Full wwPDB EM Validation Report

Nov 21, 2022 – 04:24 PM JST

PDB ID	:	7D58
EMDB ID	:	EMD-30577
Title	:	cryo-EM structure of human RNA polymerase III in elongating state
Authors	:	Wang, Q.; Wan, F.; Lan, P.; Wu, J.; Lei, M.
Deposited on	:	2020-09-25
Resolution	:	2.90 Å(reported)

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

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

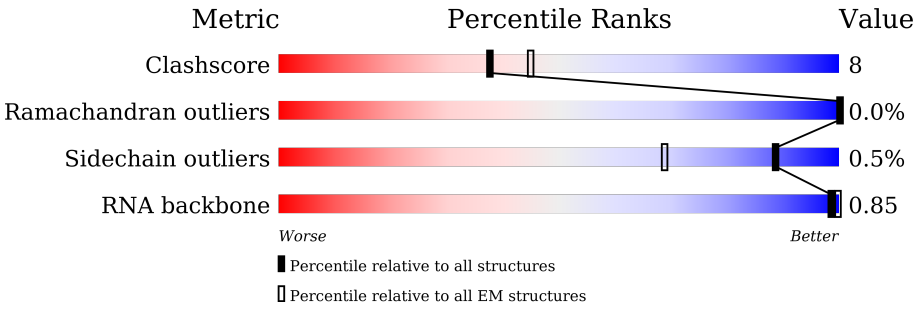
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	1390	26% 80% 19%
2	B	1133	21% 78% 18% .
3	C	346	5% 80% 20%
4	D	148	5% 61% 23% .. 15%
5	E	210	22% 82% 18%
6	F	127	10% 52% 10% 38%
7	G	204	9% 69% 22% 8%

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Mol	Chain	Length	Quality of chain
8	H	150	17% 80% 19%
9	I	108	24% 69% 30%
10	J	67	15% 90% 10%
11	K	133	5% 62% 18% 20%
12	L	58	62% 19% 19%
13	M	708	5% 24% 7% 69%
14	N	398	5% 26% 8% 66%
15	O	534	14% 72% 20% 8%
16	P	316	28% 16% 56%
17	Q	223	8% 30% 9% 61%
18	R	41	27% 15% 59%
19	S	41	7% 32% 27% 41%
20	T	20	15% 10% 15% 75%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	SF4	P	400	-	-	X	-

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 40568 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 III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1387	10886	6899	1898	2016	73	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1095	8668	5492	1513	1595	68	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	345	2752	1732	490	518	12	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	126	1013	634	176	200	3	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	210	1723	1088	301	325	9	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	79	636	407	108	116	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	187	Total	C	N	O	S	0	0
			1493	964	235	287	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	149	Total	C	N	O	S	0	0
			1197	759	195	238	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	108	Total	C	N	O	S	0	0
			857	529	158	157	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	107	Total	C	N	O	S	0	0
			856	531	153	165	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	47	Total	C	N	O	S	0	0
			397	246	77	68	6		

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	222	Total	C	N	O	S	0	0
			1797	1134	307	346	10		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	136	Total	C	N	O	S	0	0
			1038	653	188	192	5		

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	490	Total	C	N	O	S	0	0
			3913	2468	678	742	25		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	139	Total	C	N	O	S	0	0
			1103	700	178	214	11		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	86	Total	C	N	O	S	0	0
			746	482	125	133	6		

- Molecule 18 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	17	Total	C	N	O	P	0	0
			346	165	63	101	17		

- Molecule 19 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	24	Total	C	N	O	P	0	0
			493	234	90	145	24		

