



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:53 PM UTC

PDB ID : 6S1N / pdb_00006s1n
EMDB ID : EMD-10081
Title : Human polymerase delta holoenzyme Conformer 2
Authors : Lancey, C.; Hamdan, S.M.; De Biasio, A.
Deposited on : 2019-06-19
Resolution : 4.86 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

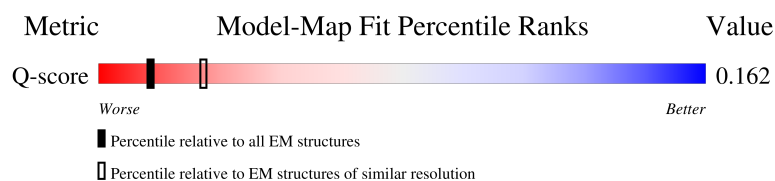
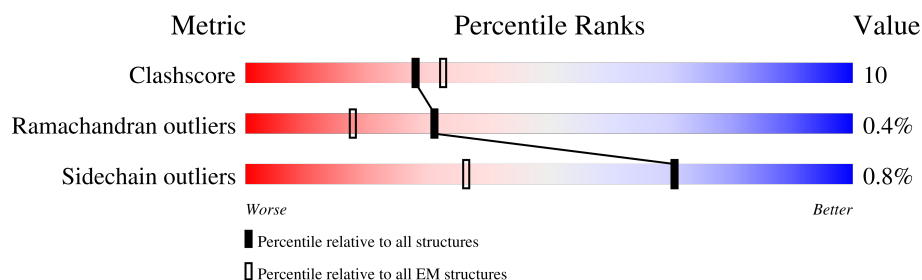
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.86 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1276 (4.36 - 5.36)

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

Mol	Chain	Length	Quality of chain
1	A	1107	15% 78% 13% 9%
2	B	469	15% 78% 13% 8%
3	C	474	9% 28% 70%
4	D	137	36% 11% 52%

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Mol	Chain	Length	Quality of chain
5	E	264	49% 70% 25% 5%
5	F	264	23% 80% 14% 6%
5	G	264	40% 73% 22% 6%
6	P	25	• 64% 24% • 8%
7	T	38	37% 34% 29%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 19726 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 polymerase delta catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1010	Total	C	N	O	S	1	0
			7926	5028	1405	1447	46		

- Molecule 2 is a protein called DNA polymerase delta subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	431	Total	C	N	O	S	0	0
			3304	2103	553	630	18		

- Molecule 3 is a protein called DNA polymerase delta subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	143	Total	C	N	O	S	0	0
			1130	715	196	214	5		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	MET	-	initiating methionine	UNP Q15054
C	-6	TRP	-	expression tag	UNP Q15054
C	-5	SER	-	expression tag	UNP Q15054
C	-4	HIS	-	expression tag	UNP Q15054
C	-3	PRO	-	expression tag	UNP Q15054
C	-2	GLN	-	expression tag	UNP Q15054
C	-1	PHE	-	expression tag	UNP Q15054
C	0	GLU	-	expression tag	UNP Q15054
C	1	LYS	-	expression tag	UNP Q15054

- Molecule 4 is a protein called DNA polymerase delta subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	66	Total	C	N	O	S	0	0
			554	359	97	94	4		

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-29	MET	-	initiating methionine	UNP Q9HCU8
D	-28	HIS	-	expression tag	UNP Q9HCU8
D	-27	HIS	-	expression tag	UNP Q9HCU8
D	-26	HIS	-	expression tag	UNP Q9HCU8
D	-25	HIS	-	expression tag	UNP Q9HCU8
D	-24	HIS	-	expression tag	UNP Q9HCU8
D	-23	HIS	-	expression tag	UNP Q9HCU8
D	-22	SER	-	expression tag	UNP Q9HCU8
D	-21	ARG	-	expression tag	UNP Q9HCU8
D	-20	ALA	-	expression tag	UNP Q9HCU8
D	-19	TRP	-	expression tag	UNP Q9HCU8
D	-18	ARG	-	expression tag	UNP Q9HCU8
D	-17	HIS	-	expression tag	UNP Q9HCU8
D	-16	PRO	-	expression tag	UNP Q9HCU8
D	-15	GLN	-	expression tag	UNP Q9HCU8
D	-14	PHE	-	expression tag	UNP Q9HCU8
D	-13	GLY	-	expression tag	UNP Q9HCU8
D	-12	GLY	-	expression tag	UNP Q9HCU8
D	-11	HIS	-	expression tag	UNP Q9HCU8
D	-10	HIS	-	expression tag	UNP Q9HCU8
D	-9	HIS	-	expression tag	UNP Q9HCU8
D	-8	HIS	-	expression tag	UNP Q9HCU8
D	-7	HIS	-	expression tag	UNP Q9HCU8
D	-6	HIS	-	expression tag	UNP Q9HCU8
D	-5	GLU	-	expression tag	UNP Q9HCU8
D	-4	ASN	-	expression tag	UNP Q9HCU8
D	-3	LEU	-	expression tag	UNP Q9HCU8
D	-2	TYR	-	expression tag	UNP Q9HCU8
D	-1	PHE	-	expression tag	UNP Q9HCU8
D	0	GLN	-	expression tag	UNP Q9HCU8
D	1	SER	-	expression tag	UNP Q9HCU8

- Molecule 5 is a protein called Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	251	Total	C	N	O	S	0	0
			1924	1211	314	383	16		
5	F	249	Total	C	N	O	S	0	0
			1913	1205	312	380	16		
5	G	249	Total	C	N	O	S	0	0
			1913	1204	314	379	16		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP P12004
E	-1	PRO	-	expression tag	UNP P12004
E	0	HIS	-	expression tag	UNP P12004
F	-2	GLY	-	expression tag	UNP P12004
F	-1	PRO	-	expression tag	UNP P12004
F	0	HIS	-	expression tag	UNP P12004
G	-2	GLY	-	expression tag	UNP P12004
G	-1	PRO	-	expression tag	UNP P12004
G	0	HIS	-	expression tag	UNP P12004

- Molecule 6 is a DNA chain called DNA primer.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	23	Total	C	N	O	P	0	0
			469	225	84	137	23		

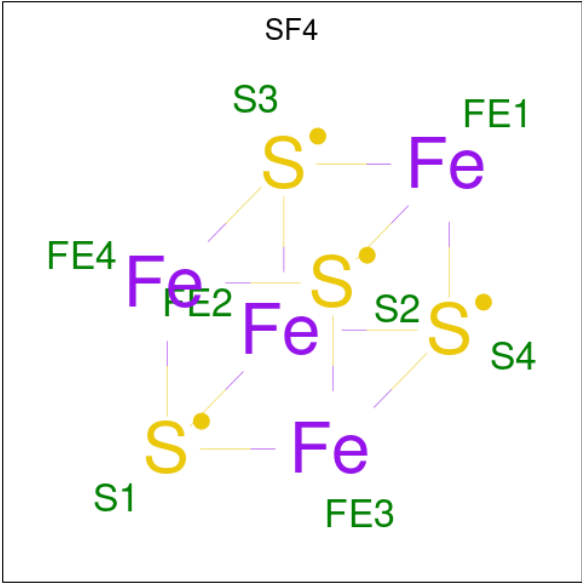
- Molecule 7 is a DNA chain called DNA template.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	27	Total	C	N	O	P	0	0
			555	266	100	162	27		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

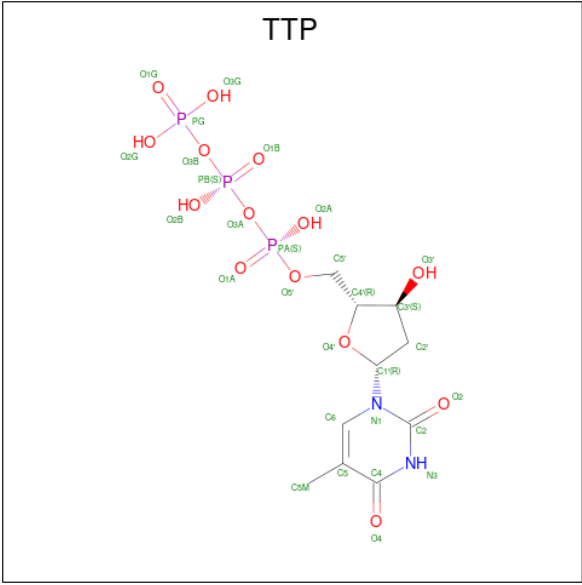
Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	Zn	0
			1	1	

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

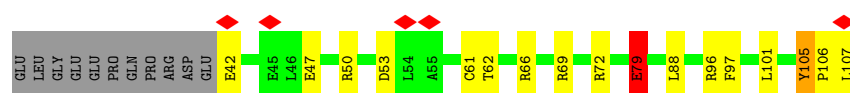


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
9	A	1	8	4	4	0

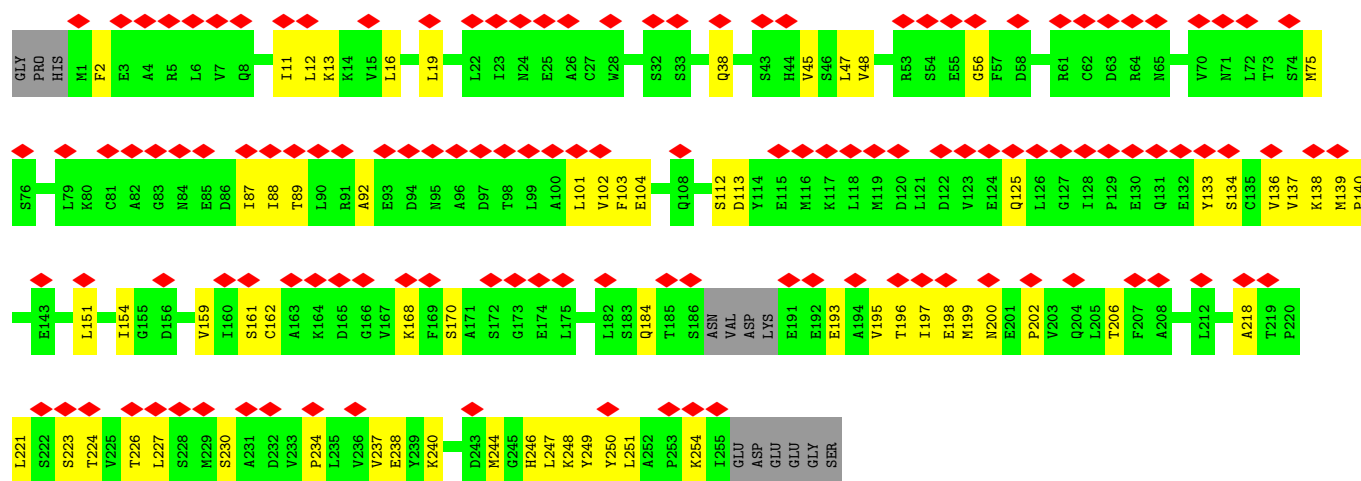
- Molecule 10 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).



