Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 11:50 pm GMT

PDB ID	:	6H67
EMDB ID	:	EMD-0146
Title	:	Yeast RNA polymerase I elongation complex stalled by cyclobutane pyrimidine dimer (CPD)
Authors	:	Sanz-Murillo, M.; Xu, J.; Gil-Carton, D.; Wang, D.; Fernandez-Tornero, C.
Deposited on	:	2018-07-26
Resolution	:	3.60 Å(reported)
Based on initial models	:	4C3I, 5M3F

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

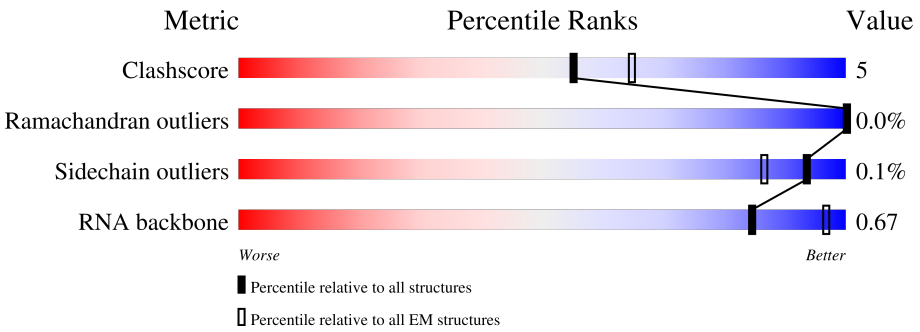
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1664	9%, 76%, 12%, 12%
2	B	1203	6%, 82%, 15%, •
3	C	335	5%, 76%, 15%, 9%
4	D	137	29%, 30%, 9%, 61%
5	E	215	13%, 92%, 7%, •
6	F	155	5%, 58%, 6%, 35%
7	G	326	30%, 42%, 10%, 48%

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Mol	Chain	Length	Quality of chain
8	H	146	8% 79% 10% 10%
9	I	125	18% 40% 10% 50%
10	J	70	74% 24%
11	K	142	58% 13% 29%
12	L	70	53% 10% 37%
13	M	415	17% 20% 6% 74%
14	N	233	39% 54% 8% 38%
15	R	10	10% 60% 10% 20% 10%
16	T	51	16% 31% 8% 59%
17	U	52	12% 19% 75%

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 33803 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1463	11565	7310	2011	2183	61	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1174	9329	5902	1637	1739	51	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	306	2431	1544	417	462	8	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	54	431	270	73	88	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	212	1734	1102	306	315	11	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	100	823	522	144	154	3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	171	1348	874	227	242	5	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	131	1051	664	176	207	4	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	63	466	292	77	93	4	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	69	569	362	101	100	6	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	101	792	496	130	161	5	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	44	351	217	70	60	4	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	M	108	856	543	142	171	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	144	1142	729	186	223	4	0	0

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
15	R	9	198	88	40	61	9	0	0

- Molecule 16 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	T	21	435	210	63	140	22	0	0

- Molecule 17 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
17	U	13	275	128	61	73	13	0	0

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
18	A	2	2	2	0
18	B	1	1	1	0
18	I	1	1	1	0
18	J	1	1	1	0
18	L	1	1	1	0

- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

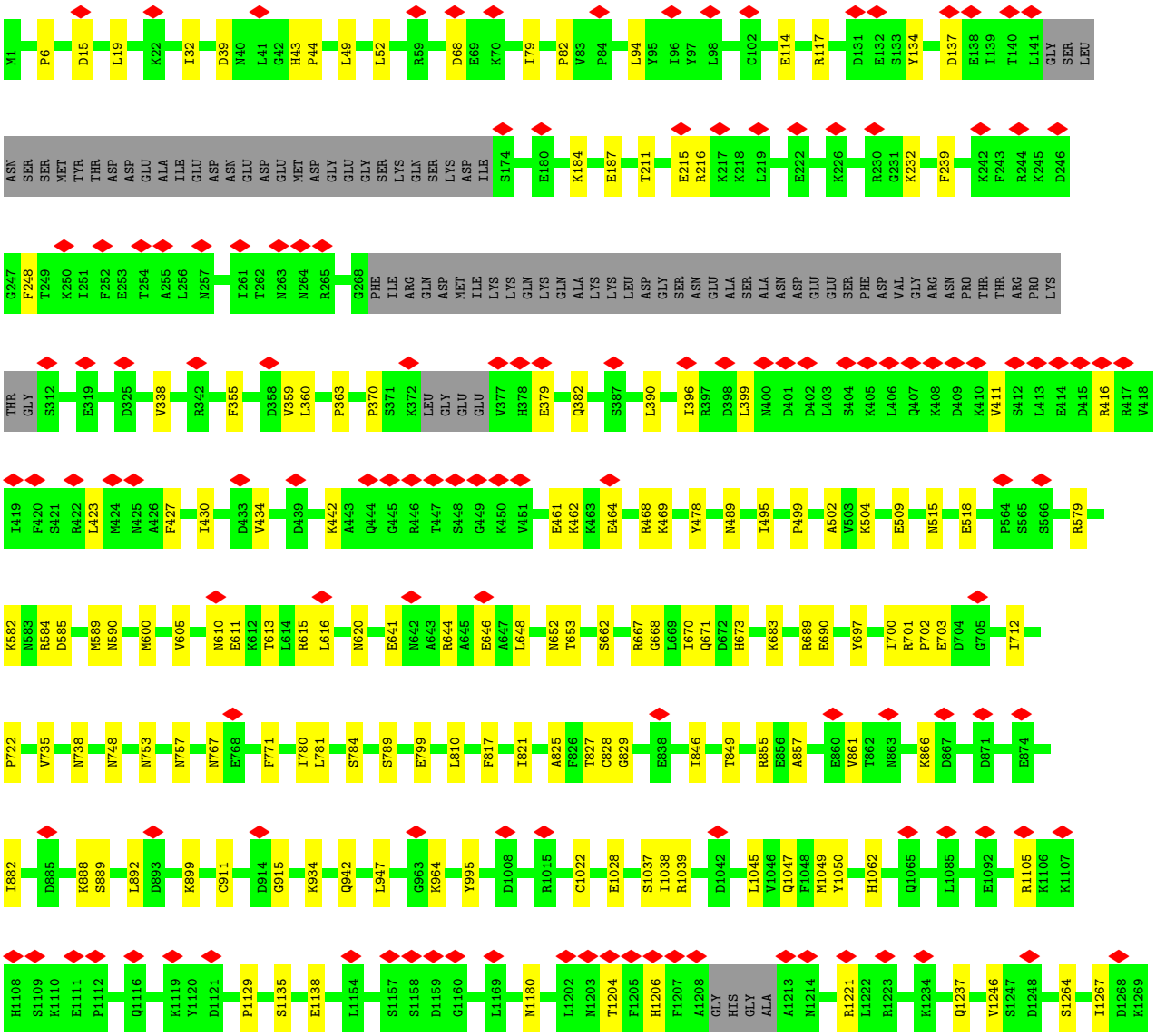
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
19	A	1	1	1	0

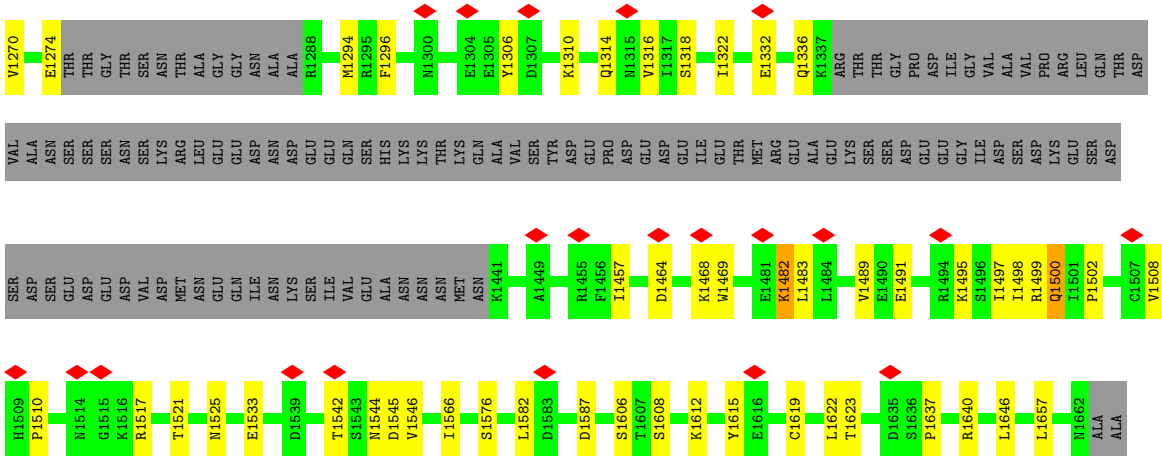
3 Residue-property plots (i)