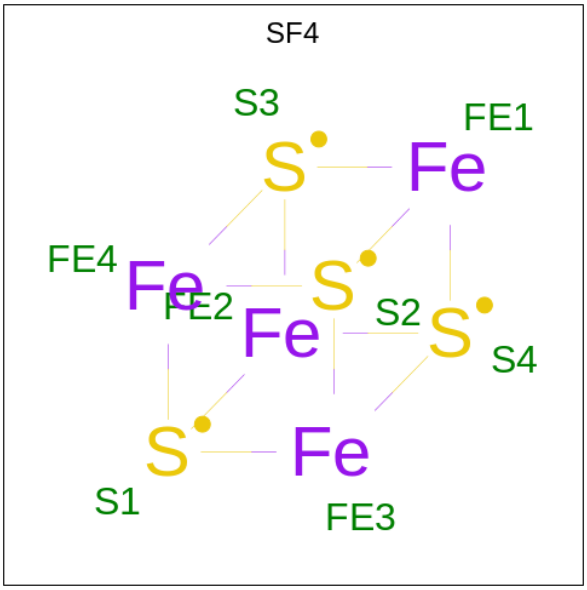
- Molecule 20 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	5	Total	C	N	O	P	0	0
			106	47	17	37	5		

- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 22 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



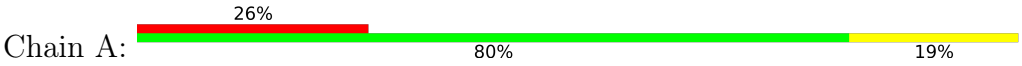
Mol	Chain	Residues	Atoms	AltConf
22	P	1	Total Fe S 8 4 4	0

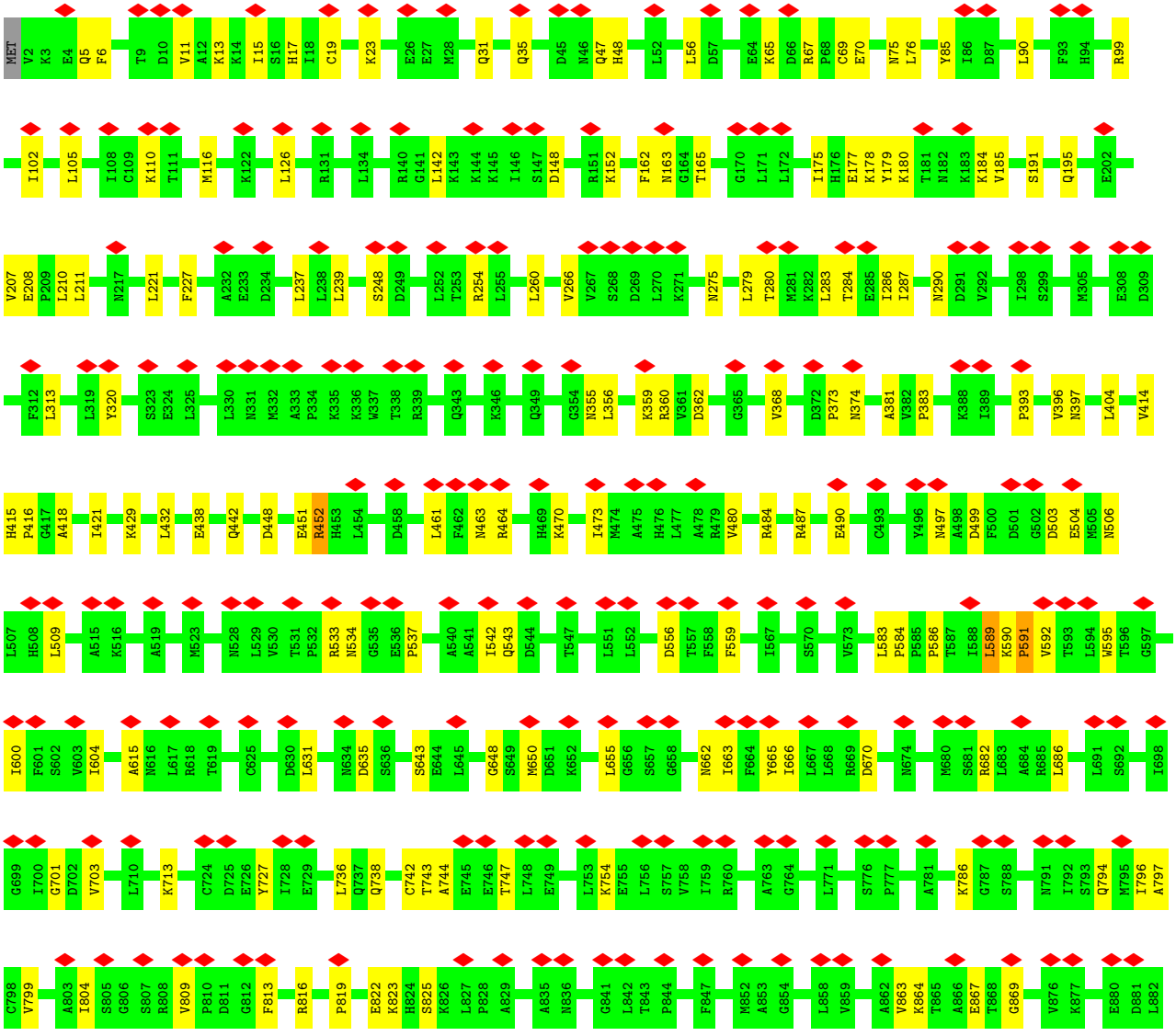
3 Residue-property plots (i)