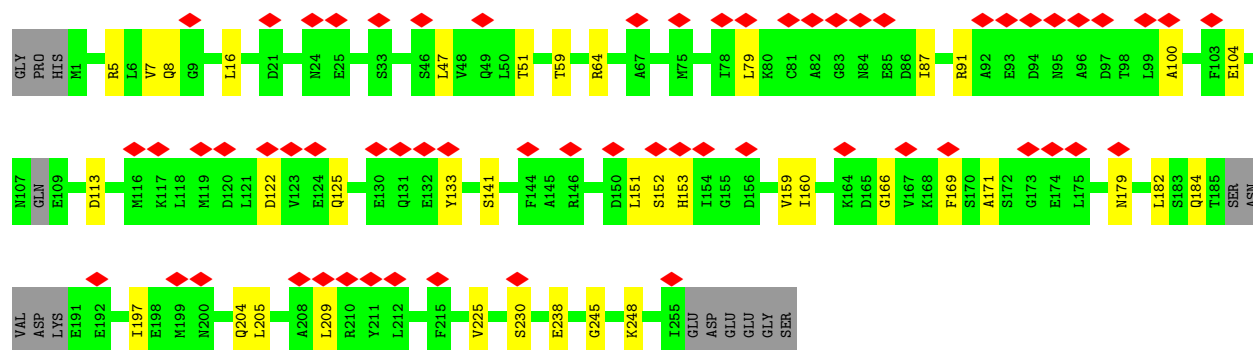
Mol	Chain	Residues	Atoms					AltConf
10	T	1	Total 29	C 10	N 2	O 14	P 3	0



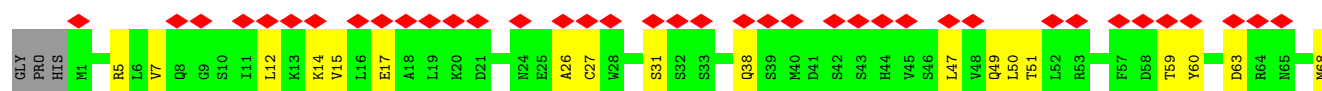
Chain E: 49% 70% 25% 5%

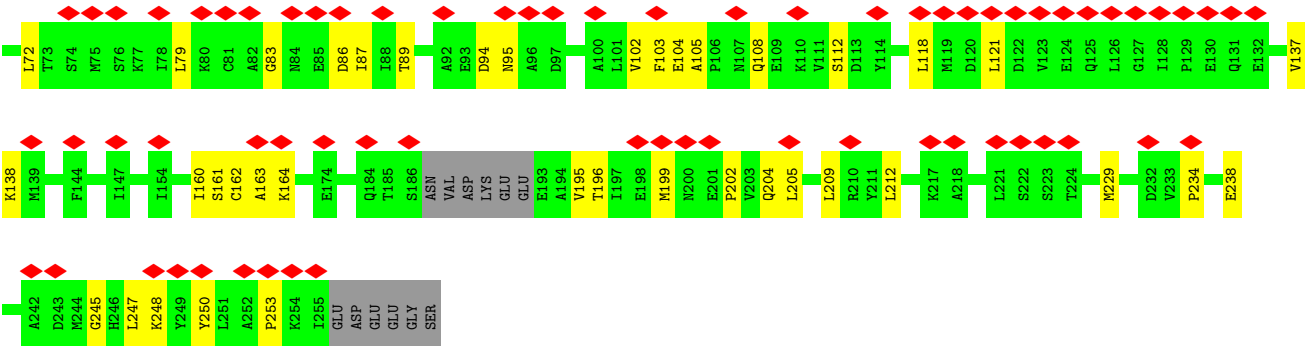


Chain F: 23% 80% 14% 6%



Chain G:

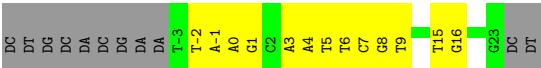




• Molecule 6: DNA primer



• Molecule 7: DNA template



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	32282	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 ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	600	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.095	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, TTP, DOC, 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	0.36	0/8094	0.70	11/10971 (0.1%)
2	B	0.38	0/3380	0.64	1/4604 (0.0%)
3	C	0.27	0/1149	0.57	0/1553
4	D	0.44	0/574	0.90	0/783
5	E	0.26	0/1949	0.59	0/2632
5	F	0.30	0/1937	0.61	0/2614
5	G	0.26	0/1938	0.58	0/2617
6	P	0.45	0/505	0.89	0/777
7	T	0.38	0/622	0.82	0/958
All	All	0.34	0/20148	0.67	12/27509 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	179	ALA	N-CA-C	7.54	119.50	111.28
1	A	1098	ARG	N-CA-C	-7.06	103.66	111.36
1	A	592	GLY	N-CA-C	6.69	119.03	110.20
1	A	1024	ALA	N-CA-C	6.62	118.49	111.28
1	A	82	PRO	CA-C-N	6.05	132.43	120.94
1	A	82	PRO	C-N-CA	6.05	132.43	120.94
1	A	1091	ASP	N-CA-C	5.47	117.32	111.36
1	A	1079	PHE	CA-C-N	5.46	131.96	121.54
1	A	1079	PHE	C-N-CA	5.46	131.96	121.54
1	A	1099	PHE	N-CA-C	-5.29	103.55	110.53
1	A	1022	GLN	N-CA-C	5.09	119.47	113.16
1	A	421	LEU	N-CA-C	5.06	118.94	112.87