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 I subunit RPA190

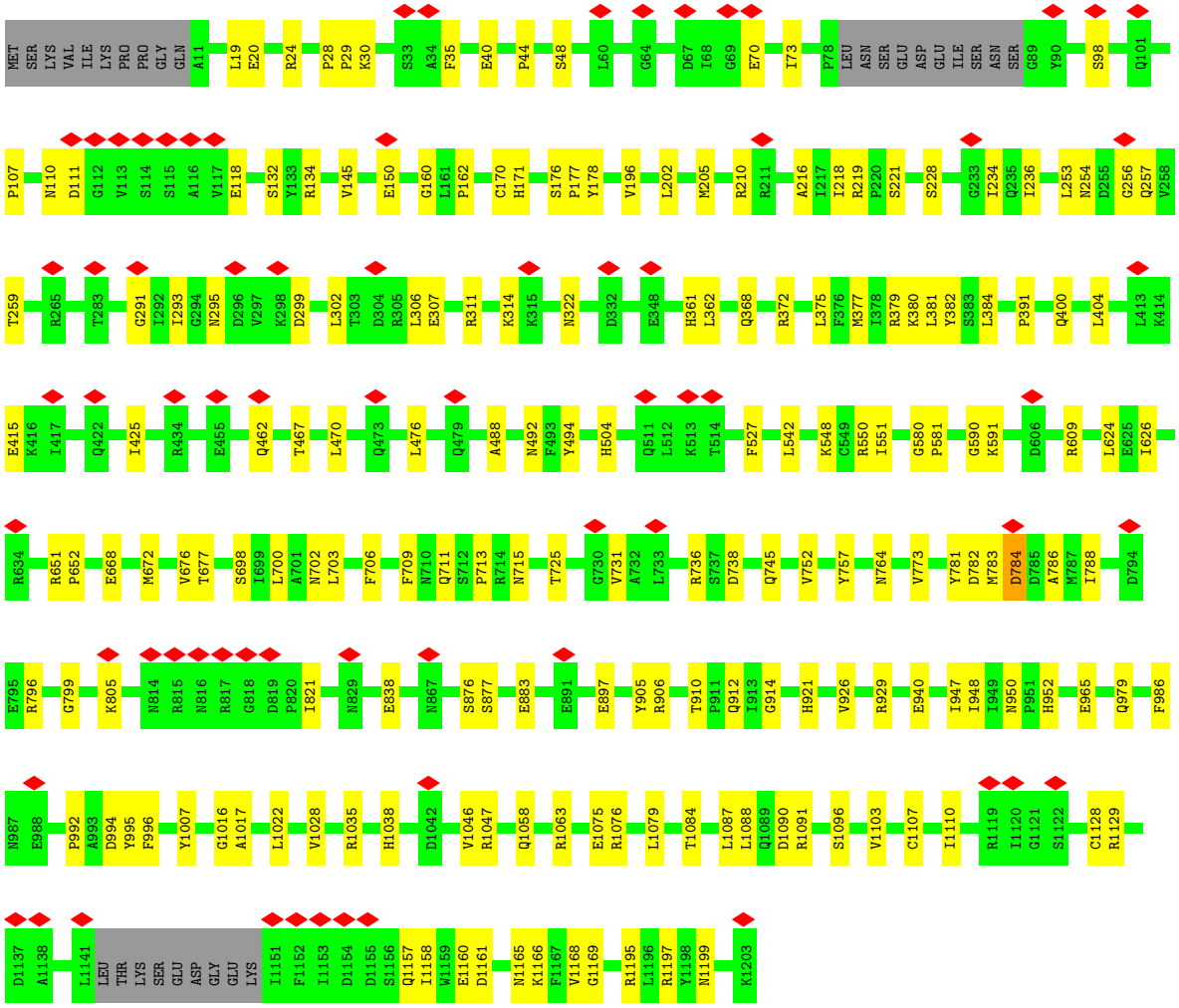
Chain A: 9% 76% 12% 12%





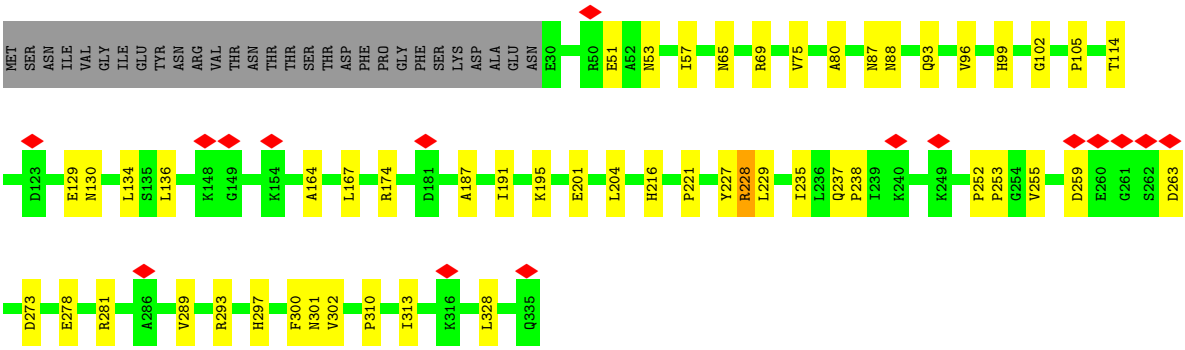
- Molecule 2: DNA-directed RNA polymerase I subunit RPA135

Chain B:



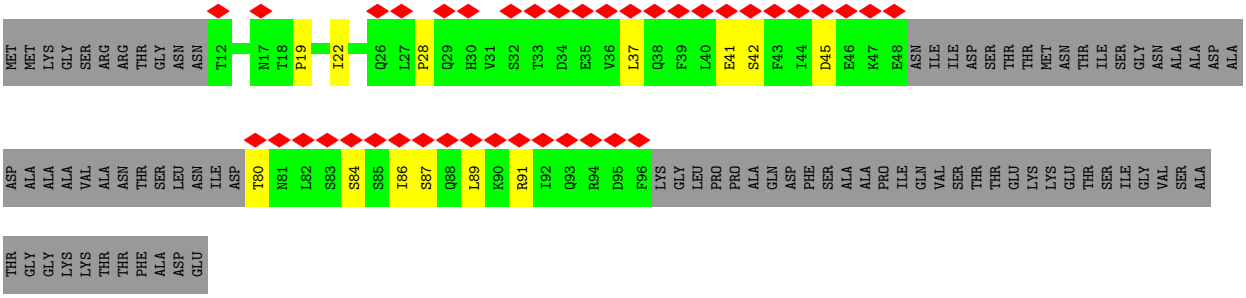
- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C:



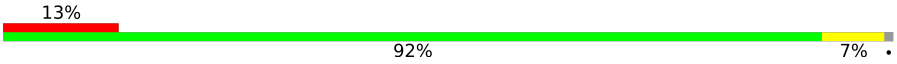
- Molecule 4: DNA-directed RNA polymerase I subunit RPA14

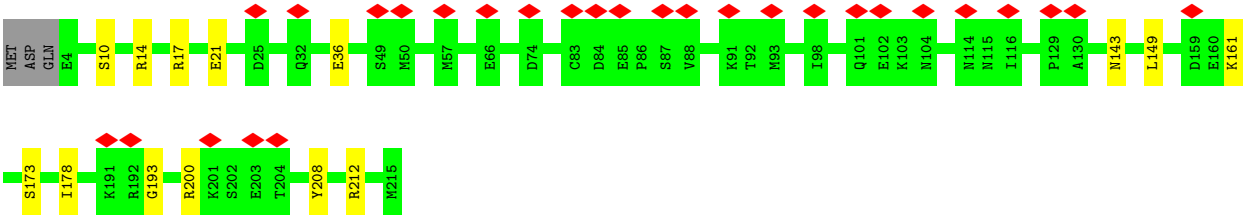
Chain D:



- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

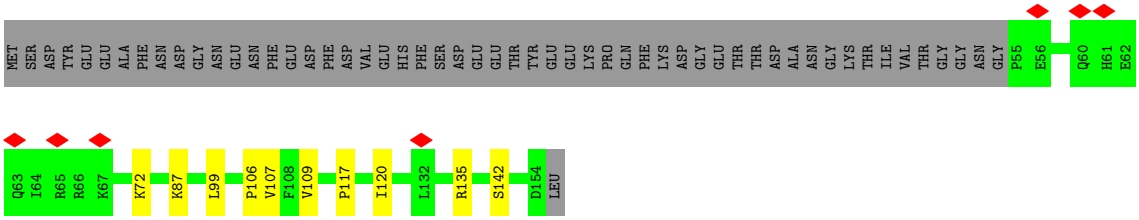
Chain E:





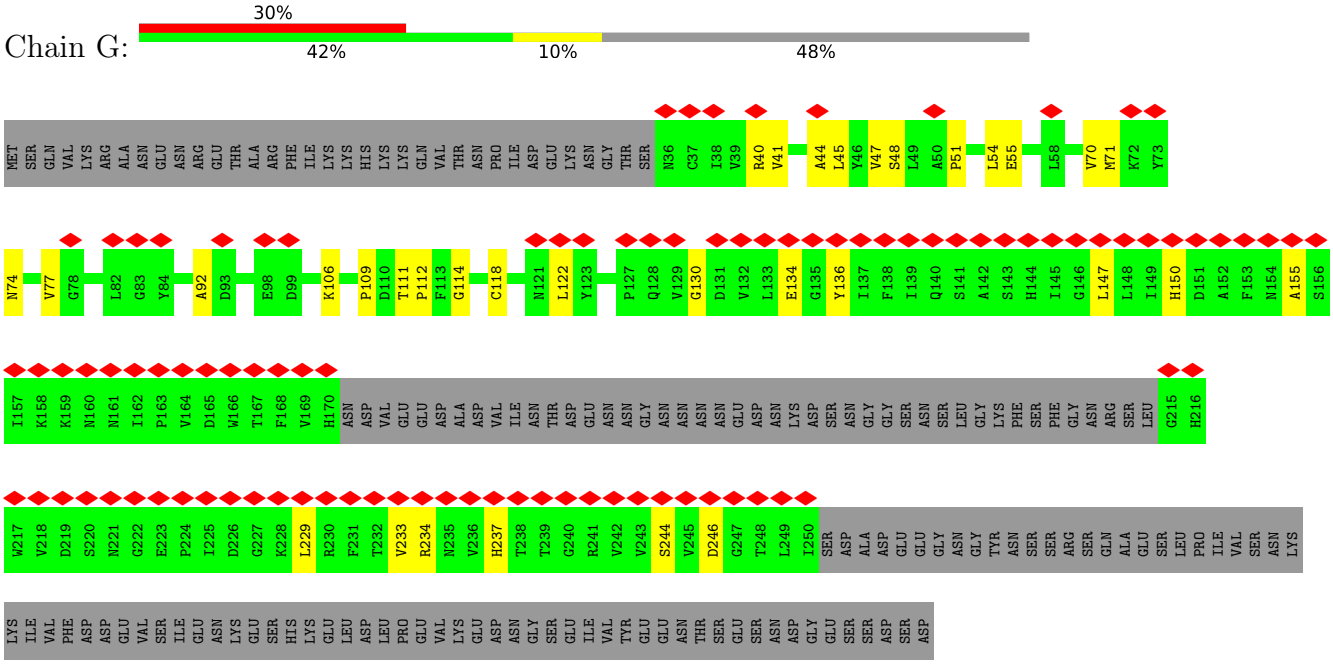
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



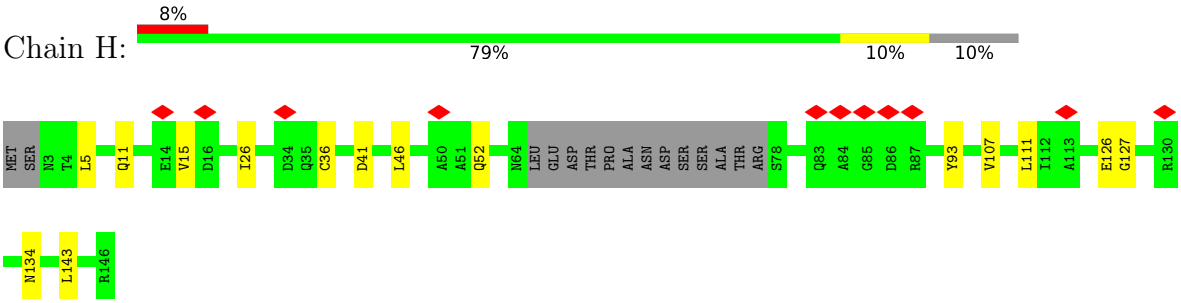
- Molecule 7: DNA-directed RNA polymerase I subunit RPA43

Chain G:



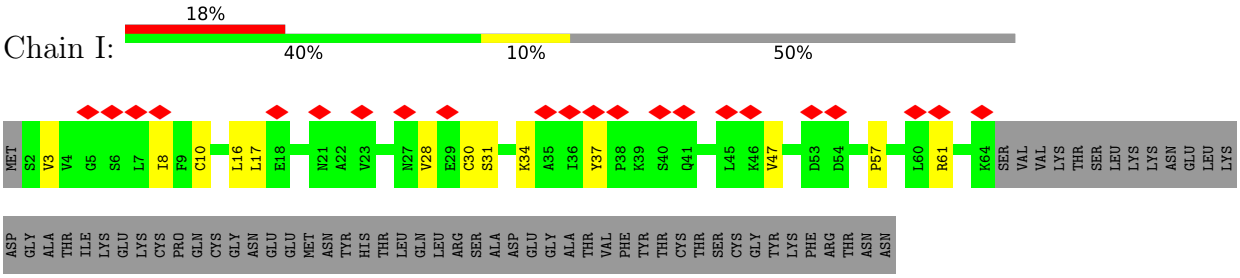
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



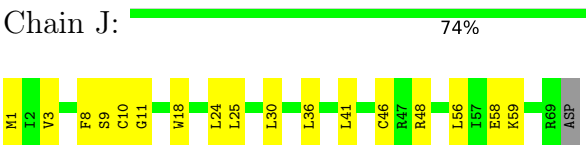
- Molecule 9: DNA-directed RNA polymerase I subunit RPA12

Chain I:



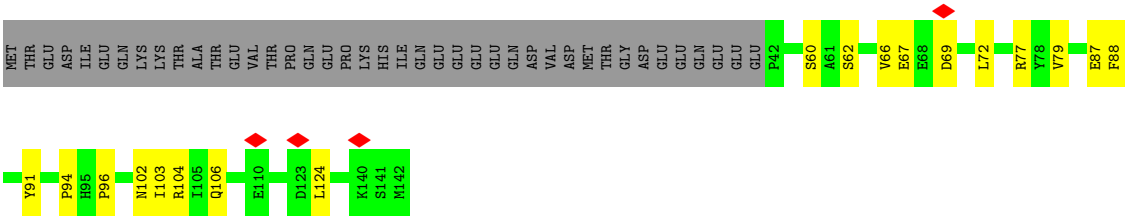
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



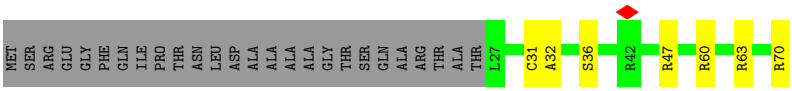
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K:



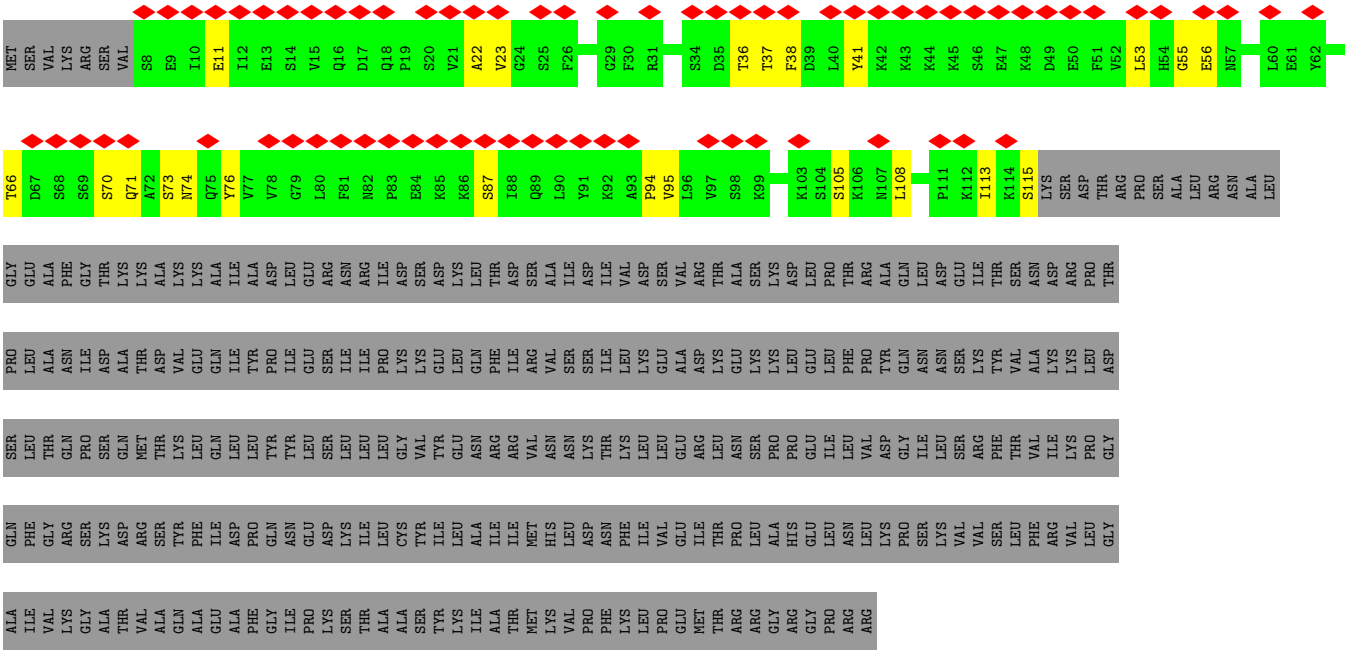
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



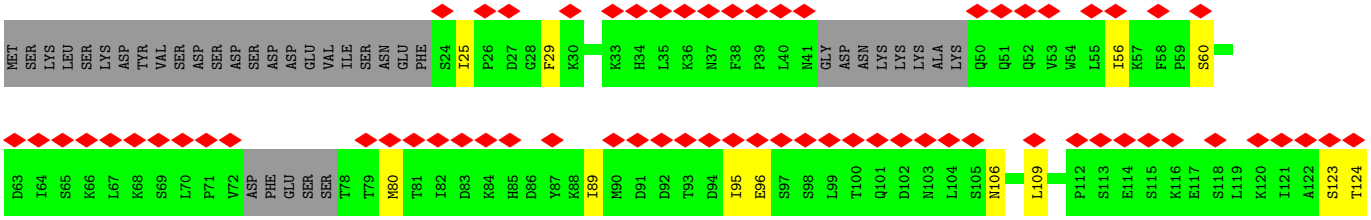
• Molecule 13: DNA-directed RNA polymerase I subunit RPA49

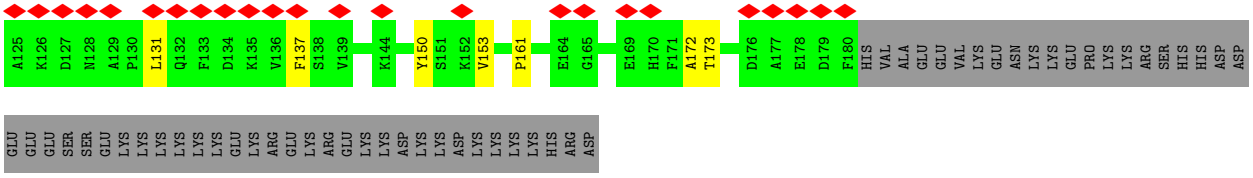
Chain M:



• Molecule 14: DNA-directed RNA polymerase I subunit RPA34

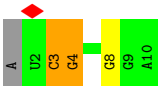
Chain N:





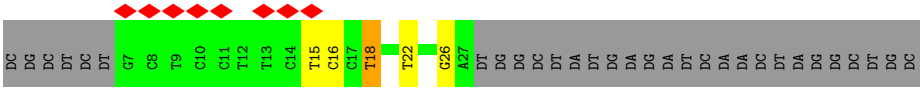
- Molecule 15: RNA

Chain R:



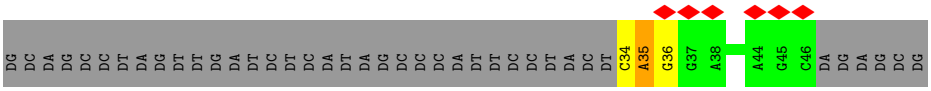
- Molecule 16: Template DNA

Chain T:



- Molecule 17: Non-template DNA

Chain U:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	254079	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	5.25	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.097	Depositor
Minimum map value	-0.054	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0162	Depositor
Map size (Å)	305.27997, 305.27997, 305.27997	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.34	0/11779	0.55	0/15907
2	B	0.36	0/9536	0.56	2/12890 (0.0%)
3	C	0.34	0/2483	0.54	0/3366
4	D	0.26	0/436	0.49	0/591
5	E	0.30	0/1770	0.50	0/2383
6	F	0.32	0/838	0.52	0/1129
7	G	0.29	0/1383	0.52	0/1886
8	H	0.32	0/1069	0.54	0/1449
9	I	0.29	0/472	0.53	0/639
10	J	0.40	0/578	0.52	0/775
11	K	0.32	0/803	0.54	0/1083
12	L	0.32	0/353	0.56	0/468
13	M	0.30	0/872	0.52	0/1170
14	N	0.26	0/1163	0.52	0/1569
15	R	0.48	0/222	1.04	1/345 (0.3%)
16	T	0.68	0/436	1.06	0/665
17	U	0.58	0/311	0.91	1/479 (0.2%)
All	All	0.35	0/34504	0.56	4/46794 (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	2
2	B	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1087	LEU	CA-CB-CG	6.43	130.09	115.30
17	U	35	DA	OP1-P-O3'	5.44	117.17	105.20
15	R	3	C	C5-C6-N1	5.12	123.56	121.00
2	B	624	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1500	GLN	Peptide
1	A	670	ILE	Peptide
2	B	783	MET	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11565	0	11657	130	0
2	B	9329	0	9227	119	0
3	C	2431	0	2418	32	0
4	D	431	0	428	8	0
5	E	1734	0	1764	11	0
6	F	823	0	841	7	0
7	G	1348	0	1351	22	0
8	H	1051	0	1021	9	0
9	I	466	0	468	10	0
10	J	569	0	586	12	0
11	K	792	0	790	15	0
12	L	351	0	374	6	0
13	M	856	0	855	15	0
14	N	1142	0	1156	14	0
15	R	198	0	98	2	0
16	T	435	0	252	5	0
17	U	275	0	144	2	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	I	1	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
19	A	1	0	0	0	0
All	All	33803	0	33430	355	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 5.