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.

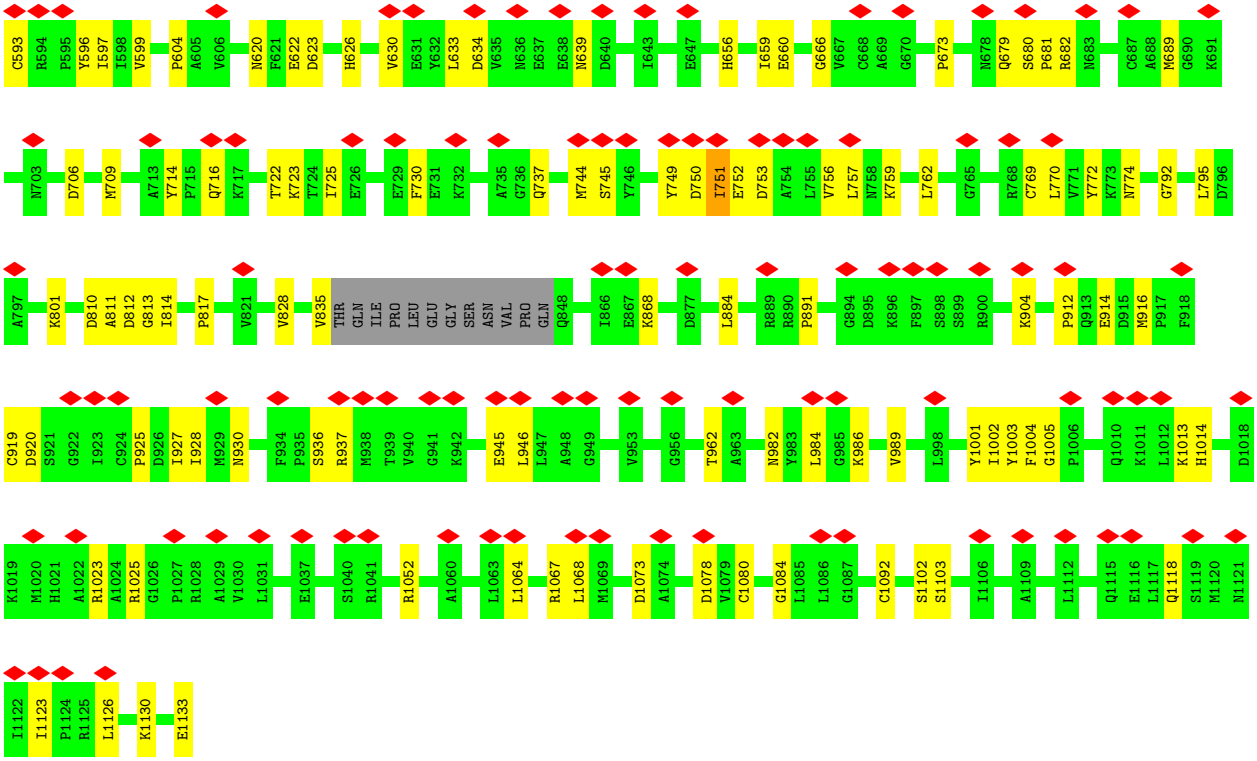
• Molecule 1: DNA-directed RNA polymerase III subunit RPC1