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7926	0	7967	162	0
2	B	3304	0	3255	57	0
3	C	1130	0	1138	7	0
4	D	554	0	537	12	0
5	E	1924	0	1930	35	0
5	F	1913	0	1922	24	0
5	G	1913	0	1928	34	0
6	P	469	0	261	9	0
7	T	555	0	307	67	0
8	A	1	0	0	0	0
9	A	8	0	0	1	0
10	T	29	0	10	0	0
All	All	19726	0	19255	372	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (372) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:4:DA:C2'	7:T:5:DT:H72	1.18	1.56
7:T:4:DA:H2''	7:T:5:DT:C5	1.41	1.51
7:T:4:DA:H2''	7:T:5:DT:C7	1.35	1.51
1:A:861:VAL:CG1	1:A:985:ARG:HD3	1.40	1.51
1:A:688:GLY:HA2	1:A:691:LEU:CD2	1.43	1.49
1:A:861:VAL:HG11	1:A:985:ARG:NE	1.27	1.48
1:A:861:VAL:CG1	1:A:985:ARG:CD	1.93	1.44
1:A:861:VAL:HG11	1:A:985:ARG:CZ	1.45	1.43
1:A:861:VAL:HG13	1:A:985:ARG:CD	1.49	1.43
1:A:968:ARG:NH2	7:T:6:DT:H3'	1.42	1.34
7:T:4:DA:C2'	7:T:5:DT:C7	1.93	1.32
2:B:308:GLN:O	2:B:329:THR:HB	1.28	1.29
7:T:6:DT:H2''	7:T:7:DC:C5	1.71	1.26
7:T:3:DA:H2''	7:T:4:DA:H5''	1.20	1.19
7:T:6:DT:H2''	7:T:7:DC:C6	1.76	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:6:DT:C2'	7:T:7:DC:C5	2.31	1.12
2:B:330:ASN:HB3	2:B:331:PRO:CD	1.77	1.11
1:A:861:VAL:CG1	1:A:985:ARG:NE	2.07	1.11
1:A:688:GLY:O	1:A:691:LEU:HG	1.53	1.09
1:A:808:ARG:NH2	7:T:6:DT:H5''	1.68	1.07
2:B:308:GLN:O	2:B:329:THR:CB	2.04	1.05
1:A:688:GLY:HA2	1:A:691:LEU:HD21	1.06	1.05
1:A:688:GLY:HA2	1:A:691:LEU:HD23	1.37	1.03
2:B:330:ASN:HB3	2:B:331:PRO:HD3	1.02	1.01
1:A:688:GLY:CA	1:A:691:LEU:CD2	2.38	1.00
1:A:861:VAL:CG1	1:A:985:ARG:CZ	2.38	1.00
7:T:4:DA:H2''	7:T:5:DT:C6	1.96	1.00
2:B:308:GLN:OE1	2:B:330:ASN:ND2	1.95	0.98
7:T:4:DA:C2'	7:T:5:DT:C5	2.35	0.96
7:T:15:DT:H2''	7:T:16:DG:C8	2.02	0.95
1:A:688:GLY:CA	1:A:691:LEU:HD21	1.96	0.93
1:A:968:ARG:NH2	7:T:6:DT:C3'	2.32	0.93
1:A:861:VAL:HG11	1:A:985:ARG:CD	1.76	0.92
1:A:968:ARG:HH21	7:T:6:DT:H3'	1.30	0.92
1:A:861:VAL:HG13	1:A:985:ARG:HD2	1.48	0.91
7:T:6:DT:C2'	7:T:7:DC:C6	2.51	0.90
1:A:808:ARG:CZ	7:T:6:DT:H5''	2.03	0.89
1:A:861:VAL:HG12	1:A:985:ARG:HD3	1.54	0.88
7:T:4:DA:H2'	7:T:5:DT:H72	0.87	0.86
2:B:295:MET:HG3	2:B:328:VAL:HG23	1.56	0.86
1:A:861:VAL:HG11	1:A:985:ARG:NH1	1.91	0.86
1:A:968:ARG:HH21	7:T:7:DC:P	1.98	0.85
1:A:808:ARG:HH22	7:T:6:DT:H4'	1.42	0.85
6:P:24:DG:H2''	6:P:25:DOC:H5'	1.57	0.85
1:A:164:LEU:HB3	1:A:190:VAL:HG11	1.59	0.84
2:B:309:GLN:C	2:B:329:THR:HG22	2.02	0.84
7:T:4:DA:H2'	7:T:5:DT:C7	1.84	0.83
2:B:310:PRO:N	2:B:329:THR:HG22	1.92	0.83
1:A:1026:CYS:O	1:A:1030:GLN:HG3	1.78	0.83
1:A:861:VAL:HG13	1:A:985:ARG:HD3	1.07	0.82
7:T:6:DT:H2''	7:T:7:DC:H5	1.41	0.81
7:T:6:DT:C2'	7:T:7:DC:H5	1.92	0.81
1:A:808:ARG:NH2	7:T:6:DT:C5'	2.44	0.81
6:P:11:DA:C2	7:T:16:DG:N2	2.49	0.81
7:T:3:DA:C2'	7:T:4:DA:H5''	2.07	0.80
1:A:188:LEU:HA	1:A:213:THR:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:15:DT:C2'	7:T:16:DG:C8	2.67	0.78
7:T:6:DT:C1'	7:T:7:DC:C5	2.67	0.78
2:B:330:ASN:CB	2:B:331:PRO:HD3	1.99	0.77
2:B:295:MET:HG2	2:B:329:THR:O	1.85	0.77
1:A:1028:PHE:CB	5:F:64:ARG:HG3	2.14	0.76
1:A:1038:GLN:HE22	2:B:273:VAL:HA	1.48	0.76
1:A:806:LYS:O	7:T:5:DT:H4'	1.85	0.76
7:T:3:DA:H2''	7:T:4:DA:C5'	2.11	0.75
1:A:861:VAL:CG1	1:A:985:ARG:NH1	2.50	0.74
1:A:968:ARG:HH21	7:T:6:DT:C3'	1.96	0.74
1:A:1078:ILE:HG13	9:A:1202:SF4:S1	2.26	0.74
1:A:188:LEU:N	1:A:188:LEU:HD23	2.04	0.73
7:T:6:DT:H2''	7:T:7:DC:H6	1.48	0.72
7:T:6:DT:C1'	7:T:7:DC:C6	2.71	0.72
1:A:164:LEU:HB3	1:A:190:VAL:HG21	1.72	0.72
7:T:6:DT:H1'	7:T:7:DC:C6	2.24	0.72
1:A:1011:CYS:O	1:A:1098:ARG:NH1	2.22	0.72
1:A:1018:VAL:CB	5:F:125:GLN:OE1	2.39	0.70
5:F:166:GLY:HA3	5:F:182:LEU:O	1.90	0.70
1:A:688:GLY:CA	1:A:691:LEU:HD23	2.13	0.69
1:A:834:ARG:NH1	6:P:23:DT:P	2.65	0.69
5:E:103:PHE:HB2	5:E:112:SER:HB2	1.75	0.69
1:A:968:ARG:HH22	7:T:6:DT:H3'	1.53	0.68
5:E:234:PRO:HA	5:E:251:LEU:O	1.94	0.68
1:A:1024:ALA:HB2	1:A:1098:ARG:HB3	1.76	0.68
7:T:5:DT:H1'	7:T:6:DT:H5'	1.76	0.68
2:B:310:PRO:CD	2:B:329:THR:CG2	2.73	0.67
1:A:1091:ASP:OD1	1:A:1092:GLN:N	2.29	0.66
2:B:310:PRO:N	2:B:329:THR:CG2	2.58	0.66
5:G:27:CYS:HB3	5:G:121:LEU:HD21	1.78	0.66
7:T:5:DT:H2''	7:T:6:DT:H5'	1.75	0.66
1:A:808:ARG:NH2	7:T:6:DT:H4'	2.11	0.66
5:F:166:GLY:HA2	5:F:197:ILE:HD13	1.77	0.65
2:B:310:PRO:HD3	2:B:329:THR:HG21	1.77	0.65
1:A:525:ARG:O	1:A:682:ARG:NH2	2.29	0.65
1:A:834:ARG:NH1	6:P:23:DT:OP2	2.30	0.64
2:B:296:PRO:CD	2:B:329:THR:HA	2.27	0.64
1:A:1002:LEU:HD21	5:F:47:LEU:HB2	1.78	0.64
2:B:309:GLN:C	2:B:329:THR:CG2	2.71	0.64
2:B:295:MET:HG3	2:B:328:VAL:CG2	2.24	0.64
5:E:238:GLU:HG3	5:E:248:LYS:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:47:LEU:HB3	5:G:250:TYR:HB2	1.80	0.63
1:A:981:ALA:O	1:A:985:ARG:HG3	1.98	0.63
2:B:296:PRO:HD2	2:B:329:THR:HA	1.80	0.62
5:E:87:ILE:HB	5:E:104:GLU:HB2	1.82	0.62
6:P:17:DA:N6	7:T:8:DG:O6	2.32	0.62
4:D:53:ASP:OD2	4:D:66:ARG:NH2	2.31	0.61
1:A:688:GLY:C	1:A:691:LEU:HG	2.24	0.61
2:B:310:PRO:HA	2:B:328:VAL:O	2.00	0.61
4:D:42:GLU:OE2	4:D:96:ARG:NH2	2.34	0.61
1:A:688:GLY:O	1:A:691:LEU:CG	2.41	0.61
2:B:73:TRP:NE1	2:B:175:ASP:OD2	2.33	0.60
1:A:674:LEU:HD13	1:A:686:LEU:HB2	1.82	0.60
1:A:583:GLY:O	1:A:725:ARG:NH1	2.34	0.60
1:A:1088:ASP:HA	1:A:1091:ASP:OD2	2.02	0.60
1:A:187:VAL:HG22	1:A:187:VAL:O	2.02	0.60
1:A:188:LEU:HD23	1:A:188:LEU:H	1.64	0.60
1:A:1030:GLN:N	1:A:1031:PRO:CD	2.65	0.60
1:A:834:ARG:NH1	6:P:23:DT:OP1	2.35	0.60
1:A:525:ARG:HG2	1:A:682:ARG:HH22	1.67	0.59
5:F:5:ARG:HB3	5:F:59:THR:HB	1.84	0.59
1:A:432:ARG:HH21	1:A:434:SER:HB2	1.66	0.59
7:T:5:DT:C2'	7:T:6:DT:H5'	2.32	0.59
5:E:226:THR:HB	5:E:238:GLU:HB2	1.83	0.59
1:A:1013:ILE:HD12	1:A:1024:ALA:HB1	1.84	0.59
4:D:61:CYS:SG	4:D:72:ARG:NH2	2.75	0.59
1:A:808:ARG:CZ	7:T:6:DT:C5'	2.79	0.59
1:A:186:ALA:HB3	1:A:188:LEU:CD2	2.33	0.59
5:E:133:TYR:HA	5:E:230:SER:HB2	1.85	0.58
1:A:357:LEU:HD11	1:A:374:GLU:HG2	1.85	0.58
1:A:1062:GLN:NE2	1:A:1068:ASP:O	2.37	0.58
6:P:17:DA:N6	7:T:8:DG:C6	2.72	0.58
5:G:238:GLU:HG3	5:G:248:LYS:HG2	1.85	0.58
1:A:986:GLY:O	1:A:990:ARG:N	2.36	0.58
1:A:806:LYS:HB2	7:T:5:DT:H5''	1.85	0.58
1:A:1039:LYS:O	1:A:1040:GLU:HG2	2.04	0.58
2:B:184:GLN:HB2	2:B:398:CYS:HB3	1.85	0.58
1:A:186:ALA:HB3	1:A:188:LEU:HD21	1.86	0.58
2:B:1:MET:HG2	2:B:441:ASN:HD22	1.69	0.57
5:G:104:GLU:HB3	5:G:108:GLN:HE22	1.69	0.57
5:E:237:VAL:HG22	5:E:249:TYR:HB2	1.86	0.57
1:A:161:MET:O	1:A:165:GLN:NE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:LEU:O	1:A:990:ARG:NH1	2.38	0.57
5:F:5:ARG:NH2	5:F:104:GLU:OE1	2.38	0.57
5:F:7:VAL:HA	5:F:87:ILE:HG23	1.86	0.57
1:A:1056:THR:HG23	1:A:1060:ARG:HH21	1.70	0.57
1:A:628:GLN:HB3	1:A:629:LYS:HD3	1.86	0.57
5:F:152:SER:HA	5:F:209:LEU:HD13	1.86	0.57
2:B:134:VAL:HG11	2:B:141:ARG:HH11	1.70	0.56
5:G:89:THR:HB	5:G:102:VAL:HB	1.87	0.56
2:B:309:GLN:HA	2:B:329:THR:HG21	1.86	0.56
7:T:8:DG:H2''	7:T:9:DT:C6	2.40	0.56
1:A:587:ILE:HD13	1:A:732:LYS:HD3	1.88	0.56
3:C:35:ASN:HA	3:C:38:LYS:HD2	1.88	0.56
1:A:968:ARG:NH1	7:T:6:DT:OP1	2.39	0.56
7:T:0:DA:H2'	7:T:1:DG:H8	1.71	0.56
1:A:1030:GLN:H	1:A:1031:PRO:CD	2.19	0.55
2:B:310:PRO:HD3	2:B:329:THR:CG2	2.35	0.55
5:E:139:MET:HE3	5:E:140:PRO:HD2	1.88	0.55
1:A:806:LYS:O	7:T:5:DT:H5''	2.06	0.55
1:A:808:ARG:NH2	7:T:6:DT:C4'	2.69	0.55
5:G:234:PRO:HA	5:G:253:PRO:HD3	1.87	0.55
1:A:153:PRO:HD2	1:A:158:PRO:HG2	1.88	0.55
1:A:539:THR:HA	1:A:558:GLN:HE21	1.69	0.55
5:F:113:ASP:OD1	5:F:113:ASP:N	2.40	0.55
5:E:113:ASP:OD1	5:E:113:ASP:N	2.40	0.55
1:A:1028:PHE:CB	5:F:64:ARG:CG	2.84	0.55
1:A:1027:GLU:HA	1:A:1030:GLN:CD	2.31	0.55
2:B:296:PRO:HD2	2:B:329:THR:CA	2.36	0.55
2:B:32:TYR:HH	2:B:332:TYR:HH	1.53	0.55
2:B:307:PRO:O	2:B:309:GLN:NE2	2.37	0.54
2:B:310:PRO:HG3	2:B:329:THR:HG23	1.90	0.54
1:A:1021:HIS:C	1:A:1021:HIS:CD2	2.85	0.54
5:E:47:LEU:HB3	5:E:250:TYR:HD2	1.72	0.54
5:E:89:THR:HB	5:E:102:VAL:HB	1.90	0.54
5:E:161:SER:HB3	5:E:168:LYS:HB2	1.90	0.54
7:T:15:DT:H2''	7:T:16:DG:H8	1.70	0.54
2:B:356:SER:OG	2:B:357:SER:N	2.40	0.54
4:D:66:ARG:NH1	4:D:97:PHE:O	2.41	0.54
5:G:162:CYS:O	5:G:202:PRO:HA	2.08	0.54
4:D:47:GLU:OE1	4:D:50:ARG:NH1	2.41	0.53
1:A:993:THR:O	5:F:122:ASP:HB2	2.08	0.53
2:B:298:GLU:HG3	2:B:347:GLN:HE21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:51:THR:O	5:G:245:GLY:HA3	2.08	0.53
3:C:110:ASP:OD1	3:C:110:ASP:N	2.42	0.53
5:E:2:PHE:HB3	5:E:92:ALA:HB3	1.91	0.53
5:G:137:VAL:HA	5:G:196:THR:O	2.09	0.53
1:A:142:HIS:NE2	1:A:289:ASP:OD1	2.38	0.52
2:B:404:CYS:SG	2:B:405:GLY:N	2.79	0.52
1:A:394:THR:HG22	1:A:457:MET:HB2	1.91	0.52
2:B:308:GLN:HB2	2:B:330:ASN:HB2	1.92	0.52