All (355) 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)
8:H:36:CYS:HA	8:H:126:GLU:O	1.75	0.86
1:A:671:GLN:HE21	1:A:934:LYS:HD3	1.59	0.68
1:A:1039:ARG:HE	1:A:1045:LEU:HD13	1.59	0.67
1:A:590:ASN:HD21	2:B:1075:GLU:HG2	1.59	0.66
13:M:73:SER:HA	14:N:60:SER:HB3	1.77	0.65
2:B:145:VAL:HB	2:B:150:GLU:HB2	1.78	0.64
3:C:228:ARG:HH22	14:N:172:ALA:HB1	1.61	0.64
2:B:379:ARG:HH21	2:B:581:PRO:HD2	1.63	0.63
13:M:41:TYR:HB3	14:N:29:PHE:HB3	1.80	0.63
1:A:15:ASP:HB2	2:B:1197:ARG:HB3	1.81	0.63
2:B:929:ARG:HH12	11:K:96:PRO:HG2	1.62	0.63
2:B:492:ASN:ND2	2:B:725:THR:OG1	2.32	0.62
2:B:1160:GLU:HG2	2:B:1166:LYS:HG2	1.82	0.62
1:A:1306:TYR:O	1:A:1499:ARG:NH2	2.33	0.61
1:A:411:VAL:HG12	1:A:416:ARG:HE	1.65	0.61
2:B:1016:GLY:O	3:C:69:ARG:NH2	2.33	0.60
10:J:8:PHE:HB2	10:J:48:ARG:HH22	1.66	0.59
9:I:30:CYS:HB3	9:I:34:LYS:H	1.67	0.59
9:I:30:CYS:SG	9:I:31:SER:N	2.75	0.59
1:A:509:GLU:OE2	1:A:584:ARG:NH2	2.36	0.59
3:C:87:ASN:ND2	3:C:201:GLU:OE2	2.36	0.59
2:B:921:HIS:NE2	2:B:965:GLU:OE1	2.34	0.59
6:F:72:LYS:HB3	6:F:142:SER:HA	1.84	0.59
11:K:60:SER:OG	11:K:104:ARG:NH2	2.36	0.59
2:B:821:ILE:HD13	2:B:897:GLU:HG2	1.84	0.58
7:G:130:GLY:HA2	7:G:233:VAL:H	1.69	0.58
13:M:37:THR:O	13:M:55:GLY:HA2	2.03	0.58
2:B:253:LEU:HD22	2:B:257:GLN:HB2	1.84	0.58
1:A:461:GLU:HG3	1:A:462:LYS:HG3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:237:HIS:HB2	7:G:244:SER:HB3	1.85	0.58
2:B:1103:VAL:HG22	2:B:1110:ILE:HG22	1.85	0.58
6:F:135:ARG:NH2	7:G:92:ALA:O	2.36	0.58
7:G:48:SER:HA	7:G:114:GLY:O	2.04	0.58
8:H:15:VAL:HG22	8:H:26:ILE:HG12	1.85	0.58
2:B:1158:ILE:HG13	2:B:1168:VAL:HG22	1.86	0.57
11:K:87:GLU:N	11:K:106:GLN:O	2.37	0.57
3:C:105:PRO:HB2	3:C:187:ALA:HB3	1.86	0.57
1:A:1028:GLU:HG3	1:A:1637:PRO:HD2	1.86	0.57
2:B:322:ASN:ND2	13:M:105:SER:O	2.37	0.57
2:B:1128:CYS:SG	2:B:1129:ARG:N	2.78	0.57
1:A:1294:MET:O	1:A:1469:TRP:HA	2.05	0.57
1:A:748:ASN:HA	1:A:771:PHE:O	2.05	0.56
11:K:88:PHE:HB3	11:K:106:GLN:HB2	1.87	0.56
12:L:31:CYS:HB3	12:L:36:SER:H	1.70	0.56
1:A:468:ARG:NH2	16:T:18:TTD:O4P	2.38	0.56
3:C:278:GLU:OE2	3:C:281:ARG:NH1	2.38	0.56
2:B:609:ARG:NH2	2:B:668:GLU:OE1	2.38	0.56
12:L:31:CYS:SG	12:L:32:ALA:N	2.78	0.56
1:A:712:ILE:H	11:K:106:GLN:HE22	1.53	0.56
2:B:70:GLU:HG2	2:B:98:SER:HB3	1.87	0.56
2:B:295:ASN:ND2	14:N:95:ILE:O	2.38	0.56
5:E:161:LYS:NZ	5:E:193:GLY:O	2.38	0.56
1:A:1316:VAL:HG21	1:A:1498:ILE:HG23	1.88	0.56
2:B:210:ARG:NH2	2:B:400:GLN:O	2.38	0.56
2:B:218:ILE:HD12	2:B:391:PRO:HB3	1.87	0.56
1:A:216:ARG:NH2	1:A:338:VAL:O	2.39	0.56
11:K:66:VAL:HG12	11:K:67:GLU:HG2	1.88	0.56
2:B:368:GLN:O	2:B:372:ARG:NH1	2.39	0.55
1:A:1180:ASN:OD1	6:F:87:LYS:NZ	2.39	0.55
2:B:1038:HIS:NE2	15:R:8:G:O2'	2.39	0.55
2:B:29:PRO:HG2	2:B:177:PRO:HG2	1.88	0.55
2:B:202:LEU:HD23	2:B:488:ALA:HB2	1.88	0.55
1:A:964:LYS:NZ	2:B:672:MET:O	2.39	0.55
1:A:94:LEU:HD12	1:A:355:PHE:HB3	1.88	0.55
2:B:736:ARG:NH2	2:B:738:ASP:OD2	2.37	0.55
3:C:129:GLU:OE2	3:C:174:ARG:NH1	2.39	0.55
1:A:1336:GLN:NE2	1:A:1482:LYS:O	2.39	0.55
2:B:883:GLU:OE1	2:B:906:ARG:NH1	2.39	0.55
1:A:1049:MET:HB2	5:E:208:TYR:HE1	1.72	0.55
2:B:782:ASP:O	2:B:950:ASN:ND2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:104:ARG:HH21	11:K:106:GLN:HE21	1.55	0.55
2:B:216:ALA:HB2	2:B:380:LYS:HE2	1.88	0.54
13:M:71:GLN:NE2	13:M:95:VAL:O	2.40	0.54
2:B:470:LEU:HD21	2:B:476:LEU:HD12	1.89	0.54
1:A:6:PRO:HA	7:G:111:THR:HG21	1.90	0.54
2:B:799:GLY:O	2:B:1035:ARG:NH1	2.39	0.54
3:C:75:VAL:HB	3:C:221:PRO:HG3	1.90	0.54
2:B:838:GLU:O	12:L:63:ARG:NH2	2.41	0.54
2:B:1017:ALA:O	3:C:65:ASN:ND2	2.40	0.54
1:A:683:LYS:NZ	8:H:41:ASP:OD2	2.39	0.54
1:A:828:CYS:SG	1:A:829:GLY:N	2.79	0.53
5:E:200:ARG:HD2	5:E:208:TYR:HD2	1.73	0.53
9:I:10:CYS:SG	9:I:37:TYR:OH	2.65	0.53
2:B:788:ILE:HB	2:B:948:ILE:HB	1.91	0.53
3:C:88:ASN:O	12:L:60:ARG:NH1	2.41	0.53
1:A:753:ASN:ND2	1:A:780:ILE:O	2.42	0.53
2:B:527:PHE:HE1	2:B:651:ARG:HB2	1.73	0.53
14:N:25:ILE:HD12	14:N:29:PHE:HB2	1.91	0.53
1:A:1237:GLN:HA	1:A:1521:THR:O	2.08	0.53
2:B:914:GLY:HA2	2:B:926:VAL:HG13	1.90	0.53
8:H:11:GLN:NE2	8:H:52:GLN:OE1	2.41	0.53
9:I:57:PRO:HA	9:I:61:ARG:HD3	1.89	0.53
2:B:1157:GLN:HE21	2:B:1169:GLY:HA2	1.73	0.53
7:G:51:PRO:HA	7:G:54:LEU:HG	1.91	0.53
1:A:648:LEU:O	1:A:652:ASN:ND2	2.42	0.52
3:C:328:LEU:HD22	11:K:72:LEU:HD21	1.90	0.52
1:A:662:SER:OG	1:A:1576:SER:O	2.27	0.52
2:B:698:SER:O	2:B:702:ASN:ND2	2.41	0.52
8:H:107:VAL:HB	8:H:111:LEU:HD11	1.90	0.52
1:A:653:THR:O	1:A:667:ARG:NH1	2.41	0.52
6:F:99:LEU:HD23	7:G:112:PRO:HD3	1.91	0.52
1:A:1608:SER:O	1:A:1612:LYS:NZ	2.40	0.52
7:G:70:VAL:HG12	7:G:71:MET:HG2	1.92	0.52
1:A:589:MET:O	1:A:600:MET:HA	2.10	0.52
1:A:995:TYR:OH	2:B:715:ASN:ND2	2.43	0.51
1:A:1491:GLU:HG3	1:A:1495:LYS:HE2	1.91	0.51
2:B:219:ARG:NH1	17:U:34:DC:OP1	2.43	0.51
1:A:697:TYR:OH	1:A:703:GLU:OE2	2.26	0.51
2:B:745:GLN:OE1	3:C:93:GLN:NE2	2.43	0.51
5:E:178:ILE:HD12	5:E:212:ARG:HG3	1.92	0.51
2:B:20:GLU:OE2	2:B:24:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:782:ASP:HA	2:B:786:ALA:HB3	1.93	0.51
1:A:495:ILE:HG22	1:A:605:VAL:HA	1.93	0.51
1:A:1047:GLN:NE2	1:A:1587:ASP:OD2	2.41	0.51
1:A:1508:VAL:HG12	1:A:1510:PRO:HD3	1.92	0.51
2:B:218:ILE:HD11	2:B:384:LEU:HD11	1.91	0.51
1:A:1482:LYS:NZ	2:B:307:GLU:OE1	2.41	0.50
5:E:200:ARG:HB2	5:E:208:TYR:HB3	1.92	0.50
13:M:70:SER:O	13:M:74:ASN:ND2	2.45	0.50
1:A:799:GLU:HG2	1:A:1062:HIS:HB2	1.93	0.50
7:G:147:LEU:HD21	7:G:229:LEU:HD23	1.94	0.50
1:A:509:GLU:OE1	1:A:515:ASN:ND2	2.44	0.50
2:B:311:ARG:HE	9:I:16:LEU:HD21	1.77	0.50
3:C:53:ASN:ND2	14:N:173:THR:O	2.45	0.50
14:N:109:LEU:HD23	14:N:131:LEU:HD23	1.93	0.50
1:A:861:VAL:HG21	1:A:892:LEU:HA	1.94	0.50
8:H:93:TYR:HD2	8:H:143:LEU:HB3	1.76	0.50
3:C:216:HIS:NE2	12:L:70:ARG:O	2.44	0.50
2:B:291:GLY:HA3	2:B:375:LEU:HD13	1.94	0.49
1:A:518:GLU:OE1	1:A:582:LYS:NZ	2.44	0.49
2:B:368:GLN:HB3	2:B:372:ARG:HH12	1.76	0.49
1:A:499:PRO:HA	1:A:502:ALA:HB3	1.93	0.49
7:G:234:ARG:HB2	7:G:246:ASP:HB3	1.94	0.49
1:A:1105:ARG:HH12	1:A:1138:GLU:HG2	1.77	0.49
1:A:114:GLU:HA	1:A:117:ARG:HG2	1.95	0.49
1:A:134:TYR:OH	1:A:215:GLU:OE1	2.31	0.49
2:B:40:GLU:OE1	2:B:550:ARG:NH2	2.43	0.49
2:B:205:MET:HG2	2:B:404:LEU:HA	1.95	0.49
1:A:1500:GLN:HG2	1:A:1502:PRO:HA	1.94	0.49
4:D:19:PRO:HG2	4:D:22:ILE:HD11	1.95	0.49
1:A:82:PRO:HG3	1:A:396:ILE:HG21	1.93	0.49
1:A:360:LEU:HD11	1:A:434:VAL:HG22	1.95	0.49
1:A:370:PRO:HB3	1:A:379:GLU:HA	1.93	0.49
2:B:676:VAL:HG12	2:B:677:THR:HG23	1.94	0.49
1:A:857:ALA:HB2	1:A:899:LYS:HD2	1.96	0.48
1:A:700:ILE:HD13	1:A:738:ASN:HB2	1.95	0.48
1:A:1657:LEU:HG	7:G:106:LYS:HA	1.95	0.48
4:D:80:THR:O	4:D:84:SER:OG	2.26	0.48
1:A:79:ILE:O	1:A:359:VAL:HA	2.13	0.48
1:A:911:CYS:O	1:A:915:GLY:N	2.44	0.48
1:A:1498:ILE:HG22	1:A:1499:ARG:HG3	1.94	0.48
5:E:10:SER:OG	5:E:14:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:66:THR:HB	13:M:71:GLN:HG3	1.93	0.48
1:A:1619:CYS:HA	1:A:1622:LEU:HB3	1.96	0.48
1:A:1646:LEU:HD22	7:G:109:PRO:HB3	1.95	0.48
2:B:111:ASP:HB3	12:L:47:ARG:HH22	1.79	0.48
6:F:106:PRO:HG2	7:G:55:GLU:HG3	1.95	0.48
11:K:62:SER:HA	11:K:103:ILE:O	2.13	0.48
13:M:11:GLU:HB3	13:M:87:SER:HA	1.96	0.48
13:M:38:PHE:HB3	13:M:53:LEU:HD11	1.95	0.48
1:A:855:ARG:NH1	1:A:866:LYS:O	2.45	0.48
1:A:690:GLU:HB3	11:K:77:ARG:HH22	1.78	0.48
2:B:19:LEU:HD11	10:J:25:LEU:HB3	1.96	0.47
2:B:35:PHE:HE2	2:B:764:ASN:HD21	1.62	0.47
2:B:253:LEU:HD11	2:B:259:THR:HG23	1.96	0.47
2:B:910:THR:OG1	2:B:912:GLN:NE2	2.40	0.47
4:D:42:SER:HA	4:D:45:ASP:HB2	1.95	0.47
4:D:84:SER:HA	4:D:87:SER:HB3	1.95	0.47
9:I:28:VAL:HB	9:I:37:TYR:HB2	1.96	0.47
3:C:96:VAL:O	3:C:99:HIS:ND1	2.48	0.47
11:K:79:VAL:HG21	11:K:124:LEU:HB2	1.96	0.47
1:A:1502:PRO:O	1:A:1525:ASN:ND2	2.45	0.47
2:B:170:CYS:SG	2:B:171:HIS:N	2.87	0.47
1:A:1296:PHE:HB2	1:A:1468:LYS:HA	1.97	0.47
1:A:689:ARG:NH2	11:K:87:GLU:O	2.48	0.47
10:J:24:LEU:HB3	10:J:30:LEU:HD12	1.97	0.47
1:A:784:SER:HA	1:A:789:SER:HB2	1.97	0.46
2:B:504:HIS:HB3	2:B:542:LEU:HD23	1.95	0.46
2:B:609:ARG:HE	2:B:626:ILE:HD12	1.80	0.46
3:C:136:LEU:HB3	3:C:204:LEU:HG	1.97	0.46
6:F:117:PRO:HA	6:F:120:ILE:HD12	1.97	0.46
2:B:467:THR:HG22	16:T:26:DG:H4'	1.98	0.46
9:I:3:VAL:HG22	9:I:8:ILE:HG12	1.97	0.46
10:J:1:MET:HA	10:J:56:LEU:HB3	1.96	0.46
16:T:18:TTD:H2"	16:T:18:TTD:H6	1.51	0.46
2:B:379:ARG:HE	2:B:580:GLY:HA2	1.80	0.46
5:E:21:GLU:OE1	5:E:143:ASN:ND2	2.43	0.46