Chain A:

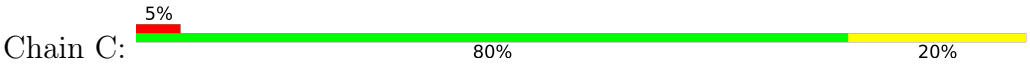


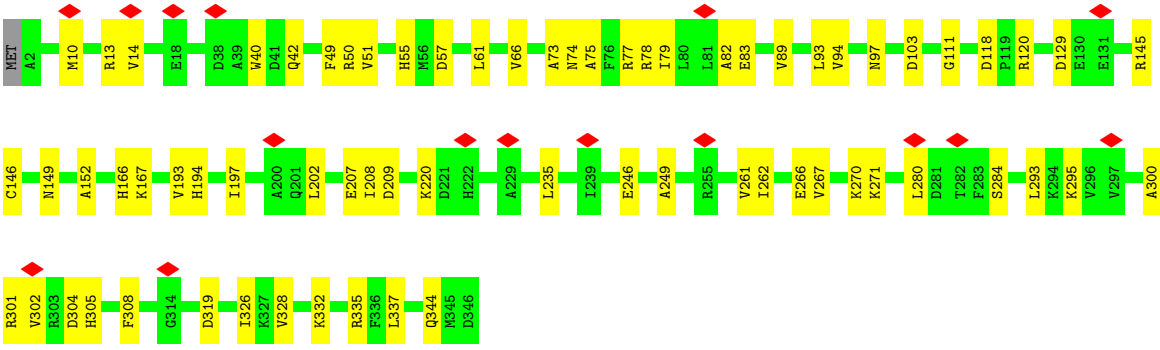


• Molecule 2: DNA-directed RNA polymerase III subunit RPC2

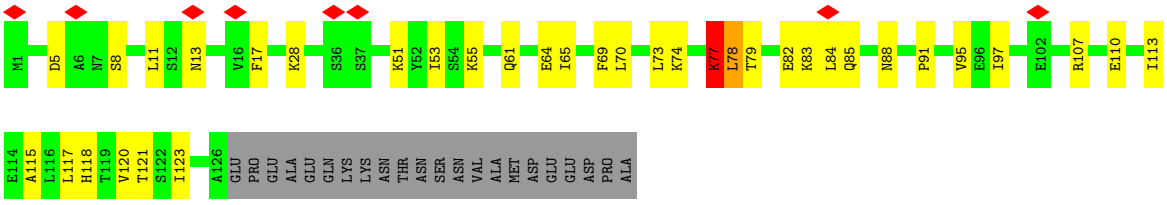


• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



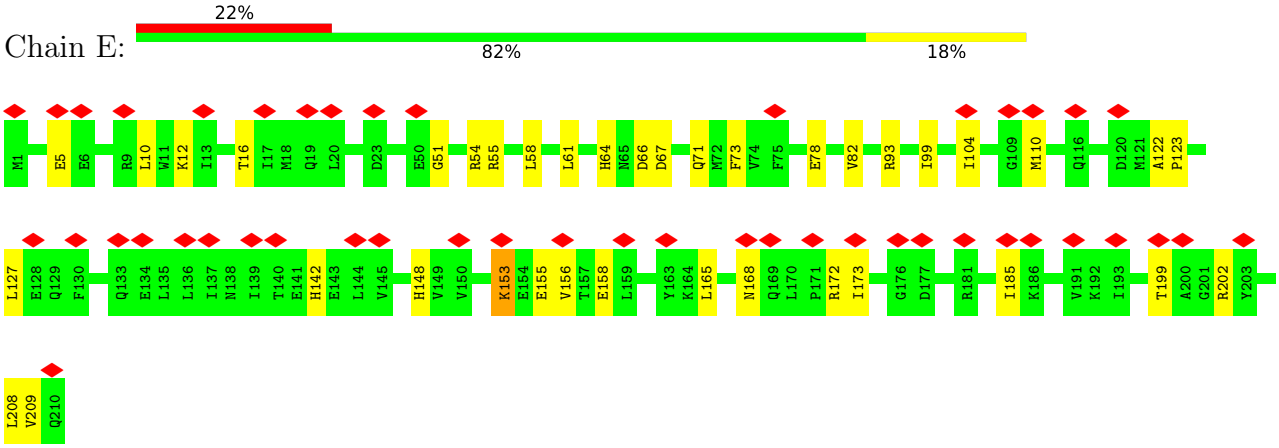