5:F:91:ARG:HB3	5:F:100:ALA:HB3	1.90	0.52
2:B:330:ASN:CB	2:B:331:PRO:CD	2.64	0.52
7:T:-2:DT:C7	7:T:-1:DA:N6	2.73	0.52
7:T:4:DA:C2'	7:T:5:DT:C6	2.83	0.52
7:T:5:DT:C1'	7:T:6:DT:H5'	2.39	0.52
3:C:59:VAL:HG12	3:C:103:ILE:HG22	1.92	0.52
1:A:164:LEU:HB3	1:A:190:VAL:CG1	2.37	0.52
1:A:164:LEU:CB	1:A:190:VAL:HG21	2.38	0.52
2:B:310:PRO:CA	2:B:329:THR:HG22	2.40	0.52
5:F:184:GLN:NE2	5:F:197:ILE:O	2.43	0.52
1:A:232:ARG:HH12	1:A:242:ALA:HB3	1.75	0.52
5:G:38:GLN:HG2	5:G:49:GLN:HG2	1.92	0.51
5:G:103:PHE:HB2	5:G:112:SER:HB2	1.92	0.51
1:A:687:ASP:O	1:A:691:LEU:HD23	2.09	0.51
1:A:171:ALA:H	1:A:180:ARG:HG3	1.75	0.51
5:E:206:THR:HG23	5:E:254:LYS:HB2	1.92	0.51
1:A:102:ASP:HB3	1:A:126:ARG:HB2	1.93	0.51
7:T:6:DT:N1	7:T:7:DC:C5	2.78	0.51
1:A:617:CYS:HB3	1:A:620:THR:HG22	1.91	0.51
5:G:7:VAL:HA	5:G:87:ILE:HG23	1.92	0.51
7:T:6:DT:C6	7:T:7:DC:N4	2.79	0.51
5:G:63:ASP:OD1	5:G:63:ASP:N	2.43	0.50
1:A:360:CYS:SG	1:A:361:ALA:N	2.85	0.50
1:A:736:GLU:HG3	1:A:751:VAL:HG23	1.94	0.50
7:T:15:DT:C4	7:T:16:DG:C6	2.99	0.50
7:T:6:DT:C5	7:T:7:DC:N4	2.79	0.50
1:A:191:GLU:HB3	1:A:211:ARG:HB3	1.93	0.50
1:A:984:LEU:HA	1:A:987:ASP:HB2	1.94	0.50
5:F:16:LEU:HD22	5:F:79:LEU:HD12	1.93	0.50
2:B:49:GLN:NE2	4:D:62:THR:OG1	2.45	0.50
2:B:301:PRO:HG2	2:B:315:MET:HE1	1.93	0.50
5:E:184:GLN:HG3	5:E:197:ILE:HD12	1.94	0.49
1:A:587:ILE:HD12	1:A:754:GLY:HA3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:GLN:NE2	1:A:985:ARG:HH11	2.10	0.49
1:A:1039:LYS:O	1:A:1040:GLU:CG	2.61	0.49
5:G:68:MET:HB3	5:G:118:LEU:HD11	1.94	0.49
7:T:7:DC:H2"	7:T:8:DG:C8	2.48	0.49
5:E:16:LEU:HA	5:E:19:LEU:HB2	1.94	0.49
5:G:161:SER:HB3	5:G:204:GLN:HE21	1.78	0.49
5:F:160:ILE:O	5:F:204:GLN:HA	2.13	0.49
1:A:974:LEU:HD22	1:A:978:ARG:HD3	1.95	0.49
5:G:105:ALA:O	5:G:108:GLN:NE2	2.46	0.49
7:T:6:DT:C6	7:T:7:DC:C4	3.01	0.49
1:A:964:LYS:HG3	1:A:965:PRO:HD3	1.95	0.48
1:A:248:VAL:HG11	1:A:560:LEU:HD11	1.95	0.48
1:A:1026:CYS:O	1:A:1030:GLN:CG	2.55	0.48
2:B:240:ARG:NH2	2:B:293:ASP:OD2	2.37	0.48
5:E:12:LEU:HD23	5:E:88:ILE:HG21	1.96	0.48
5:G:138:LYS:O	5:G:195:VAL:HA	2.12	0.48
2:B:18:SER:OG	2:B:19:ALA:N	2.45	0.48
5:G:160:ILE:HD11	5:G:229:MET:HE3	1.96	0.48
5:G:205:LEU:HD13	5:G:253:PRO:HG3	1.95	0.48
5:E:218:ALA:HA	5:E:221:LEU:HD23	1.96	0.48
1:A:421:LEU:H	1:A:421:LEU:HD22	1.78	0.48
1:A:1039:LYS:O	1:A:1040:GLU:CB	2.62	0.48
5:E:75:MET:HE1	5:E:101:LEU:HD11	1.94	0.48
5:F:169:PHE:O	5:F:179:ASN:HA	2.14	0.48
2:B:328:VAL:C	2:B:329:THR:HG23	2.39	0.48
2:B:99:LYS:H	2:B:155:THR:HB	1.77	0.47
3:C:6:TYR:OH	3:C:43:ASP:OD2	2.32	0.47
1:A:861:VAL:HG12	1:A:985:ARG:NH1	2.29	0.47
1:A:1054:LEU:HD23	2:B:107:ILE:HD13	1.95	0.47
1:A:1047:LEU:HB3	1:A:1089:LEU:HD13	1.96	0.47
1:A:688:GLY:HA2	1:A:691:LEU:CG	2.34	0.47
1:A:188:LEU:N	1:A:188:LEU:CD2	2.73	0.47
2:B:276:VAL:HG11	2:B:315:MET:HB3	1.95	0.47
5:E:138:LYS:O	5:E:195:VAL:HA	2.15	0.47
1:A:810:ALA:HA	1:A:825:ASP:O	2.15	0.47
4:D:50:ARG:HG3	4:D:101:LEU:HD21	1.97	0.47
1:A:1088:ASP:O	1:A:1091:ASP:OD1	2.32	0.47
5:E:162:CYS:O	5:E:202:PRO:HA	2.14	0.47
5:E:240:LYS:HD3	5:E:246:HIS:HB3	1.96	0.47
5:F:159:VAL:HA	5:F:205:LEU:O	2.15	0.46
2:B:296:PRO:HD2	2:B:329:THR:C	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:GLU:HA	1:A:1030:GLN:NE2	2.31	0.46
2:B:439:LEU:HG	2:B:450:ILE:HD11	1.98	0.46
1:A:806:LYS:O	7:T:5:DT:C5'	2.64	0.46
2:B:83:CYS:HB3	2:B:140:GLN:HE22	1.80	0.46
5:E:137:VAL:HA	5:E:196:THR:O	2.16	0.46
5:E:13:LYS:HE2	5:E:13:LYS:HB3	1.80	0.45
3:C:104:GLN:NE2	3:C:106:ALA:O	2.49	0.45
5:E:134:SER:HA	5:E:200:ASN:HD21	1.81	0.45
5:F:51:THR:O	5:F:245:GLY:HA3	2.16	0.45
5:G:5:ARG:HB3	5:G:59:THR:HB	1.99	0.45
4:D:79:GLU:OE1	4:D:79:GLU:HA	2.13	0.45
5:E:140:PRO:HG3	5:E:193:GLU:HA	1.98	0.45
1:A:186:ALA:C	1:A:188:LEU:HD23	2.41	0.45
1:A:467:TYR:O	1:A:472:TYR:OH	2.32	0.45
1:A:163:ASP:HA	1:A:166:ARG:HB2	1.98	0.45
1:A:843:LEU:HD22	1:A:867:VAL:HG11	1.99	0.45
1:A:1098:ARG:HG2	1:A:1098:ARG:NH2	2.31	0.45
5:G:50:LEU:HD13	5:G:247:LEU:HD13	1.98	0.45
1:A:861:VAL:CG1	1:A:985:ARG:HH11	2.30	0.45
2:B:70:GLN:HG2	2:B:77:VAL:HG11	1.99	0.45
5:G:79:LEU:HA	5:G:103:PHE:HZ	1.82	0.44
2:B:193:ASP:N	2:B:193:ASP:OD1	2.49	0.44
1:A:187:VAL:O	1:A:187:VAL:HG13	2.18	0.44
1:A:594:TYR:HB2	1:A:801:TYR:HB3	2.00	0.44
1:A:1030:GLN:N	1:A:1031:PRO:HD2	2.33	0.44
5:E:56:GLY:HA3	5:E:244:MET:HA	1.99	0.44
5:G:26:ALA:HB3	5:G:72:LEU:HD21	1.99	0.44
1:A:164:LEU:HB3	1:A:190:VAL:CG2	2.46	0.44
1:A:815:SER:OG	1:A:819:ASP:OD2	2.35	0.44
2:B:246:ASN:H	2:B:297:GLY:HA3	1.82	0.44
5:G:94:ASP:OD1	5:G:94:ASP:N	2.50	0.44
2:B:161:VAL:HG23	2:B:176:TYR:HB3	2.00	0.44
7:T:5:DT:H1'	7:T:6:DT:C5'	2.45	0.44
5:F:133:TYR:HA	5:F:230:SER:HB2	1.99	0.44
5:F:151:LEU:HD22	5:F:171:ALA:HB3	1.99	0.44
7:T:-2:DT:C5	7:T:-1:DA:N6	2.86	0.44
2:B:366:GLU:HG3	2:B:415:ILE:HD13	1.99	0.43
7:T:6:DT:C6	7:T:7:DC:C5	3.06	0.43
1:A:736:GLU:OE2	1:A:751:VAL:N	2.39	0.43
1:A:806:LYS:O	7:T:5:DT:C4'	2.61	0.43
1:A:1107:TRP:CD1	1:A:1107:TRP:H	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:0:DA:H2'	7:T:1:DG:C8	2.50	0.43
1:A:830:GLU:HG3	1:A:965:PRO:HB3	1.99	0.43
1:A:421:LEU:HD22	1:A:421:LEU:N	2.34	0.43
1:A:617:CYS:SG	1:A:618:TYR:N	2.92	0.43
4:D:66:ARG:HG2	4:D:88:LEU:HD11	2.00	0.43
1:A:1098:ARG:CG	1:A:1098:ARG:HH21	2.32	0.43
1:A:137:VAL:HG22	1:A:286:LEU:HB2	2.00	0.43
5:F:141:SER:HB3	5:F:225:VAL:HG13	2.01	0.43
5:E:199:MET:HB2	5:E:199:MET:HE2	1.69	0.43
1:A:834:ARG:HH21	1:A:921:ARG:HH11	1.65	0.43
2:B:137:ASP:OD1	2:B:138:GLU:N	2.45	0.43
3:C:128:ASN:N	3:C:128:ASN:OD1	2.51	0.43
1:A:682:ARG:HA	1:A:685:VAL:HG22	2.00	0.43
1:A:740:THR:HA	1:A:748:SER:HA	2.01	0.43
5:G:83:GLY:N	5:G:86:ASP:OD2	2.52	0.43
1:A:618:TYR:OH	1:A:711:LEU:O	2.31	0.42
1:A:687:ASP:C	1:A:691:LEU:HD23	2.44	0.42
2:B:407:THR:HG21	2:B:427:THR:HB	2.01	0.42
4:D:61:CYS:HB2	4:D:69:ARG:HH21	1.85	0.42
5:E:223:SER:OG	5:E:224:THR:N	2.53	0.42
2:B:417:GLY:N	2:B:421:GLN:O	2.51	0.42
7:T:6:DT:N1	7:T:7:DC:C4	2.87	0.42
1:A:594:TYR:HE2	1:A:762:ARG:HH11	1.67	0.42
2:B:328:VAL:HB	2:B:329:THR:H	1.70	0.42
3:C:62:LEU:HD12	3:C:79:VAL:HG22	2.01	0.42
5:G:95:ASN:OD1	5:G:95:ASN:N	2.52	0.42
2:B:360:ASP:OD1	2:B:363:GLU:N	2.49	0.42
5:G:12:LEU:HA	5:G:15:VAL:HB	2.00	0.42
5:G:14:LYS:HA	5:G:17:GLU:HB2	2.02	0.42
1:A:260:ILE:HG22	1:A:297:SER:HB2	2.01	0.41
1:A:682:ARG:O	1:A:686:LEU:HG	2.20	0.41
1:A:865:GLN:HE21	1:A:985:ARG:HD3	1.84	0.41
5:F:238:GLU:HG3	5:F:248:LYS:HG2	2.00	0.41
1:A:385:ILE:HG21	1:A:421:LEU:HD12	2.02	0.41
1:A:523:LEU:HD12	1:A:528:VAL:HB	2.02	0.41
1:A:1082:ARG:HH22	4:D:107:LEU:HA	1.86	0.41
5:E:162:CYS:HB3	5:E:199:MET:HE1	2.02	0.41
1:A:157:GLY:HA3	1:A:237:GLY:HA2	2.03	0.41
1:A:597:PRO:HD2	1:A:766:SER:HA	2.02	0.41
1:A:1039:LYS:N	1:A:1039:LYS:HD3	2.33	0.41
2:B:35:SER:O	2:B:333:GLN:NE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:162:CYS:SG	5:G:163:ALA:N	2.94	0.41
1:A:367:LYS:HE3	1:A:369:GLN:HE21	1.85	0.41
1:A:1078:ILE:HD13	1:A:1078:ILE:HA	1.83	0.41
5:E:159:VAL:HG13	5:E:170:SER:HB3	2.03	0.41
5:G:164:LYS:HA	5:G:199:MET:HE3	2.03	0.41
5:G:209:LEU:HD23	5:G:212:LEU:HD12	2.03	0.41
5:E:38:GLN:HE21	5:E:125:GLN:NE2	2.19	0.41
5:G:138:LYS:HB3	5:G:196:THR:HG22	2.02	0.41
1:A:732:LYS:HB3	1:A:732:LYS:HE2	1.90	0.41
1:A:886:GLU:OE1	6:P:22:DT:OP2	2.39	0.41
5:E:151:LEU:HA	5:E:154:ILE:HD12	2.03	0.41
1:A:560:LEU:HD23	1:A:560:LEU:HA	1.92	0.41
5:E:227:LEU:HD13	5:E:237:VAL:HG12	2.03	0.41
6:P:11:DA:H2''	6:P:12:DT:C6	2.55	0.41
7:T:6:DT:H2'	7:T:7:DC:H5	1.82	0.41
1:A:400:ASN:HD21	1:A:446:THR:HG23	1.85	0.40
1:A:457:MET:HE2	1:A:457:MET:HB3	1.99	0.40
1:A:632:LEU:HD23	1:A:632:LEU:HA	1.96	0.40
1:A:809:TYR:CZ	1:A:827:LYS:HG3	2.57	0.40
4:D:105:TYR:O	4:D:107:LEU:N	2.54	0.40
5:F:7:VAL:HG23	5:F:8:GLN:HG3	2.02	0.40
1:A:240:SER:HA	1:A:241:PHE:HA	1.62	0.40
1:A:651:VAL:HG12	1:A:652:ARG:HG2	2.03	0.40
7:T:4:DA:C3'	7:T:5:DT:C7	2.86	0.40
1:A:188:LEU:CA	1:A:213:THR:O	2.62	0.40
1:A:579:GLU:O	1:A:707:GLN:NE2	2.51	0.40
5:E:136:VAL:HG23	5:E:198:GLU:HB3	2.03	0.40
5:G:31:SER:O	5:G:60:TYR:OH	2.34	0.40
5:G:102:VAL:HG12	5:G:104:GLU:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1003/1107 (91%)	934 (93%)	65 (6%)	4 (0%)	30	67
2	B	425/469 (91%)	392 (92%)	31 (7%)	2 (0%)	24	62
3	C	141/474 (30%)	131 (93%)	10 (7%)	0	100	100
4	D	64/137 (47%)	49 (77%)	12 (19%)	3 (5%)	2	16
5	E	247/264 (94%)	239 (97%)	8 (3%)	0	100	100
5	F	243/264 (92%)	237 (98%)	6 (2%)	0	100	100
5	G	245/264 (93%)	229 (94%)	16 (6%)	0	100	100
All	All	2368/2979 (80%)	2211 (93%)	148 (6%)	9 (0%)	31	67