2:B:548:LYS:HE2	2:B:652:PRO:HG3	1.97	0.46
2:B:979:GLN:HE21	2:B:996:PHE:HE1	1.62	0.46
2:B:1090:ASP:O	2:B:1091:ARG:NE	2.46	0.46
2:B:107:PRO:O	2:B:171:HIS:NE2	2.38	0.46
11:K:91:TYR:HA	11:K:102:ASN:O	2.15	0.46
1:A:248:PHE:HB2	1:A:442:LYS:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:GLN:NE2	2:B:784:ASP:OD1	2.47	0.46
2:B:711:GLN:HG2	2:B:713:PRO:HD2	1.98	0.46
16:T:15:DT:H2"	16:T:16:DC:H5"	1.98	0.46
2:B:132:SER:OG	2:B:462:GLN:NE2	2.48	0.46
2:B:415:GLU:HG3	2:B:476:LEU:HD21	1.98	0.46
2:B:134:ARG:HA	2:B:162:PRO:HA	1.99	0.45
13:M:22:ALA:HA	13:M:94:PRO:HG2	1.98	0.45
13:M:113:ILE:HG22	13:M:115:SER:H	1.81	0.45
1:A:882:ILE:HG13	1:A:888:LYS:HB3	1.98	0.45
4:D:91:ARG:HB3	7:G:136:TYR:HE2	1.81	0.45
5:E:17:ARG:HH12	5:E:36:GLU:HA	1.81	0.45
2:B:322:ASN:HD22	13:M:108:LEU:HB2	1.81	0.45
6:F:107:VAL:HG12	6:F:109:VAL:H	1.81	0.45
7:G:45:LEU:HD13	7:G:47:VAL:HG13	1.99	0.45
1:A:613:THR:OG1	1:A:615:ARG:NH2	2.50	0.45
2:B:788:ILE:O	2:B:947:ILE:HA	2.16	0.45
14:N:96:GLU:OE2	14:N:106:ASN:N	2.48	0.45
1:A:464:GLU:HA	1:A:469:LYS:HD2	1.99	0.45
1:A:671:GLN:HB3	2:B:952:HIS:CG	2.52	0.45
2:B:134:ARG:HD3	2:B:160:GLY:HA3	1.97	0.45
2:B:773:VAL:O	2:B:1028:VAL:HA	2.17	0.45
1:A:1129:PRO:HA	1:A:1135:SER:HB3	1.98	0.45
1:A:1606:SER:HB3	1:A:1612:LYS:HZ2	1.80	0.45
1:A:1640:ARG:NE	1:A:1646:LEU:O	2.46	0.45
1:A:701:ARG:HA	1:A:702:PRO:HD3	1.80	0.45
9:I:8:ILE:HG22	9:I:17:LEU:HD12	1.98	0.45
7:G:134:GLU:O	7:G:150:HIS:NE2	2.50	0.45
7:G:147:LEU:HB2	7:G:155:ALA:HB3	1.99	0.45
14:N:150:TYR:HA	14:N:153:VAL:HG12	1.98	0.45
1:A:827:THR:OG1	1:A:828:CYS:N	2.49	0.44
1:A:1497:ILE:HG21	1:A:1500:GLN:HB2	1.99	0.44
10:J:36:LEU:HD22	10:J:41:LEU:HD12	1.99	0.44
1:A:821:ILE:HD13	1:A:821:ILE:HA	1.88	0.44
2:B:494:TYR:HB3	2:B:700:LEU:HD21	1.99	0.44
2:B:1076:ARG:HG3	2:B:1088:LEU:HD11	2.00	0.44
1:A:616:LEU:HD23	1:A:620:ASN:HD22	1.82	0.44
2:B:805:LYS:HB2	2:B:905:TYR:HB2	1.99	0.44
13:M:23:VAL:HB	13:M:95:VAL:HG22	1.97	0.44
1:A:15:ASP:OD2	2:B:1199:ASN:ND2	2.44	0.44
1:A:363:PRO:HG2	1:A:382:GLN:HE22	1.82	0.44
1:A:646:GLU:HB3	2:B:1084:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:995:TYR:OH	14:N:161:PRO:O	2.32	0.44
2:B:1058:GLN:HB2	2:B:1096:SER:HB2	2.00	0.44
4:D:86:ILE:HA	4:D:89:LEU:HB2	2.00	0.44
2:B:28:PRO:HG2	2:B:178:TYR:HD1	1.83	0.44
1:A:211:THR:HB	5:E:173:SER:HB2	1.98	0.44
1:A:499:PRO:HG2	1:A:610:ASN:H	1.82	0.44
1:A:1246:VAL:O	1:A:1517:ARG:NH2	2.51	0.44
1:A:1542:THR:HG22	5:E:149:LEU:HD11	2.00	0.44
2:B:796:ARG:NH2	10:J:8:PHE:O	2.46	0.44
3:C:51:GLU:HA	3:C:302:VAL:O	2.18	0.44
1:A:1264:SER:HA	1:A:1267:ILE:HD12	2.00	0.43
1:A:44:PRO:HG2	1:A:52:LEU:HD21	2.00	0.43
1:A:427:PHE:HA	1:A:430:ILE:HG22	2.00	0.43
1:A:722:PRO:HD2	8:H:46:LEU:HD13	1.99	0.43
2:B:940:GLU:OE2	3:C:228:ARG:NH1	2.46	0.43
2:B:1063:ARG:HB2	16:T:22:DT:H5”	1.99	0.43
3:C:255:VAL:HG11	3:C:273:ASP:HB2	2.00	0.43
1:A:1533:GLU:OE2	5:E:14:ARG:NE	2.51	0.43
2:B:703:LEU:HD22	2:B:757:TYR:HD1	1.84	0.43
2:B:709:PHE:CZ	2:B:992:PRO:HG3	2.53	0.43
7:G:44:ALA:HA	7:G:118:CYS:O	2.18	0.43
2:B:73:ILE:HB	2:B:425:ILE:HG23	2.00	0.43
3:C:227:TYR:HB3	3:C:300:PHE:CD1	2.54	0.43
7:G:45:LEU:HD12	7:G:118:CYS:HB2	2.01	0.43
1:A:478:TYR:H	2:B:1047:ARG:HB2	1.84	0.43
2:B:362:LEU:HD21	2:B:591:LYS:HB3	2.01	0.43
1:A:757:ASN:ND2	1:A:767:ASN:OD1	2.52	0.43
1:A:1038:ILE:HD11	1:A:1050:TYR:HB2	2.01	0.43
1:A:1274:GLU:HB2	9:I:47:VAL:HB	2.01	0.43
2:B:994:ASP:OD1	2:B:1007:TYR:OH	2.35	0.43
1:A:611:GLU:HB3	1:A:615:ARG:HH22	1.84	0.42
1:A:668:GLY:HA2	1:A:810:LEU:HD21	2.01	0.42
1:A:32:ILE:HG21	1:A:49:LEU:HD23	2.01	0.42
1:A:673:HIS:HD2	1:A:817:PHE:HB2	1.84	0.42
1:A:1310:LYS:NZ	1:A:1464:ASP:O	2.39	0.42
2:B:30:LYS:HA	2:B:176:SER:HB2	2.02	0.42
11:K:69:ASP:N	11:K:69:ASP:OD1	2.50	0.42
1:A:117:ARG:NH2	1:A:137:ASP:OD1	2.49	0.42
1:A:1022:CYS:HG	1:A:1615:TYR:HH	1.66	0.42
2:B:876:SER:OG	2:B:877:SER:N	2.52	0.42
14:N:80:MET:HB3	14:N:89:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:ARG:HG2	2:B:221:SER:H	1.84	0.42
2:B:314:LYS:NZ	9:I:16:LEU:O	2.47	0.42
2:B:731:VAL:HG21	10:J:59:LYS:HE3	2.00	0.42
3:C:229:LEU:HB2	3:C:293:ARG:HD3	2.01	0.42
15:R:3:C:H2'	15:R:4:G:C8	2.54	0.42
1:A:39:ASP:OD1	1:A:43:HIS:N	2.53	0.42
1:A:504:LYS:HG2	2:B:1046:VAL:HG11	2.02	0.42
1:A:942:GLN:HG2	1:A:947:LEU:HA	2.02	0.42
3:C:235:ILE:HG12	3:C:289:VAL:HG22	2.02	0.42
1:A:399:LEU:HD22	1:A:423:LEU:HD21	2.01	0.42
7:G:40:ARG:HA	7:G:122:LEU:O	2.19	0.42
10:J:41:LEU:HD22	10:J:46:CYS:HB3	2.01	0.42
1:A:390:LEU:HA	1:A:390:LEU:HD23	1.87	0.42
1:A:1037:SER:HB2	1:A:1045:LEU:HD11	2.02	0.42
2:B:236:ILE:HG21	2:B:377:MET:HE1	2.00	0.42
3:C:164:ALA:HB2	3:C:191:ILE:HB	2.01	0.42
1:A:700:ILE:HD11	1:A:735:VAL:HA	2.02	0.42
1:A:1332:GLU:HG2	1:A:1483:LEU:HD13	2.02	0.42
1:A:1322:ILE:HG21	1:A:1457:ILE:HD11	2.01	0.42
13:M:76:TYR:HD2	13:M:95:VAL:HG21	1.85	0.42
1:A:232:LYS:HG2	1:A:239:PHE:CE1	2.55	0.41
1:A:641:GLU:HA	1:A:644:ARG:HG2	2.02	0.41
1:A:1267:ILE:HG12	1:A:1296:PHE:HE1	1.85	0.41
2:B:110:ASN:HA	2:B:118:GLU:HG2	2.01	0.41
2:B:706:PHE:HE1	2:B:986:PHE:HE2	1.67	0.41
3:C:57:ILE:HG13	3:C:297:HIS:CD2	2.55	0.41
1:A:19:LEU:HG	2:B:1195:ARG:HB2	2.01	0.41
2:B:48:SER:HB3	2:B:404:LEU:HD22	2.02	0.41
2:B:228:SER:O	2:B:254:ASN:N	2.52	0.41
2:B:782:ASP:HB2	2:B:950:ASN:HB2	2.02	0.41
1:A:1314:GLN:OE1	1:A:1318:SER:OG	2.32	0.41
2:B:293:ILE:HD11	2:B:306:LEU:HD13	2.02	0.41
2:B:361:HIS:NE2	2:B:590:GLY:O	2.40	0.41
3:C:114:THR:OG1	3:C:130:ASN:OD1	2.32	0.41
8:H:111:LEU:HA	8:H:127:GLY:O	2.20	0.41
10:J:9:SER:OG	10:J:48:ARG:NH2	2.38	0.41
1:A:882:ILE:O	1:A:889:SER:OG	2.29	0.41
1:A:1270:VAL:HG11	1:A:1489:VAL:HG11	2.03	0.41
2:B:256:GLY:O	2:B:382:TYR:OH	2.36	0.41
14:N:56:ILE:HG12	14:N:137:PHE:HB2	2.00	0.41
2:B:44:PRO:HG3	2:B:551:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:752:VAL:HG21	2:B:965:GLU:HG3	2.03	0.41
3:C:301:ASN:HD22	14:N:173:THR:HB	1.85	0.41
13:M:36:THR:HA	13:M:56:GLU:O	2.21	0.41
14:N:123:SER:OG	14:N:124:THR:N	2.52	0.41
1:A:579:ARG:HH22	1:A:585:ASP:CG	2.23	0.41
3:C:134:LEU:HD13	3:C:167:LEU:HD13	2.03	0.41
3:C:237:GLN:HA	3:C:238:PRO:HD3	1.92	0.41
3:C:310:PRO:HA	3:C:313:ILE:HD12	2.02	0.41
10:J:10:CYS:SG	10:J:11:GLY:N	2.93	0.41
2:B:196:VAL:HG13	2:B:462:GLN:HG3	2.02	0.41
2:B:1079:LEU:HB2	2:B:1088:LEU:HD12	2.01	0.41
7:G:74:ASN:HB3	7:G:77:VAL:HG22	2.01	0.41
1:A:771:PHE:HZ	1:A:781:LEU:HD21	1.86	0.41
1:A:1022:CYS:SG	1:A:1615:TYR:OH	2.77	0.41
3:C:80:ALA:HB3	3:C:102:GLY:HA2	2.02	0.41
1:A:68:ASP:OD1	1:A:68:ASP:N	2.53	0.41
3:C:259:ASP:O	3:C:263:ASP:N	2.54	0.41
1:A:846:ILE:O	1:A:849:THR:OG1	2.31	0.41
1:A:1221:ARG:NH2	1:A:1544:ASN:OD1	2.54	0.41
1:A:1619:CYS:O	1:A:1623:THR:OG1	2.30	0.41
2:B:1161:ASP:OD1	2:B:1165:ASN:N	2.53	0.41
2:B:299:ASP:HB3	2:B:302:LEU:HD12	2.02	0.40
2:B:302:LEU:HD11	2:B:379:ARG:HH12	1.85	0.40
1:A:701:ARG:HH12	11:K:94:PRO:HB3	1.86	0.40
1:A:1204:THR:HG22	1:A:1206:HIS:HB3	2.02	0.40
2:B:1107:CYS:O	2:B:1197:ARG:NH1	2.54	0.40
1:A:825:ALA:HB3	2:B:1022:LEU:HD13	2.03	0.40
1:A:1566:ILE:HG21	1:A:1582:LEU:HD22	2.03	0.40
2:B:234:ILE:HG12	2:B:381:LEU:HD13	2.02	0.40
4:D:28:PRO:HB3	7:G:41:VAL:HB	2.02	0.40
1:A:1545:ASP:OD1	1:A:1546:VAL:N	2.55	0.40
3:C:195:LYS:NZ	10:J:58:GLU:OE2	2.44	0.40
3:C:252:PRO:HA	3:C:253:PRO:HD3	1.89	0.40
4:D:37:LEU:HD22	4:D:41:GLU:HB2	2.03	0.40
8:H:5:LEU:HD22	8:H:134:ASN:HB3	2.03	0.40
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.56	0.40
17:U:35:DA:H2'	17:U:36:DG:C8	2.56	0.40
1:A:184:LYS:HA	1:A:187:GLU:HG2	2.04	0.40
1:A:489:ASN:ND2	2:B:781:TYR:OH	2.55	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	1449/1664 (87%)	1341 (92%)	108 (8%)	0	100	100
2	B	1168/1203 (97%)	1077 (92%)	90 (8%)	1 (0%)	51	83
3	C	304/335 (91%)	292 (96%)	12 (4%)	0	100	100
4	D	50/137 (36%)	46 (92%)	4 (8%)	0	100	100
5	E	210/215 (98%)	194 (92%)	16 (8%)	0	100	100
6	F	98/155 (63%)	94 (96%)	4 (4%)	0	100	100
7	G	167/326 (51%)	149 (89%)	18 (11%)	0	100	100
8	H	127/146 (87%)	115 (91%)	12 (9%)	0	100	100
9	I	61/125 (49%)	56 (92%)	5 (8%)	0	100	100
10	J	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
11	K	99/142 (70%)	91 (92%)	8 (8%)	0	100	100
12	L	42/70 (60%)	37 (88%)	5 (12%)	0	100	100
13	M	106/415 (26%)	95 (90%)	11 (10%)	0	100	100
14	N	138/233 (59%)	126 (91%)	12 (9%)	0	100	100
All	All	4086/5236 (78%)	3779 (92%)	306 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	784	ASP