• Molecule 4: DNA-directed RNA polymerase III subunit RPC9



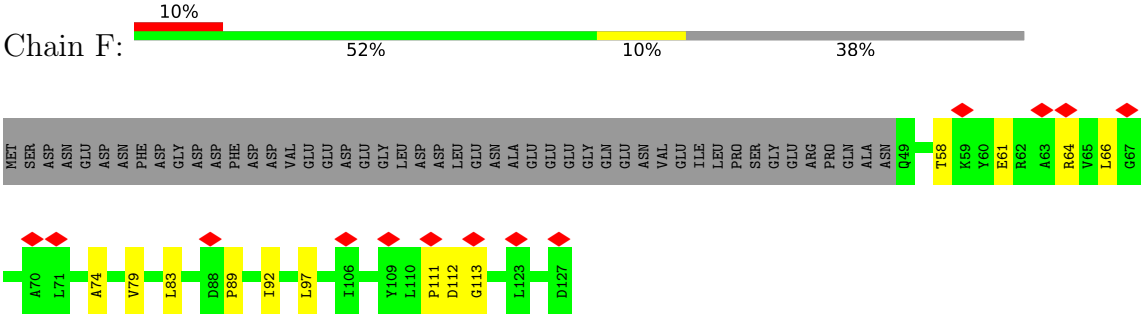
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



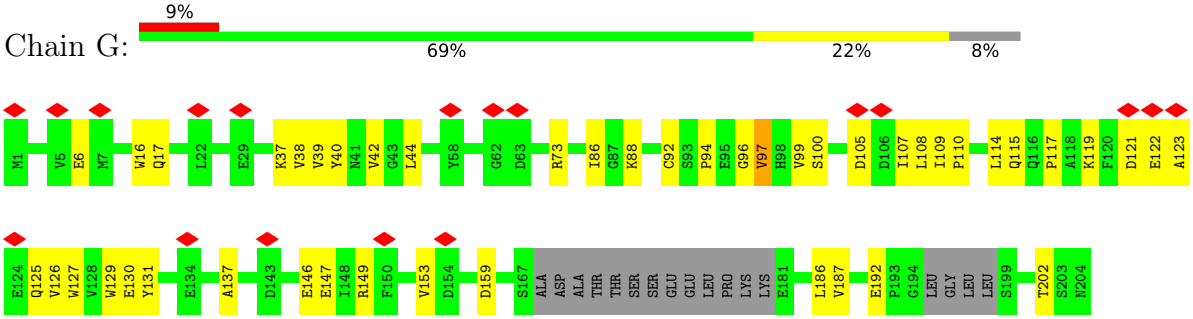
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