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	330	ASN
4	D	79	GLU
1	A	85	PRO
1	A	756	THR
1	A	1021	HIS
1	A	1040	GLU
2	B	328	VAL
4	D	106	PRO
4	D	105	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	857/944 (91%)	849 (99%)	8 (1%)	70	77
2	B	367/403 (91%)	364 (99%)	3 (1%)	73	78
3	C	125/413 (30%)	125 (100%)	0	100	100
4	D	59/120 (49%)	58 (98%)	1 (2%)	53	68
5	E	217/230 (94%)	213 (98%)	4 (2%)	51	67
5	F	216/230 (94%)	215 (100%)	1 (0%)	81	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	G	217/230 (94%)	217 (100%)	0	100	100
All	All	2058/2570 (80%)	2041 (99%)	17 (1%)	70	78

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	LEU
1	A	190	VAL
1	A	1019	LEU
1	A	1021	HIS
1	A	1032	ARG
1	A	1038	GLN
1	A	1039	LYS
1	A	1098	ARG
2	B	180	ASP
2	B	220	ASP
2	B	328	VAL
4	D	79	GLU
5	E	11	ILE
5	E	45	VAL
5	E	48	VAL
5	E	247	LEU
5	F	153	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	369	GLN
1	A	397	ASN
1	A	400	ASN
1	A	430	ASN
1	A	558	GLN
1	A	614	HIS
1	A	842	ASN
1	A	865	GLN
1	A	880	GLN
1	A	961	GLN
1	A	1021	HIS
1	A	1038	GLN
1	A	1043	HIS

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Mol	Chain	Res	Type
1	A	1045	ASN
1	A	1092	GLN
2	B	21	ASN
2	B	70	GLN
2	B	140	GLN
2	B	184	GLN
2	B	330	ASN
3	C	116	ASN
4	D	86	GLN
5	E	84	ASN
5	E	125	GLN
5	F	65	ASN
5	F	71	ASN
5	F	179	ASN
5	G	36	ASN
5	G	38	GLN
5	G	71	ASN
5	G	108	GLN
5	G	125	GLN
5	G	204	GLN
5	G	213	ASN
5	G	246	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
6	DOC	P	25	7,6	16,19,20	0.90	0	20,26,29	1.32	1 (5%)

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
6	DOC	P	25	7,6	-	2/7/18/19	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	25	DOC	C3'-C2'-C1'	2.85	106.15	102.87

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	P	25	DOC	C3'-C4'-C5'-O5'
6	P	25	DOC	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	P	25	DOC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is 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
10	TTP	T	101	-	29,30,30	4.51	17 (58%)	43,47,47	1.93	12 (27%)
9	SF4	A	1202	1	0,12,12	-	-	-		

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
10	TTP	T	101	-	-	4/22/34/34	0/2/2/2
9	SF4	A	1202	1	-	-	0/6/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	T	101	TTP	C2'-C3'	-12.11	1.22	1.52
10	T	101	TTP	C6-C5	8.31	1.48	1.34
10	T	101	TTP	O4'-C4'	-7.92	1.27	1.45
10	T	101	TTP	C2-N3	6.51	1.49	1.38
10	T	101	TTP	PA-O3A	6.27	1.66	1.59
10	T	101	TTP	C2-N1	6.21	1.48	1.38
10	T	101	TTP	PB-O3A	5.97	1.65	1.59
10	T	101	TTP	C1'-N1	-5.35	1.34	1.48
10	T	101	TTP	PB-O3B	5.04	1.64	1.59
10	T	101	TTP	C3'-C4'	4.61	1.65	1.53
10	T	101	TTP	C6-N1	3.74	1.44	1.38
10	T	101	TTP	O4'-C1'	3.40	1.49	1.42
10	T	101	TTP	C4-N3	3.31	1.45	1.38
10	T	101	TTP	O3'-C3'	2.99	1.49	1.43
10	T	101	TTP	O4-C4	-2.93	1.18	1.23
10	T	101	TTP	O2-C2	-2.88	1.18	1.23
10	T	101	TTP	C4-C5	2.41	1.48	1.44

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	T	101	TTP	C4-N3-C2	-5.94	119.56	127.34
10	T	101	TTP	C5-C4-N3	4.76	119.46	115.32
10	T	101	TTP	N3-C2-N1	4.64	120.93	114.89
10	T	101	TTP	O4-C4-C5	-3.84	120.52	124.92
10	T	101	TTP	C6-C5-C4	2.82	120.34	118.02
10	T	101	TTP	C5M-C5-C6	-2.58	119.36	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	T	101	TTP	O2-C2-N1	-2.47	119.58	122.80
10	T	101	TTP	C5-C6-N1	-2.41	120.69	123.31
10	T	101	TTP	C6-N1-C2	-2.30	119.01	121.30
10	T	101	TTP	O4'-C1'-N1	2.18	111.73	107.86
10	T	101	TTP	C3'-C2'-C1'	2.13	107.81	102.60
10	T	101	TTP	C2'-C1'-N1	-2.12	108.52	113.81

There are no chirality outliers.