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	1294/1465 (88%)	1293 (100%)	1 (0%)	93	98
2	B	1026/1053 (97%)	1026 (100%)	0	100	100
3	C	270/296 (91%)	269 (100%)	1 (0%)	91	97
4	D	52/116 (45%)	52 (100%)	0	100	100
5	E	194/197 (98%)	194 (100%)	0	100	100
6	F	90/137 (66%)	90 (100%)	0	100	100
7	G	151/291 (52%)	151 (100%)	0	100	100
8	H	115/128 (90%)	115 (100%)	0	100	100
9	I	55/110 (50%)	55 (100%)	0	100	100
10	J	64/65 (98%)	64 (100%)	0	100	100
11	K	91/130 (70%)	91 (100%)	0	100	100
12	L	39/57 (68%)	39 (100%)	0	100	100
13	M	98/371 (26%)	98 (100%)	0	100	100
14	N	134/220 (61%)	134 (100%)	0	100	100
All	All	3673/4636 (79%)	3671 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1482	LYS
3	C	228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	470	HIS
1	A	489	ASN
1	A	525	ASN
1	A	590	ASN
1	A	620	ASN
1	A	639	GLN
1	A	671	GLN
1	A	673	HIS
1	A	998	HIS
2	B	182	GLN

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Mol	Chain	Res	Type
2	B	213	HIS
2	B	243	GLN
2	B	368	GLN
2	B	399	HIS
2	B	462	GLN
2	B	646	HIS
2	B	695	ASN
2	B	702	ASN
2	B	715	ASN
2	B	745	GLN
2	B	764	ASN
2	B	770	ASN
2	B	875	HIS
2	B	912	GLN
2	B	979	GLN
2	B	1089	GLN
2	B	1157	GLN
3	C	53	ASN
3	C	93	GLN
5	E	106	GLN
5	E	153	HIS
5	E	179	GLN
8	H	11	GLN
10	J	53	HIS
11	K	70	HIS
11	K	106	GLN
13	M	54	HIS
13	M	74	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	R	8/10 (80%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	R	4	G

There are no RNA pucker outliers to report.

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

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	$\#\|Z\| > 2$
16	TTD	T	18	16	42,45,46	3.25	19 (45%)	62,74,77	2.59	24 (38%)

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
16	TTD	T	18	16	-	13/22/109/110	0/5/6/6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	T	18	TTD	C2-N1	7.78	1.52	1.36
16	T	18	TTD	C5T-C6T	-7.26	1.46	1.55
16	T	18	TTD	C5-C6	-7.15	1.46	1.55
16	T	18	TTD	C2-N3	6.49	1.49	1.38
16	T	18	TTD	C2T-N3T	6.21	1.49	1.38
16	T	18	TTD	C2T-N1T	6.04	1.48	1.36
16	T	18	TTD	C2'-C3R	-5.89	1.39	1.52
16	T	18	TTD	C4T-N3T	5.33	1.45	1.37
16	T	18	TTD	C4-N3	5.10	1.45	1.37
16	T	18	TTD	C6-N1	2.90	1.51	1.46
16	T	18	TTD	C3'-C4'	-2.60	1.45	1.53
16	T	18	TTD	O2T-C2T	-2.41	1.18	1.23
16	T	18	TTD	O4-C4	-2.34	1.18	1.22
16	T	18	TTD	C6T-C6	2.27	1.63	1.56
16	T	18	TTD	O4T-C4T	-2.22	1.19	1.22
16	T	18	TTD	O2-C2	-2.20	1.19	1.23
16	T	18	TTD	C2'-C1'	-2.10	1.46	1.52
16	T	18	TTD	PB-O3R	2.10	1.66	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	T	18	TTD	C1R-N1T	-2.04	1.43	1.45

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	T	18	TTD	O4R-C1R-N1T	9.00	119.32	108.65
16	T	18	TTD	O4'-C1'-N1	5.62	115.31	108.65
16	T	18	TTD	N3-C2-N1	5.05	121.93	116.69
16	T	18	TTD	C3R-C2'-C1'	4.84	112.16	102.91
16	T	18	TTD	C4-N3-C2	-4.78	119.32	126.67
16	T	18	TTD	O2-C2-N3	-4.26	113.56	121.50
16	T	18	TTD	C5T-C6T-N1T	4.05	121.28	115.61
16	T	18	TTD	C4T-N3T-C2T	-3.96	120.58	126.67
16	T	18	TTD	C5T-C4T-N3T	3.84	119.40	116.06
16	T	18	TTD	C2'-C1'-N1	-3.78	110.48	115.59
16	T	18	TTD	C6-C5-C4	3.56	124.65	114.50
16	T	18	TTD	N3T-C2T-N1T	3.32	120.14	116.69
16	T	18	TTD	C4'-O4R-C1R	-3.26	101.57	109.45
16	T	18	TTD	C5T-C6T-C6	-3.22	84.01	89.28
16	T	18	TTD	O4-C4-C5	-3.07	120.42	122.88
16	T	18	TTD	C5-C4-N3	2.81	118.50	116.06
16	T	18	TTD	C5-C5T-C4T	2.71	122.16	113.21
16	T	18	TTD	O4'-C1'-C2'	-2.56	101.42	106.25
16	T	18	TTD	O4P-PB-O3R	2.51	116.70	106.78
16	T	18	TTD	C5M-C5T-C6T	-2.36	106.92	114.16
16	T	18	TTD	C5T-C5-C6	-2.28	85.54	88.38
16	T	18	TTD	PB-O5R-C5R	-2.26	108.42	121.68
16	T	18	TTD	O2T-C2T-N1T	-2.25	119.99	123.49
16	T	18	TTD	O4T-C4T-N3T	-2.25	116.92	120.50

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	T	18	TTD	C4R-C5'-O5'-P
16	T	18	TTD	O4'-C1'-N1-C2
16	T	18	TTD	C5R-O5R-PB-O3R
16	T	18	TTD	O4R-C4'-C5R-O5R
16	T	18	TTD	C3'-C4'-C5R-O5R
16	T	18	TTD	O4'-C1'-N1-C6
16	T	18	TTD	C2R-C1R-N1T-C6T
16	T	18	TTD	C2R-C1R-N1T-C2T

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Mol	Chain	Res	Type	Atoms
16	T	18	TTD	O4R-C1R-N1T-C6T
16	T	18	TTD	O4R-C1R-N1T-C2T
16	T	18	TTD	C2'-C3R-O3R-PB
16	T	18	TTD	O4'-C4R-C5'-O5'
16	T	18	TTD	C3R-C4R-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	T	18	TTD	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

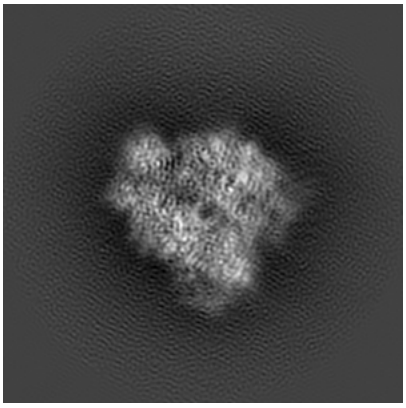
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0146. These allow visual inspection of the internal detail of the map and identification of artifacts.

