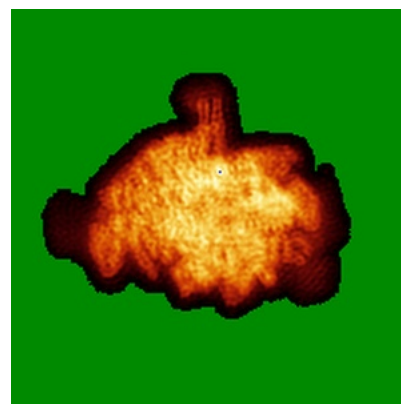
### 6.4.1 Primary map



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 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

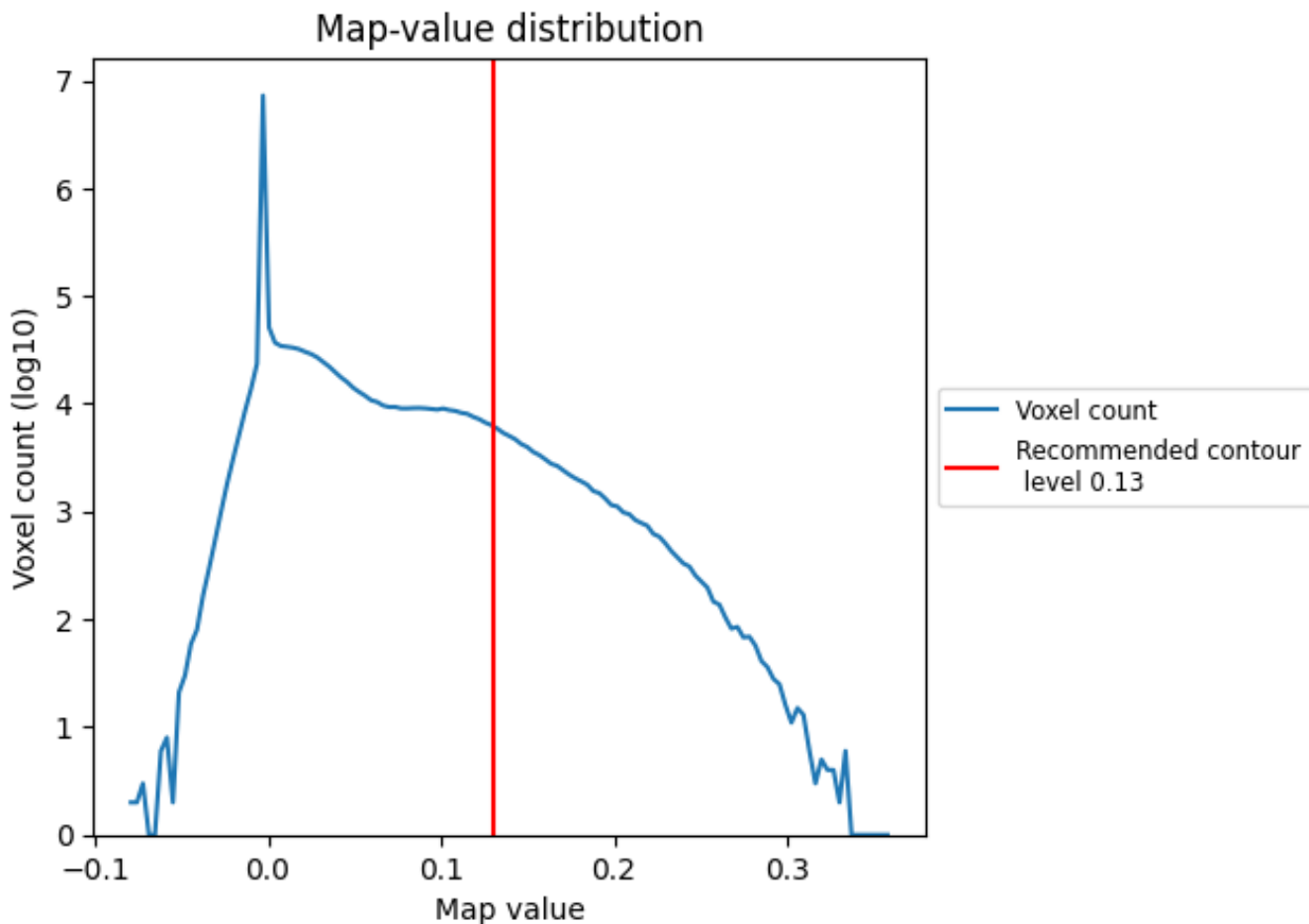
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