All (4) torsion outliers are listed below:

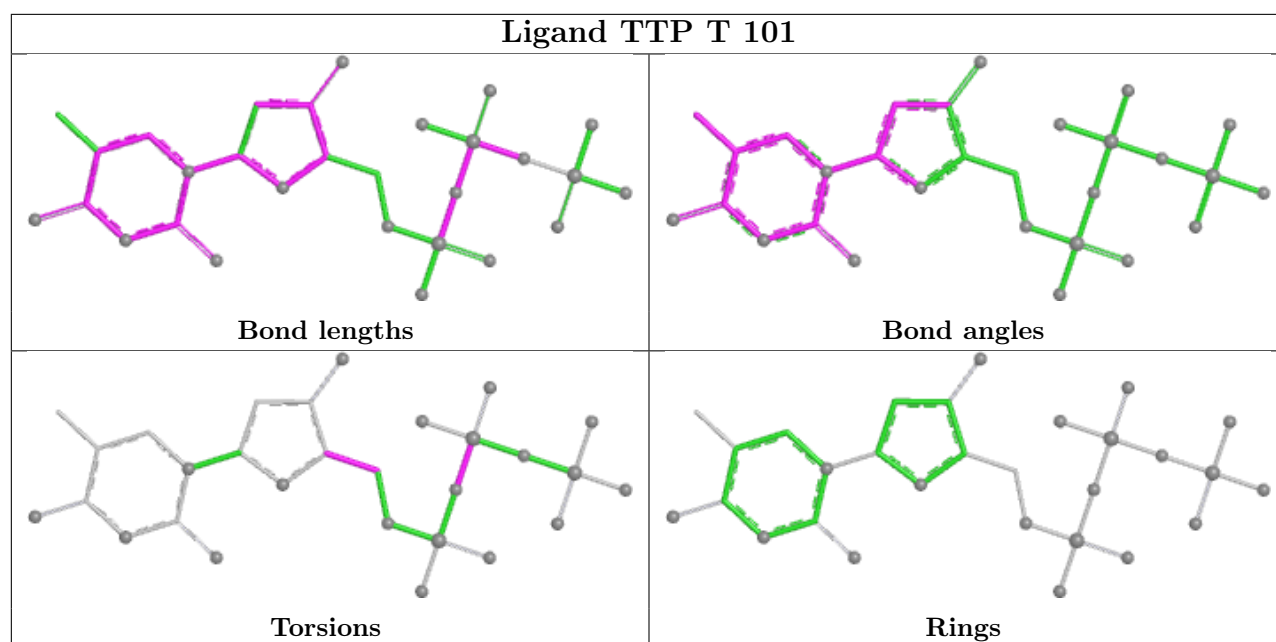
Mol	Chain	Res	Type	Atoms
10	T	101	TTP	O4'-C4'-C5'-O5'
10	T	101	TTP	C3'-C4'-C5'-O5'
10	T	101	TTP	PA-O3A-PB-O1B
10	T	101	TTP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1202	SF4	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

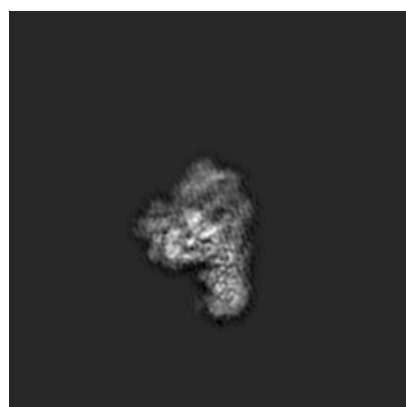
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10081. These allow visual inspection of the internal detail of the map and identification of artifacts.

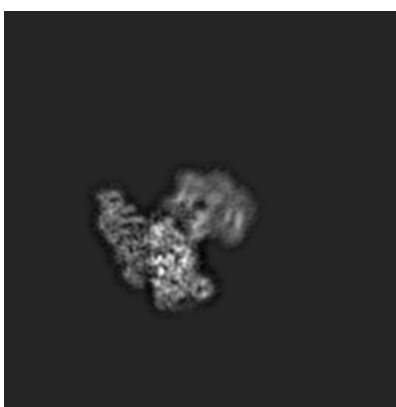
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

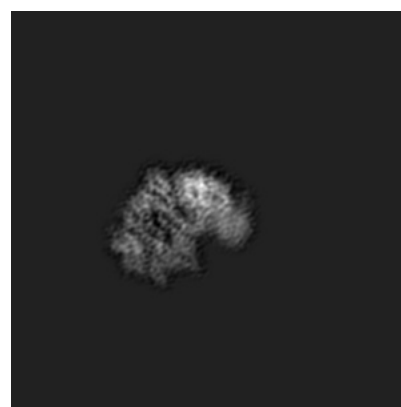
6.1.1 Primary map



X



Y



Z

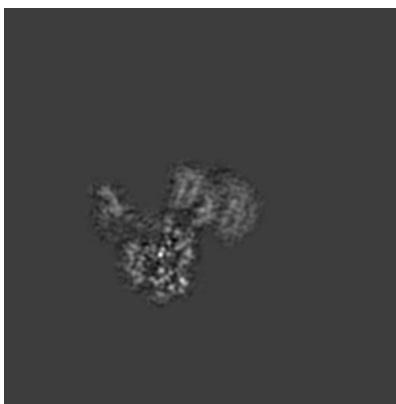
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

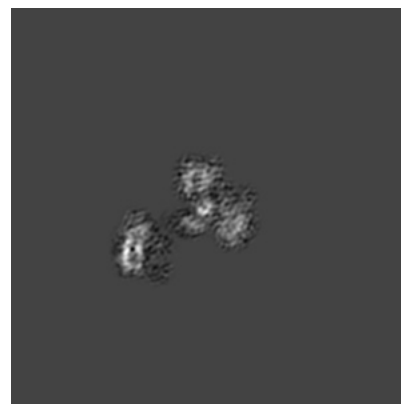
6.2.1 Primary map



X Index: 180



Y Index: 180

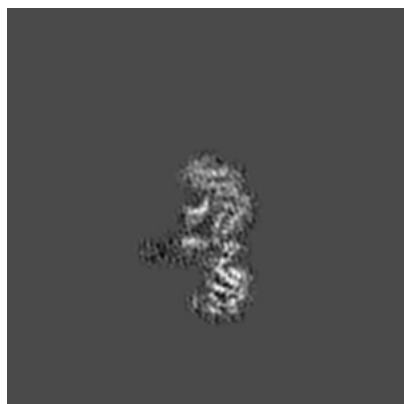


Z Index: 180

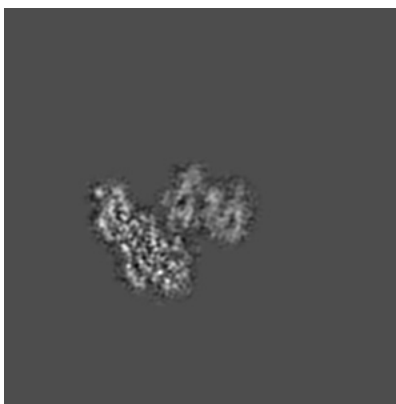
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 171



Y Index: 188

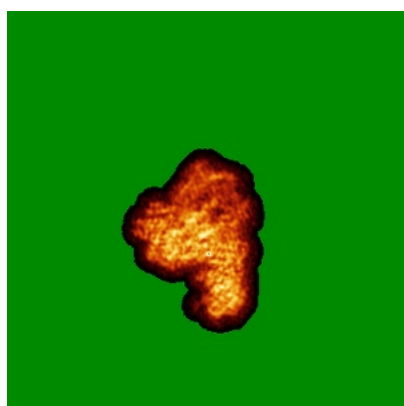


Z Index: 140

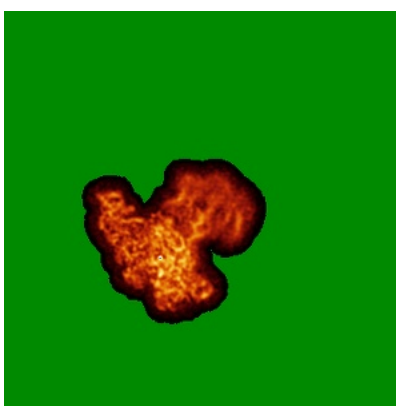
The images above show the largest variance slices of the map in three orthogonal directions.

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

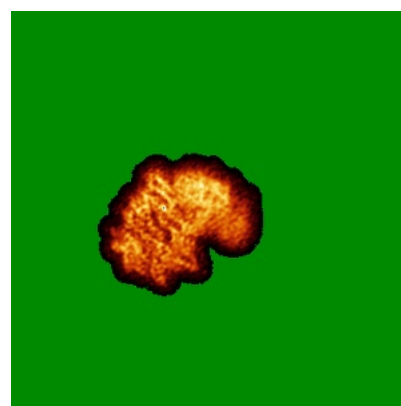
6.4.1 Primary map



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

This section was not generated.