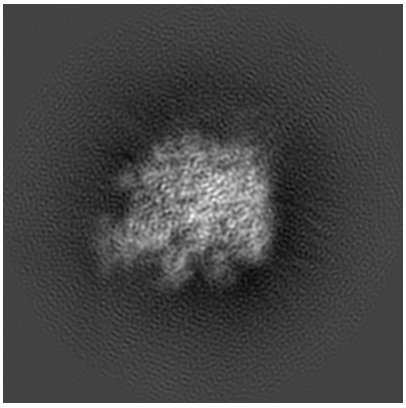
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

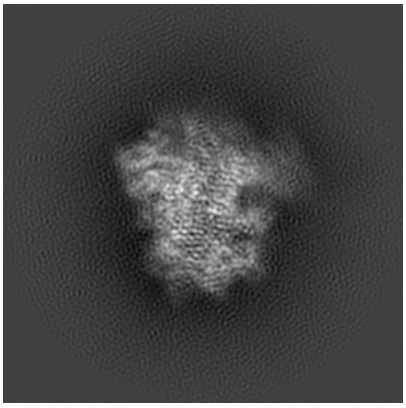
6.1.1 Primary map



X



Y

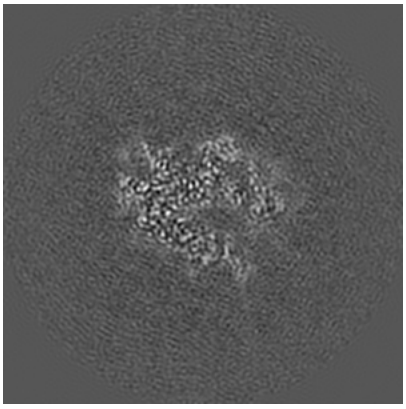


Z

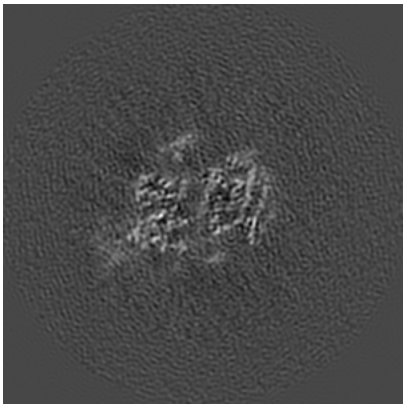
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

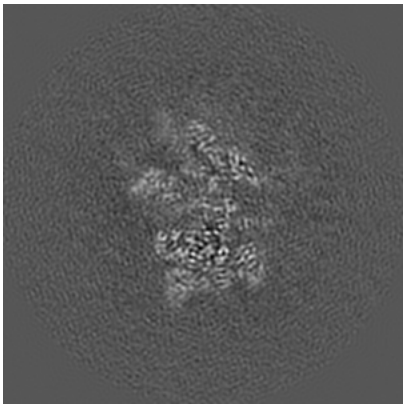
6.2.1 Primary map



X Index: 144



Y Index: 144

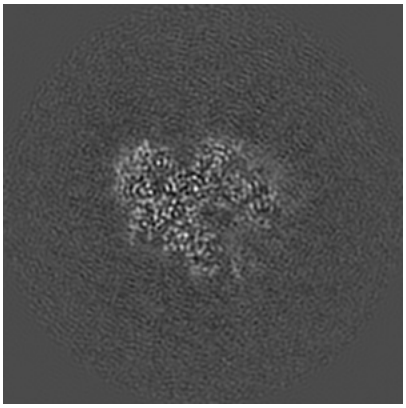


Z Index: 144

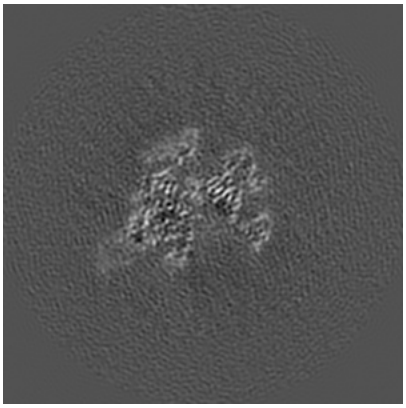
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

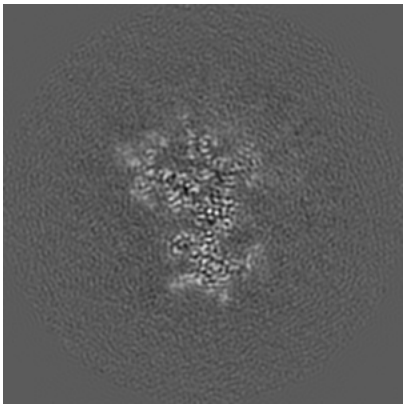
6.3.1 Primary map



X Index: 148



Y Index: 137



Z Index: 155

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0162. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

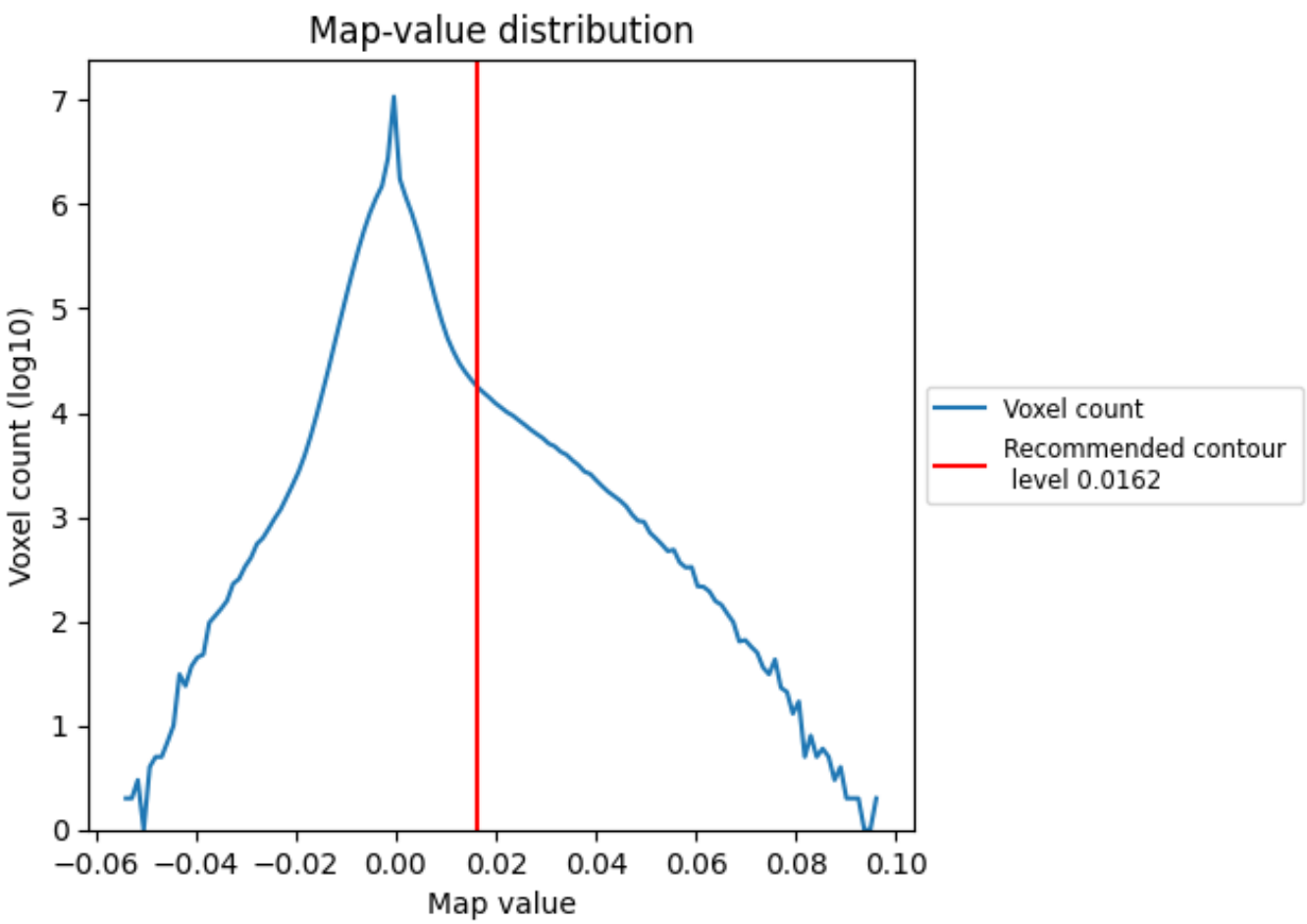
6.5 Mask visualisation (i)

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

7 Map analysis (i)

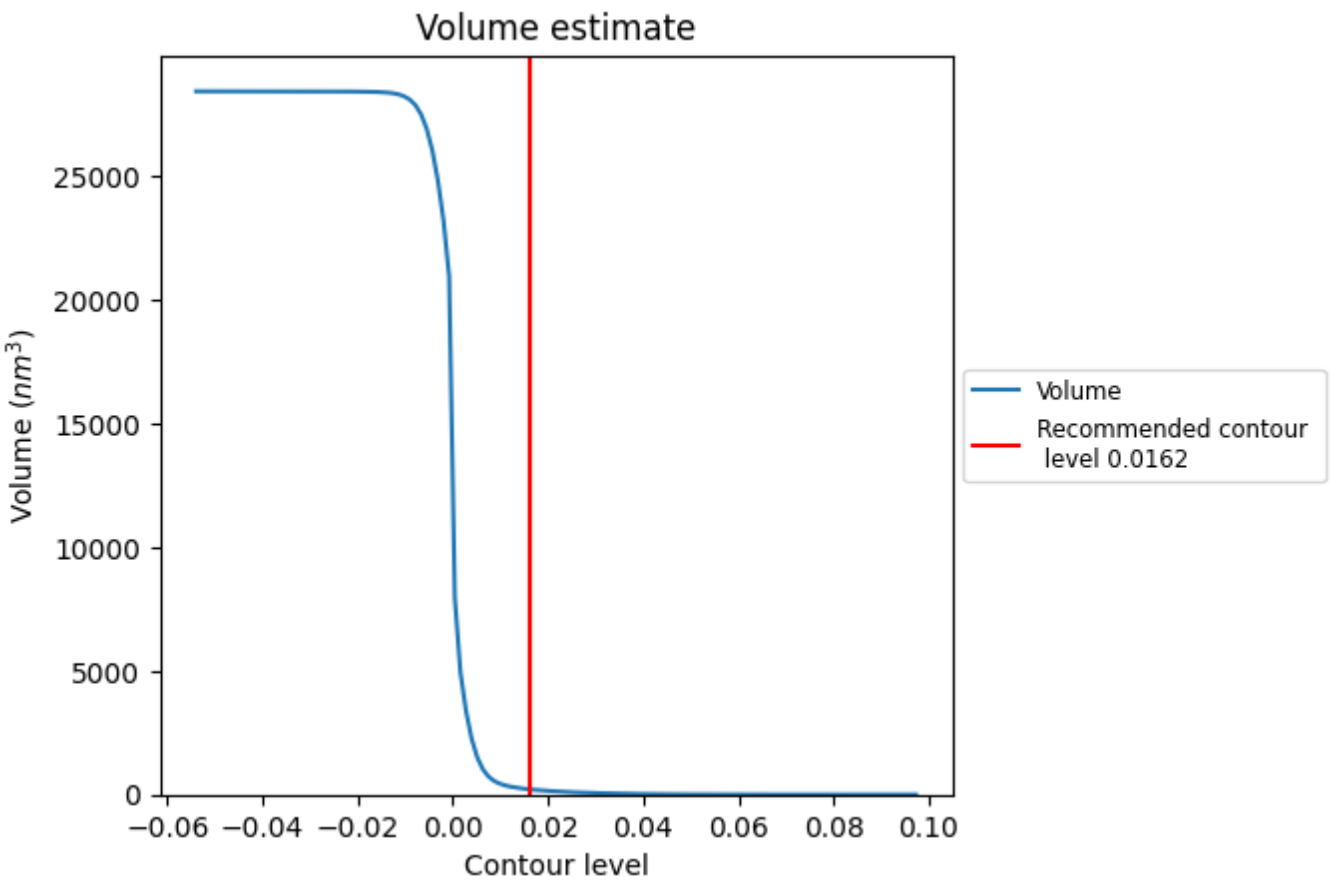
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