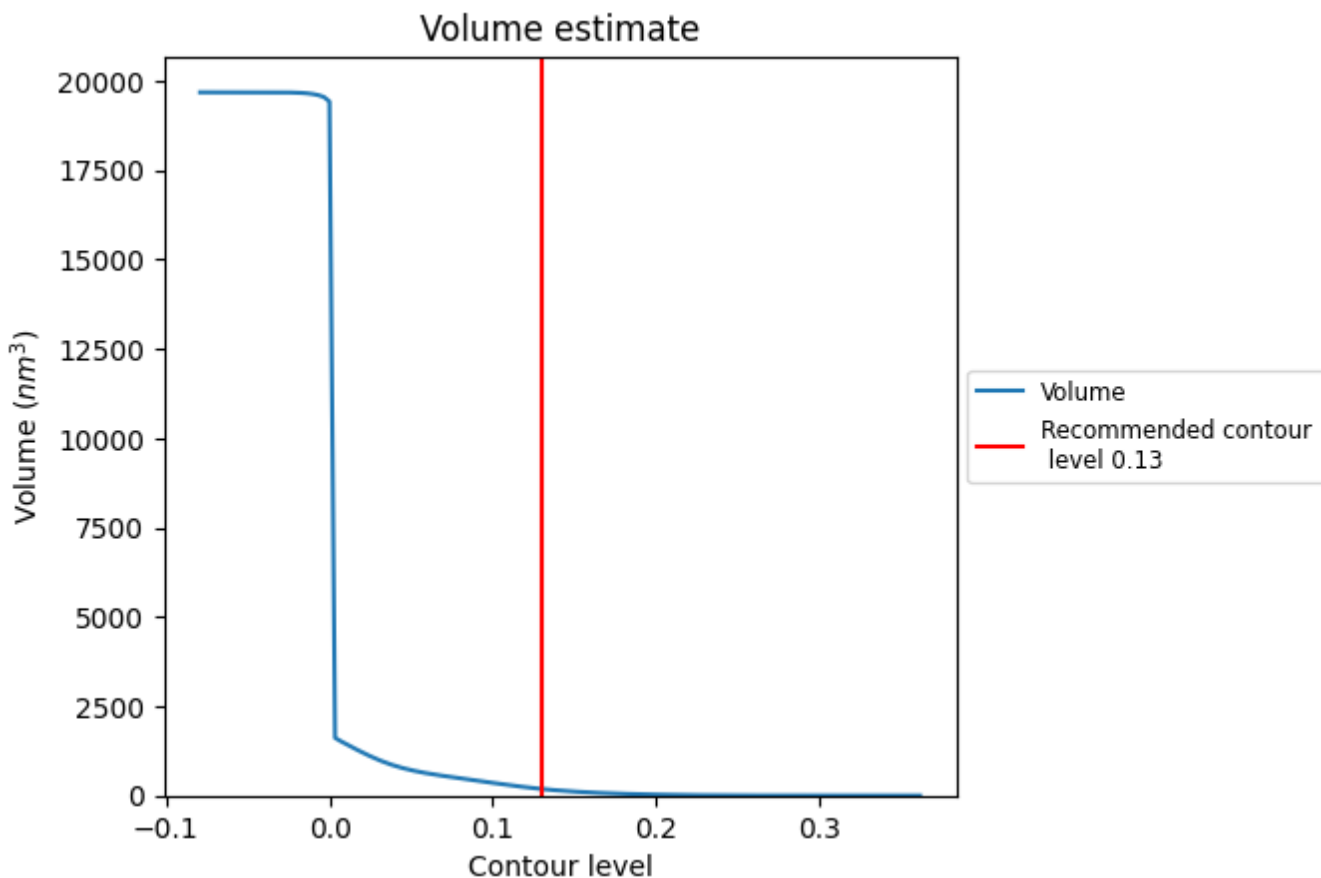
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