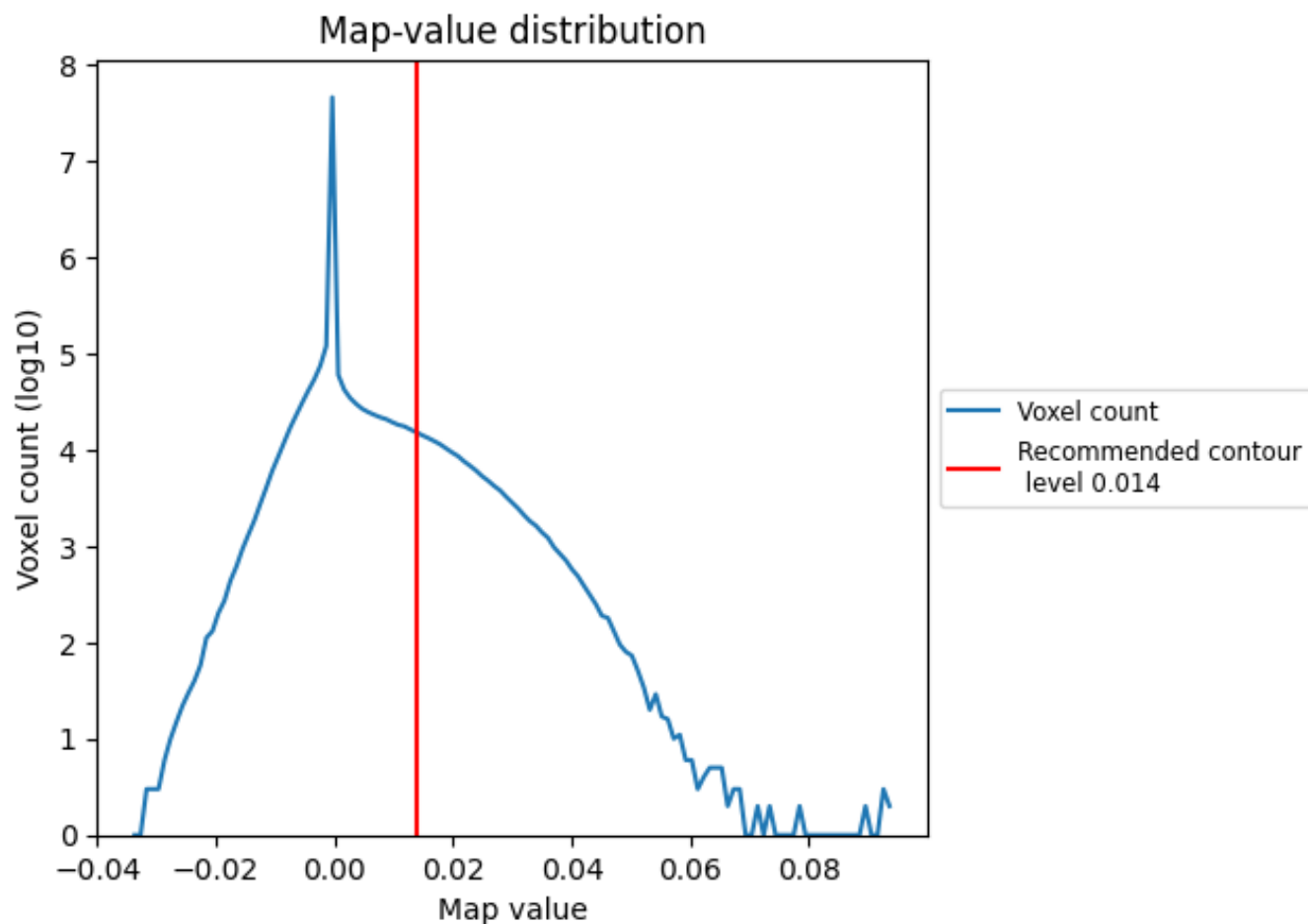
6.6 Mask visualisation

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

7 Map analysis [i](#)

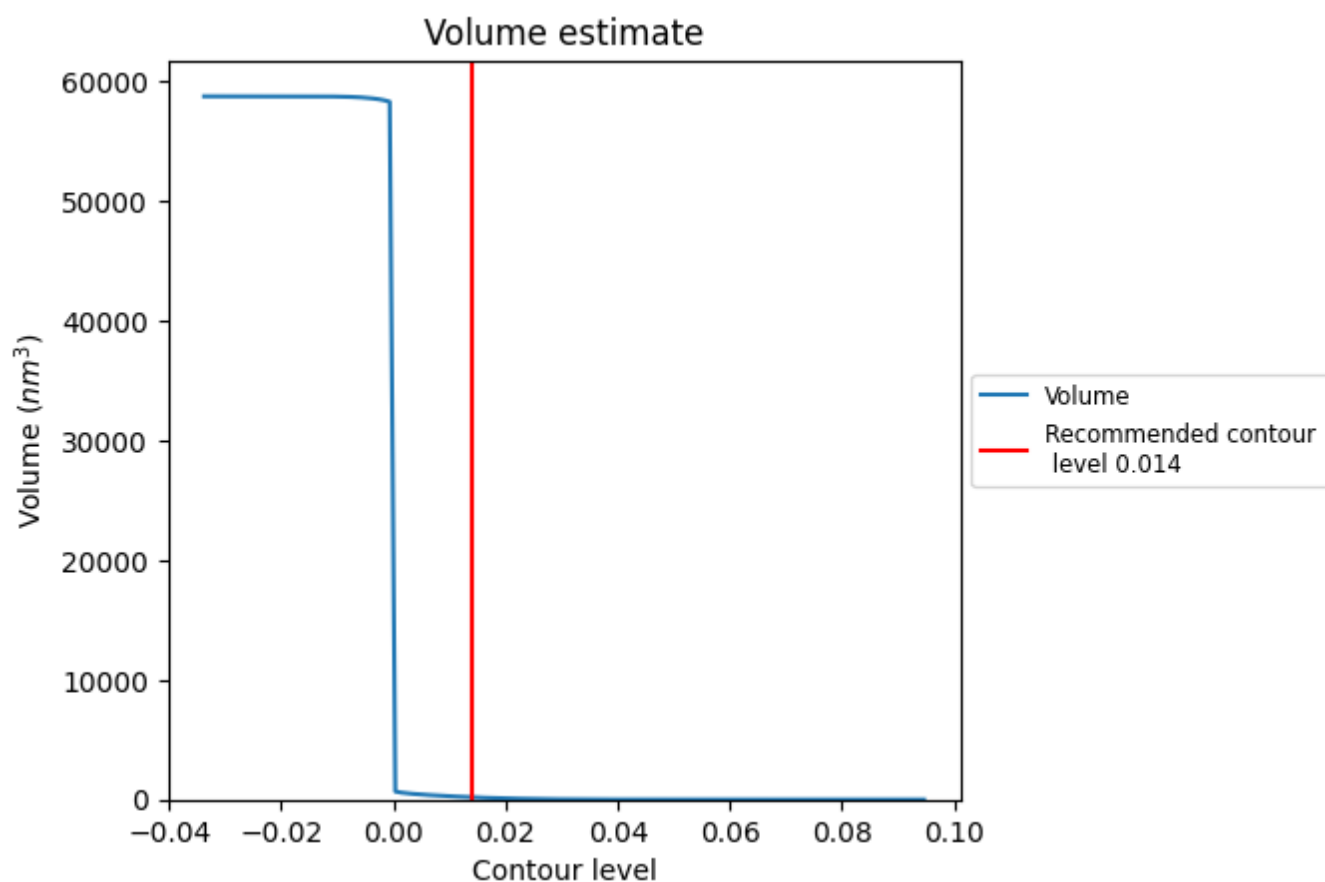
This section contains the results of statistical analysis of the map.

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.

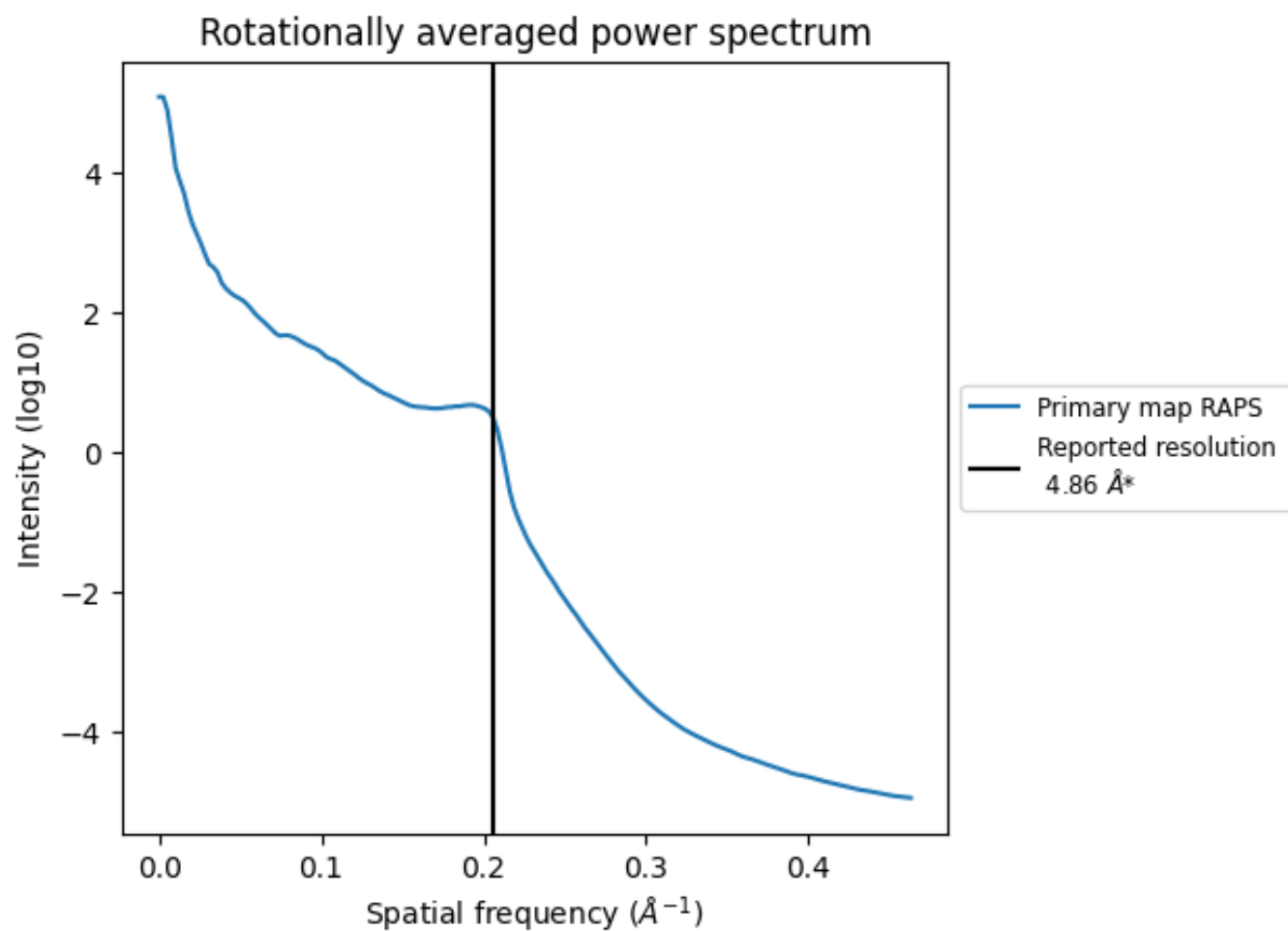
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm³; this corresponds to an approximate mass of 173 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