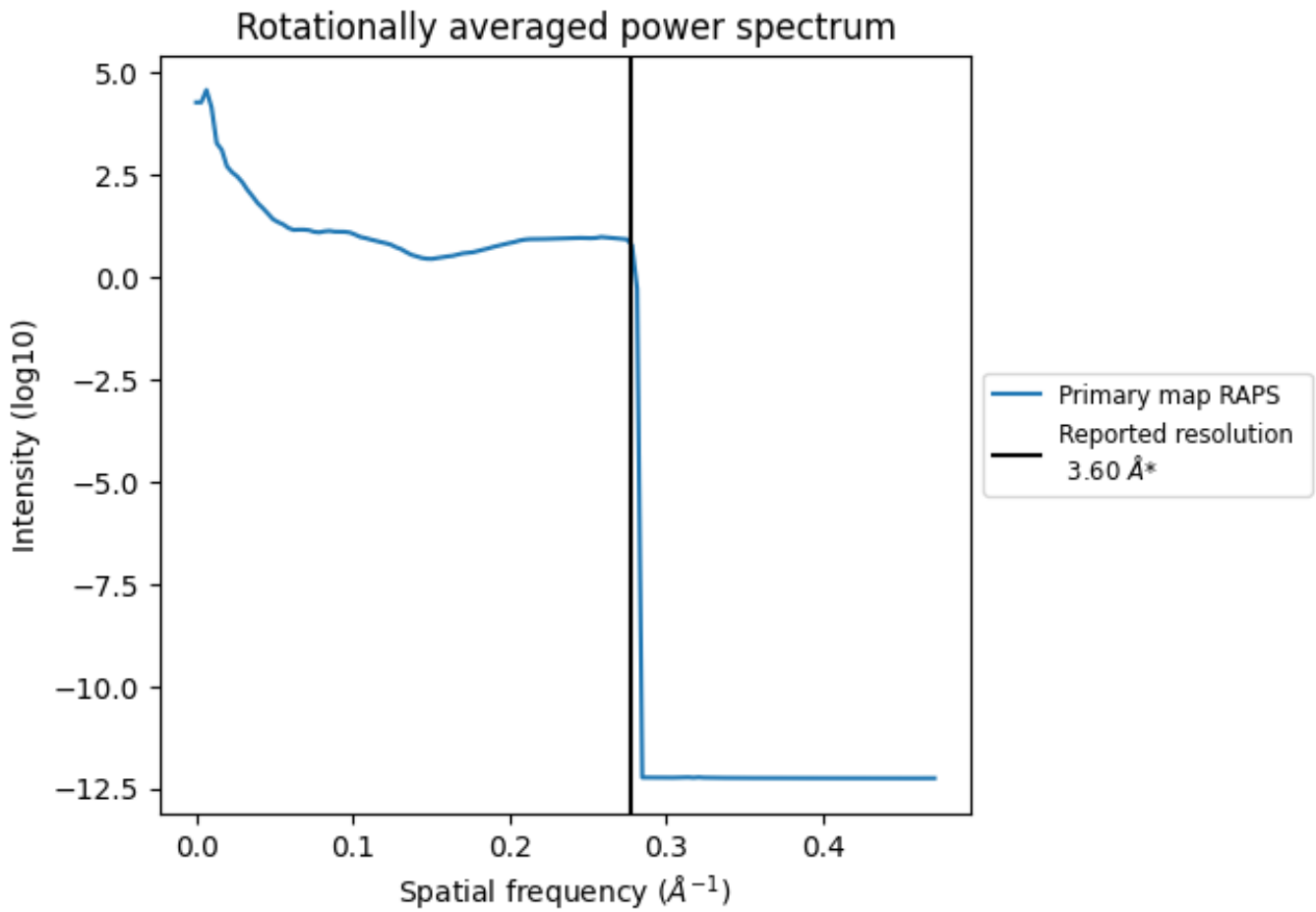
7.2 Volume estimate (i)



The volume at the recommended contour level is 210 nm^3; this corresponds to an approximate mass of 190 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 0.278 Å^{-1}

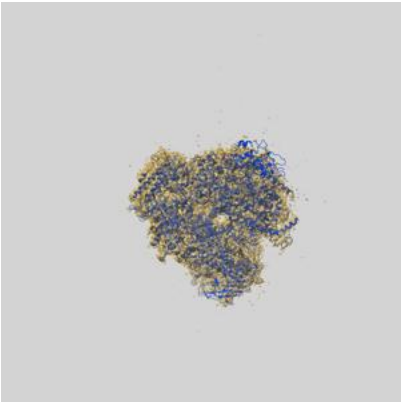
8 Fourier-Shell correlation (i)

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

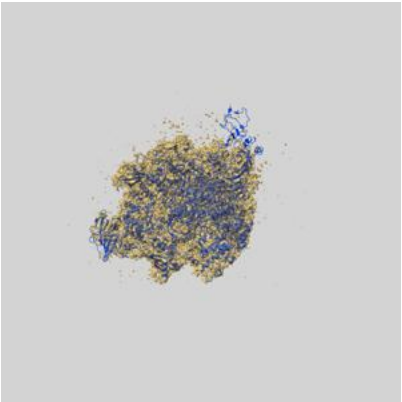
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0146 and PDB model 6H67. Per-residue inclusion information can be found in section 3 on page 7.

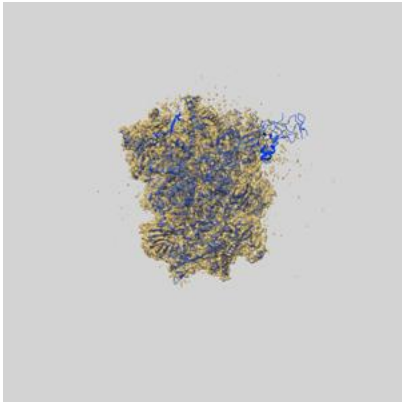
9.1 Map-model overlay (i)



X



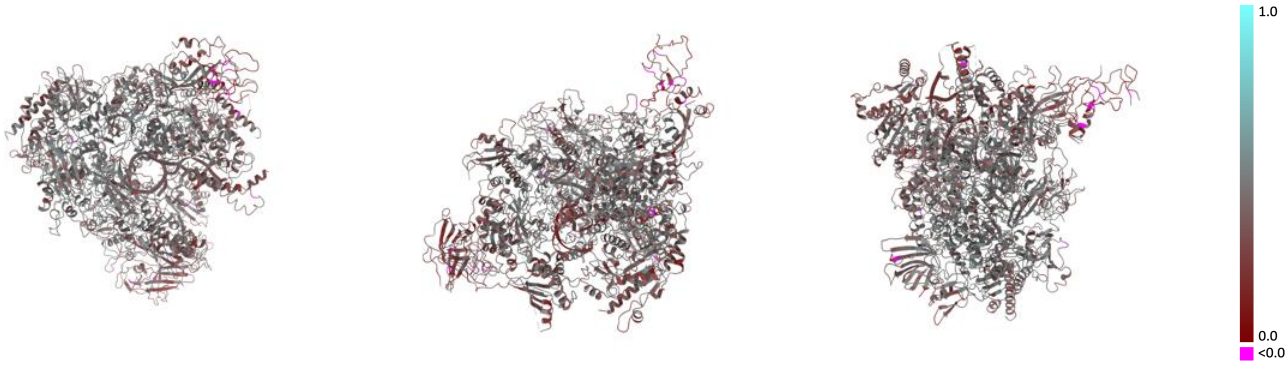
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0162 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

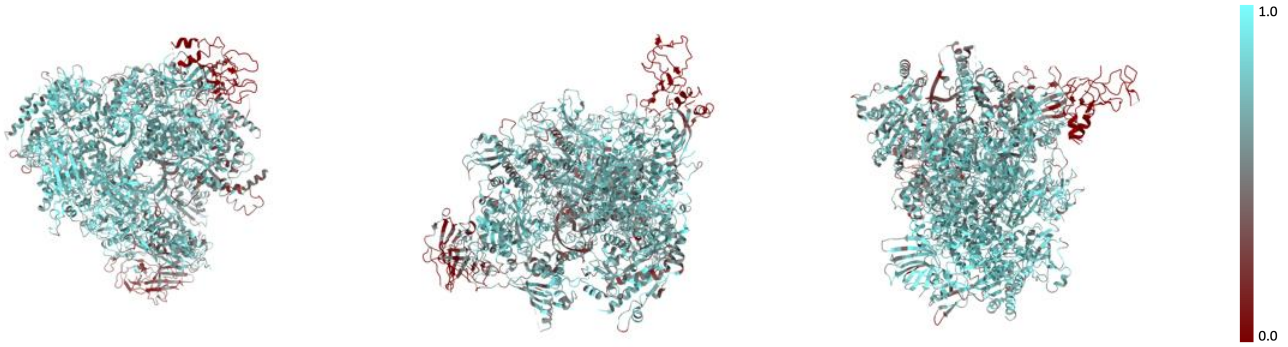
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

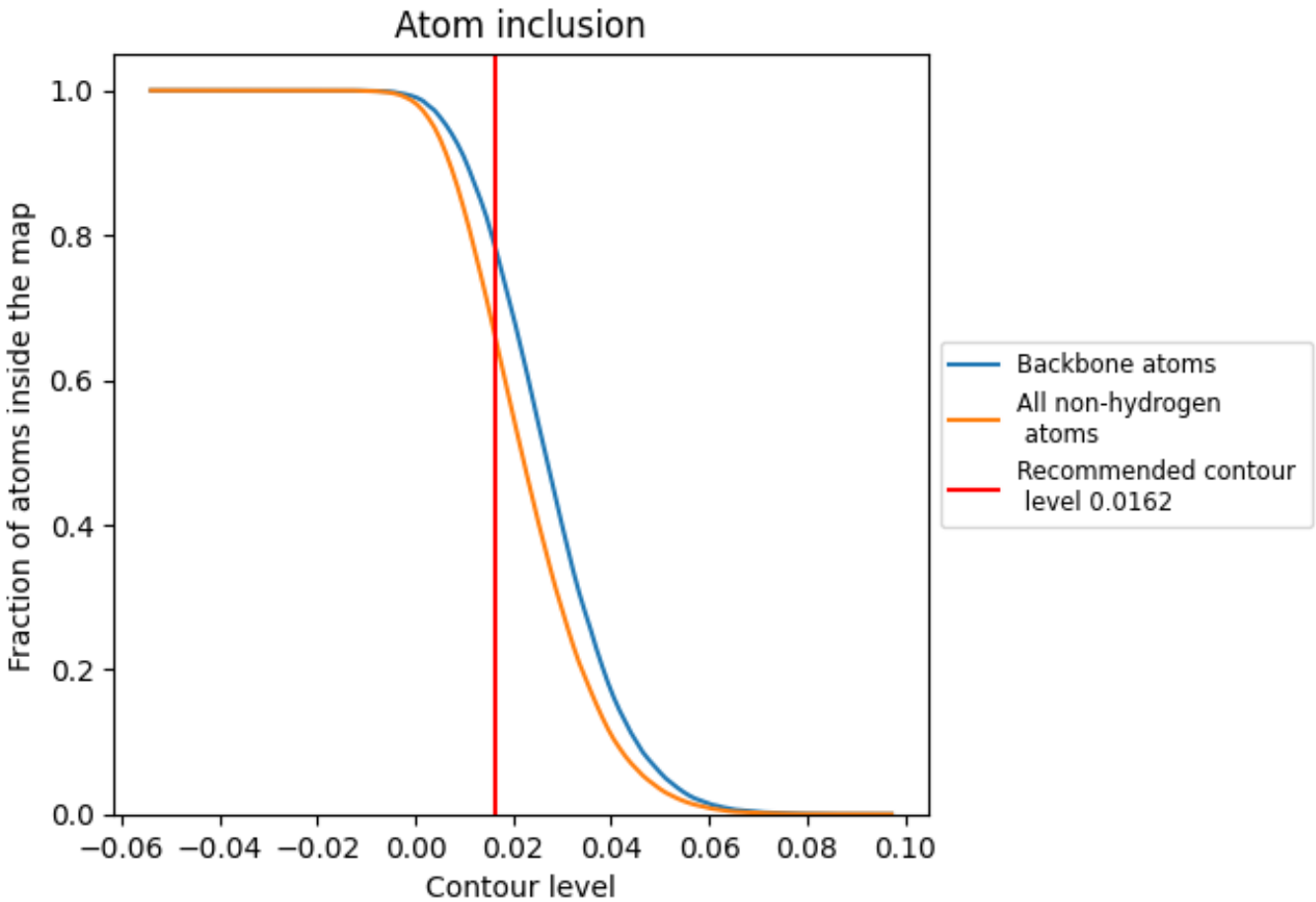
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0162).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 66% 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 (0.0162) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6634	0.4090
A	0.6925	0.4220
B	0.7425	0.4380
C	0.7398	0.4310
D	0.2061	0.3130
E	0.6404	0.3760
F	0.7253	0.4070
G	0.3421	0.3150
H	0.7220	0.4030
I	0.5086	0.3450
J	0.8116	0.4610
K	0.7510	0.4190
L	0.7670	0.4380
M	0.2698	0.2800
N	0.3219	0.3260
R	0.7475	0.4380
T	0.5724	0.3100
U	0.4655	0.2830