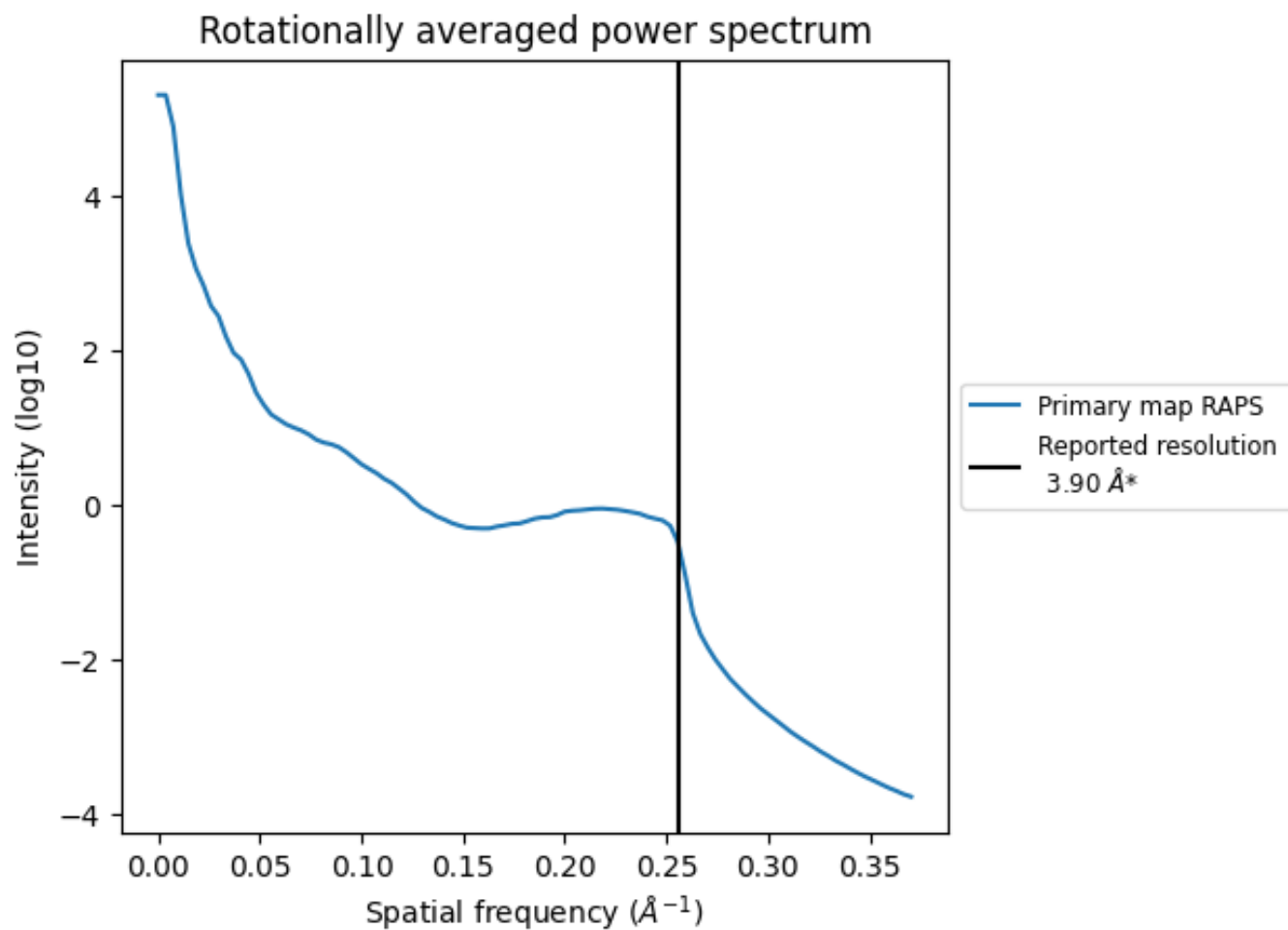
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 185 nm<sup>3</sup>; this corresponds to an approximate mass of 167 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](#)