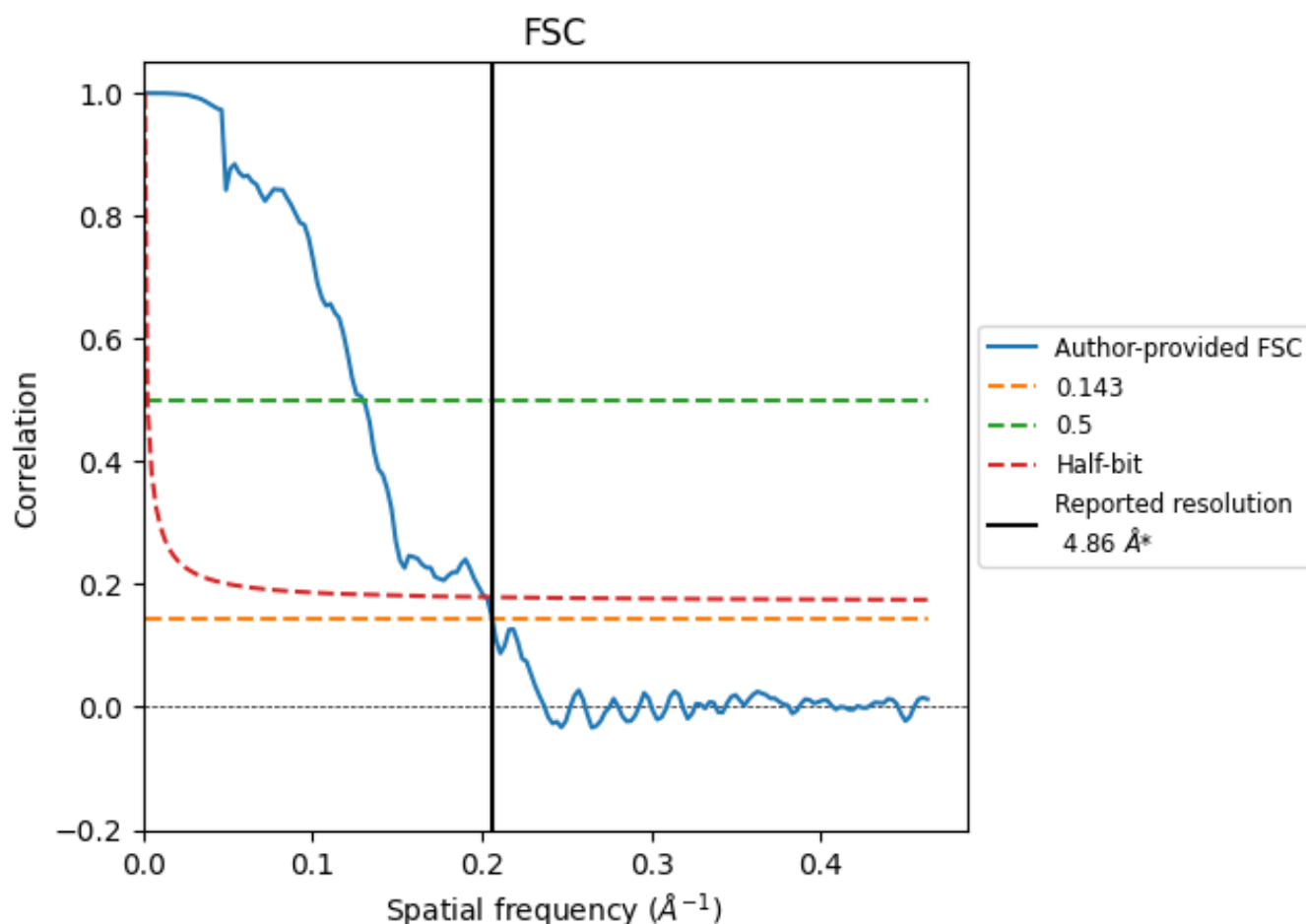


*Reported resolution corresponds to spatial frequency of 0.206 Å⁻¹

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 0.206 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.86	-	-
Author-provided FSC curve	4.85	7.70	4.95
Unmasked-calculated*	-	-	-

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

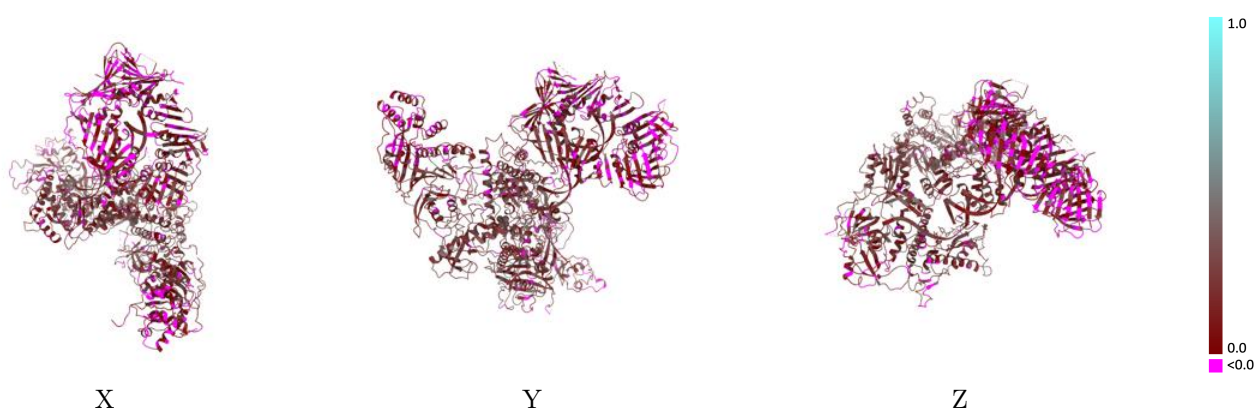
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10081 and PDB model 6S1N. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

This section was not generated.

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

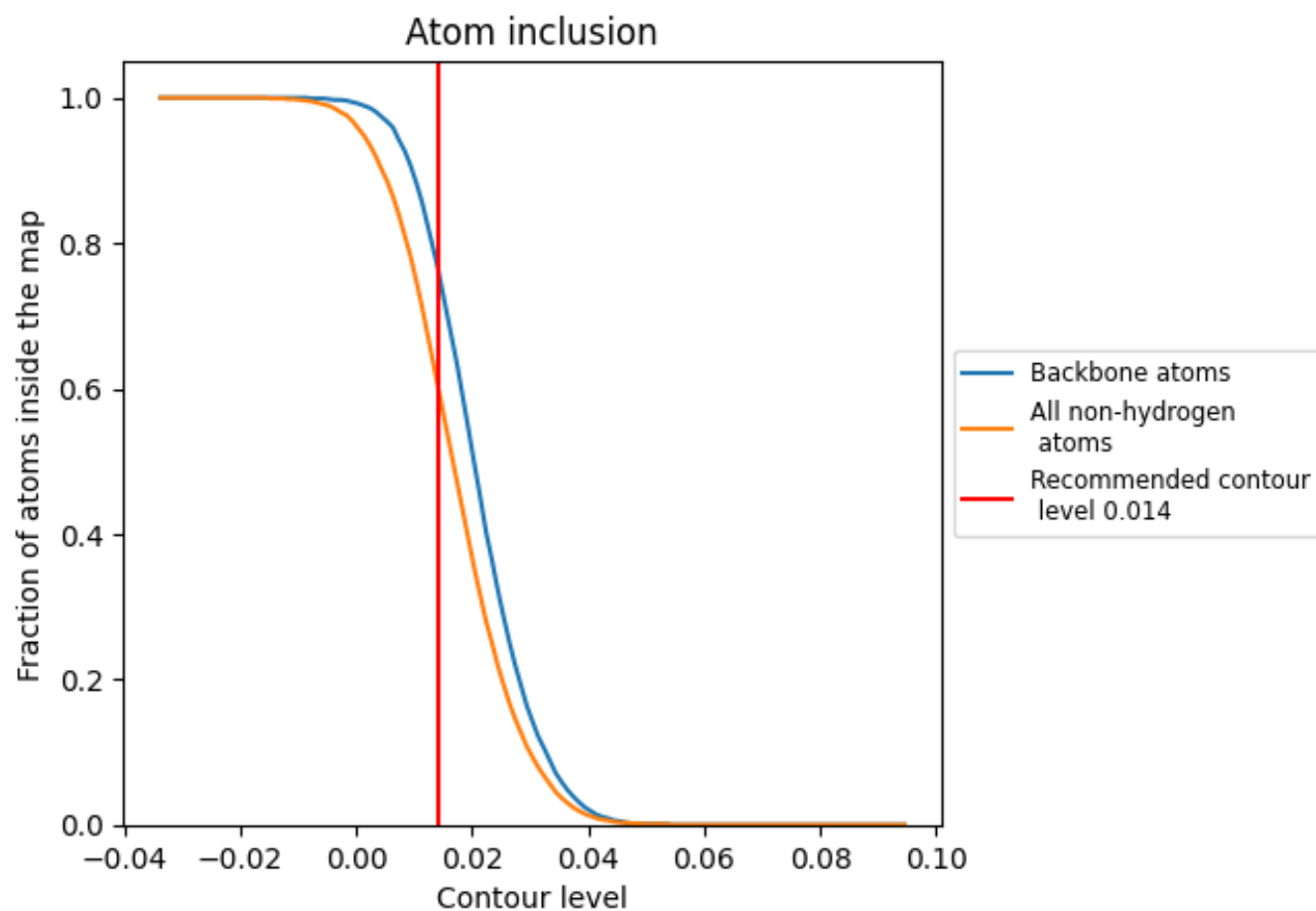


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 77% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6080	0.1620
A	0.6490	0.1990
B	0.6360	0.2010
C	0.5760	0.0760
D	0.7490	0.2670
E	0.4260	0.0590
F	0.5850	0.1530
G	0.4710	0.0610
P	0.7630	0.1650
T	0.8270	0.2170

1.0

0.0

<0.0