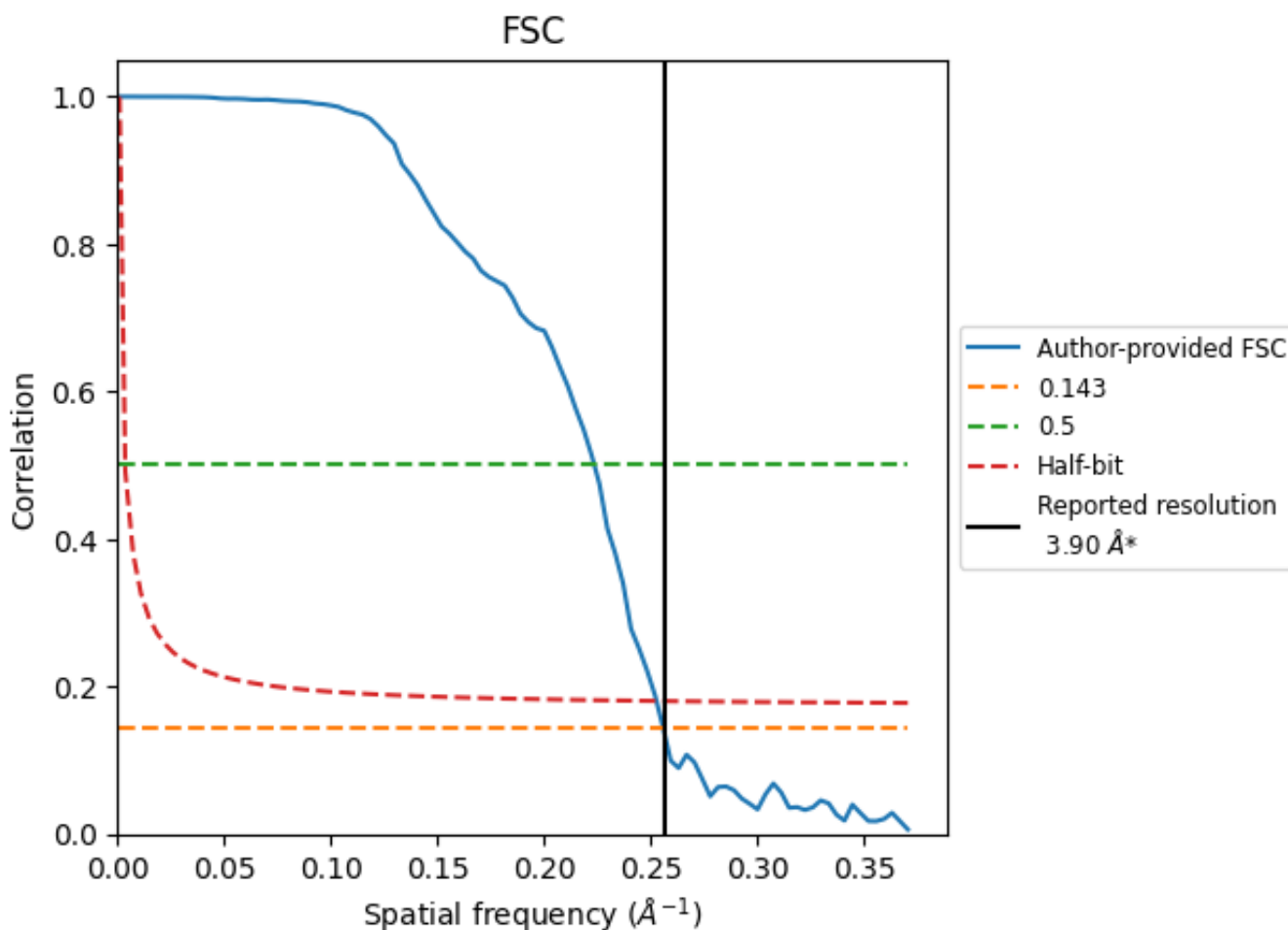


\*Reported resolution corresponds to spatial frequency of  $0.256 \text{\AA}^{-1}$

## 8 Fourier-Shell correlation [\(i\)](#)

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

### 8.1 FSC [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.91	4.47	3.96
Unmasked-calculated*	-	-	-

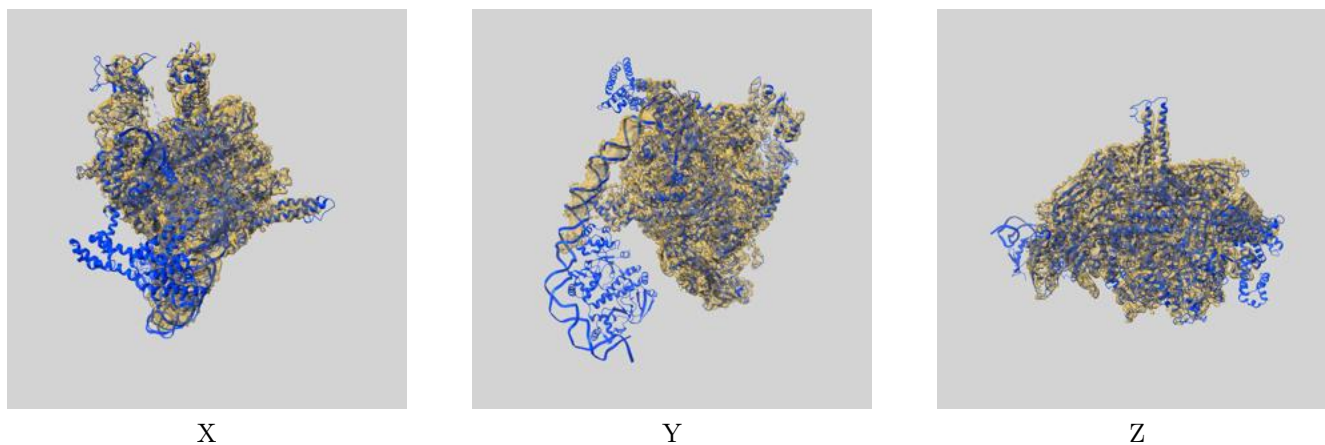
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



## 9 Map-model fit [i](#)

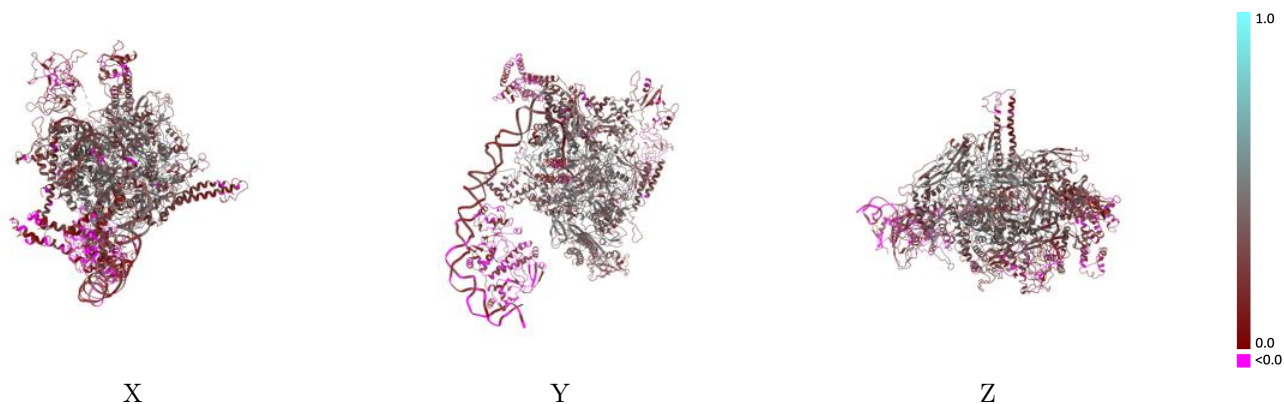
This section contains information regarding the fit between EMDB map EMD-7059 and PDB model 6B6H. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlay [i](#)



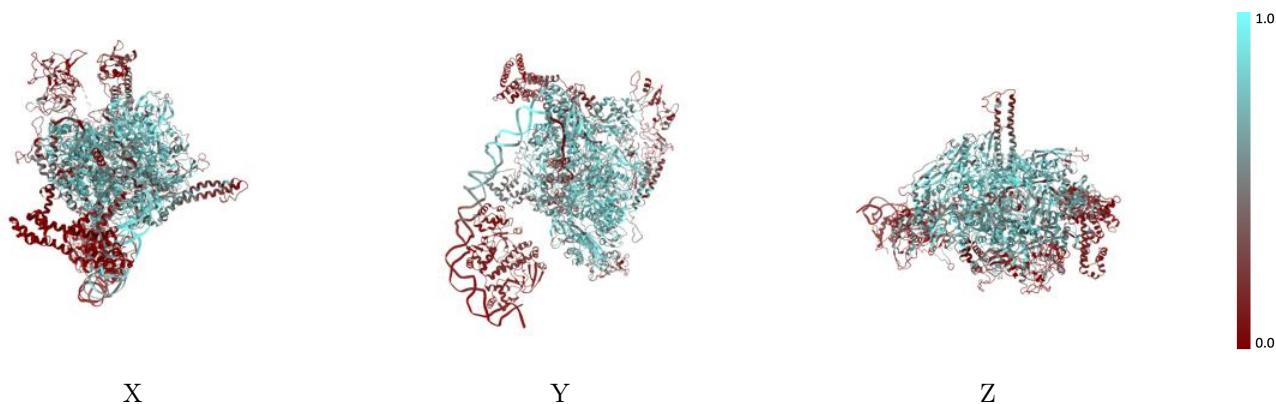
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



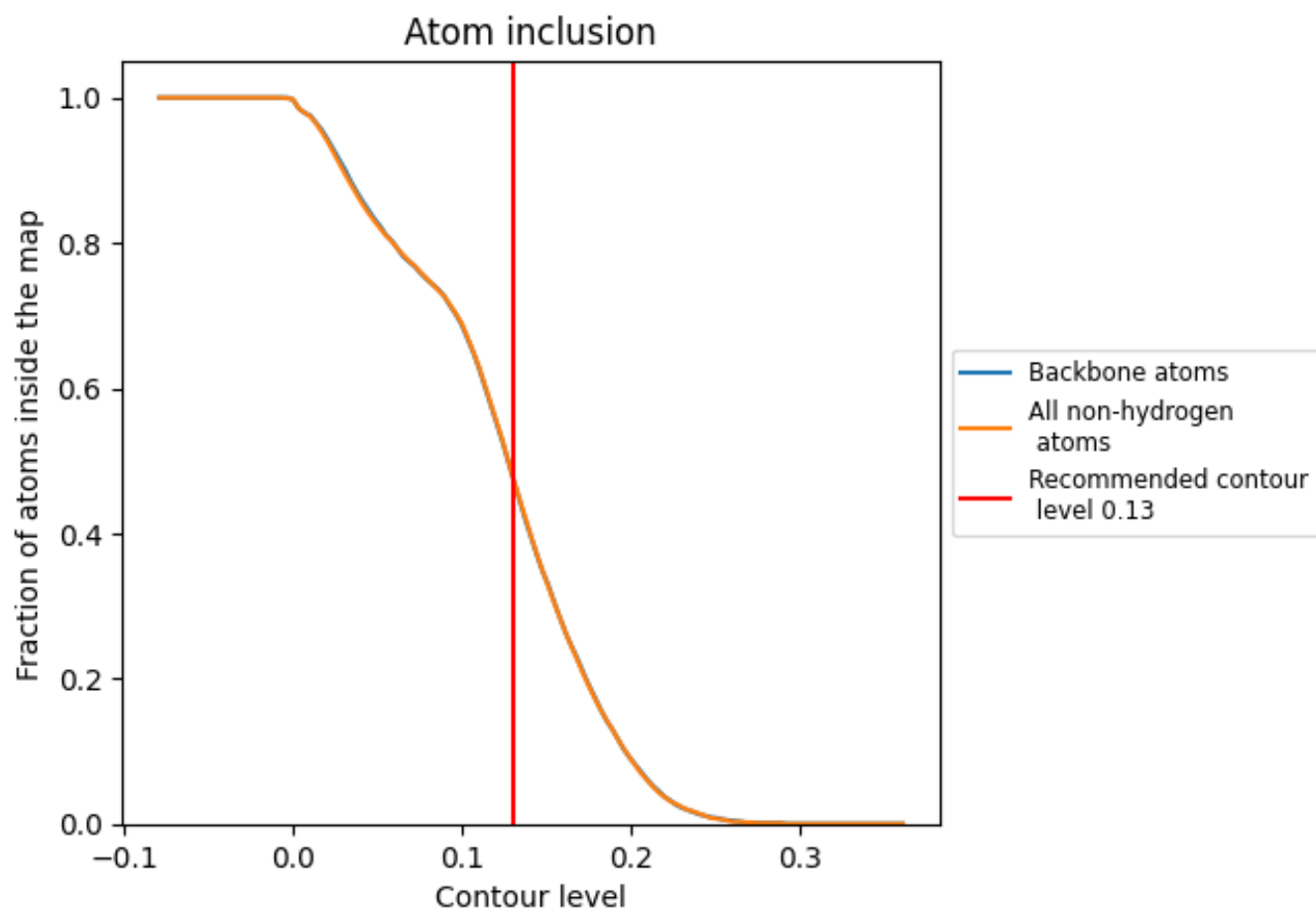
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).



























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 48% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4800	 0.2830
1	 0.3960	 0.1720
2	 0.3900	 0.1820
3	 0.4160	 0.4040
A	 0.6450	 0.3730
B	 0.5030	 0.3280
C	 0.6540	 0.3620
D	 0.5790	 0.3370
E	 0.0110	 0.2460
F	 0.3250	 0.2140
G	 0.0000	 0.0160
H	 0.0000	 0.0160
I	 0.0140	 0.1000