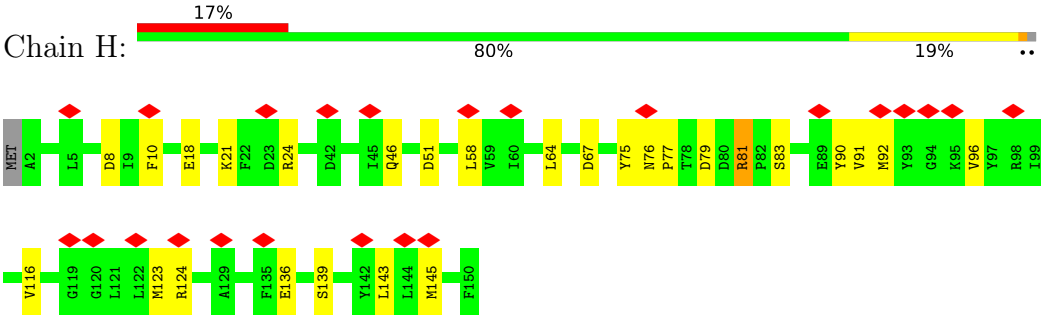
• Molecule 7: DNA-directed RNA polymerase III subunit RPC8

Chain G:



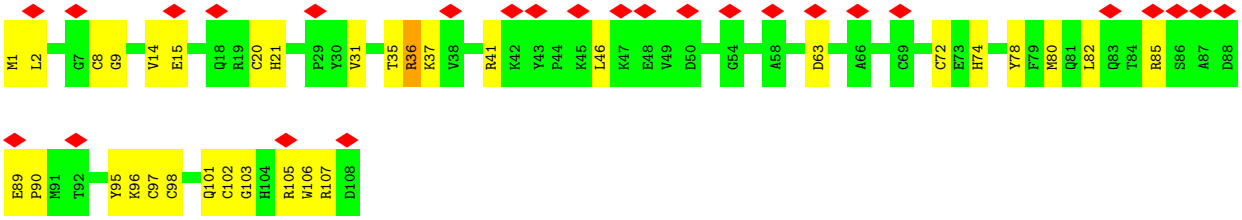
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:

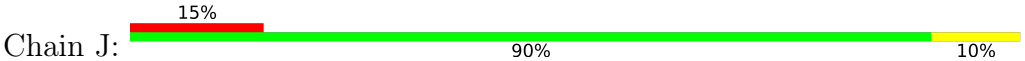


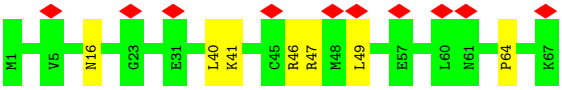
• Molecule 9: DNA-directed RNA polymerase III subunit RPC10

Chain I:

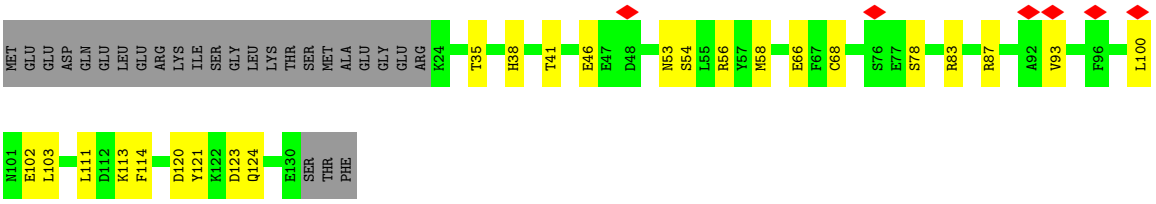


• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

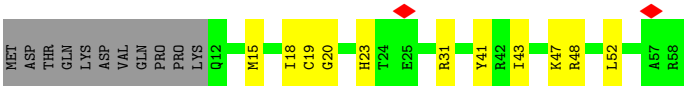




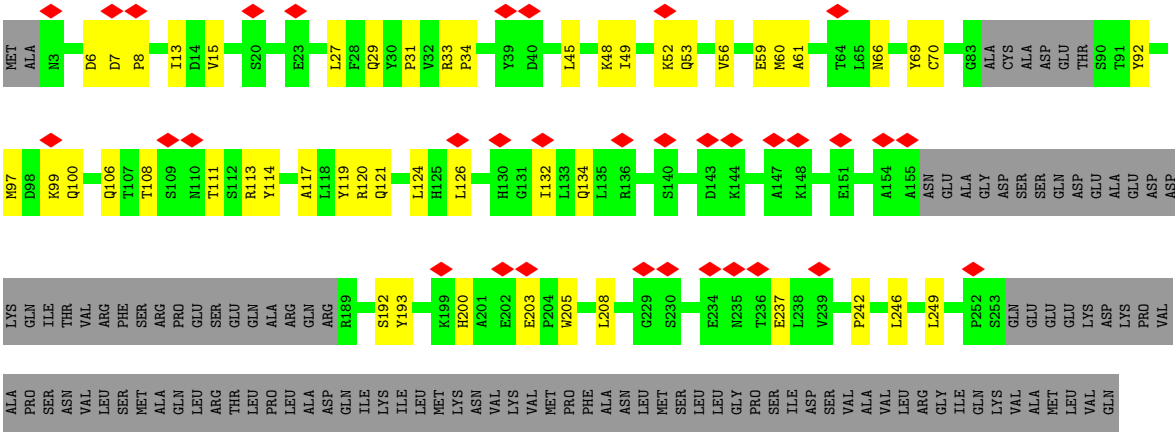
• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

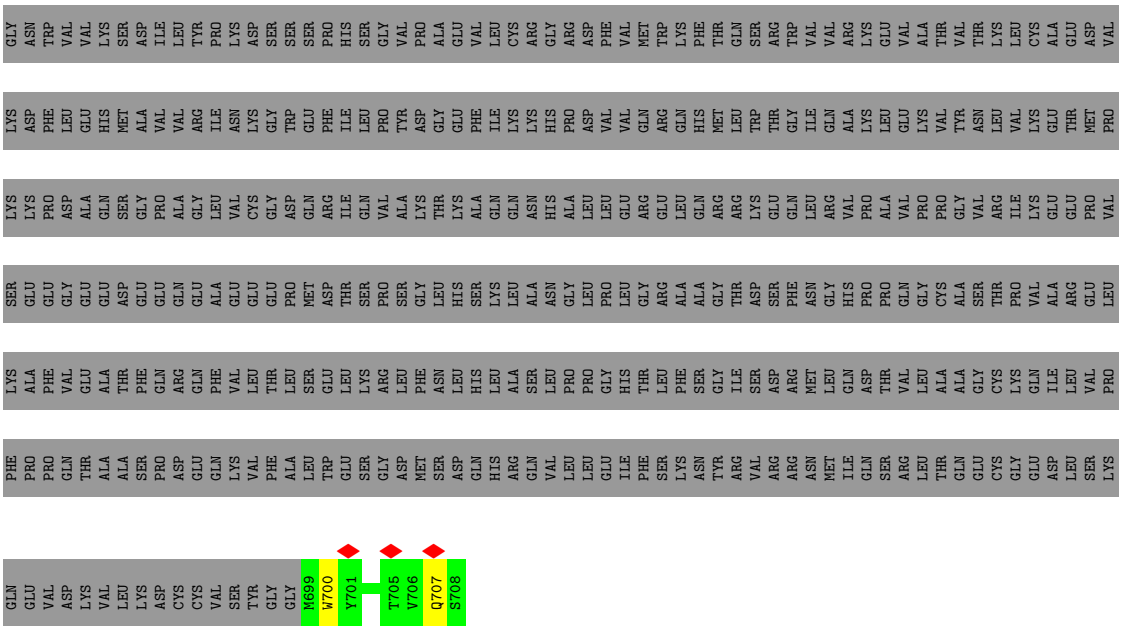


• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

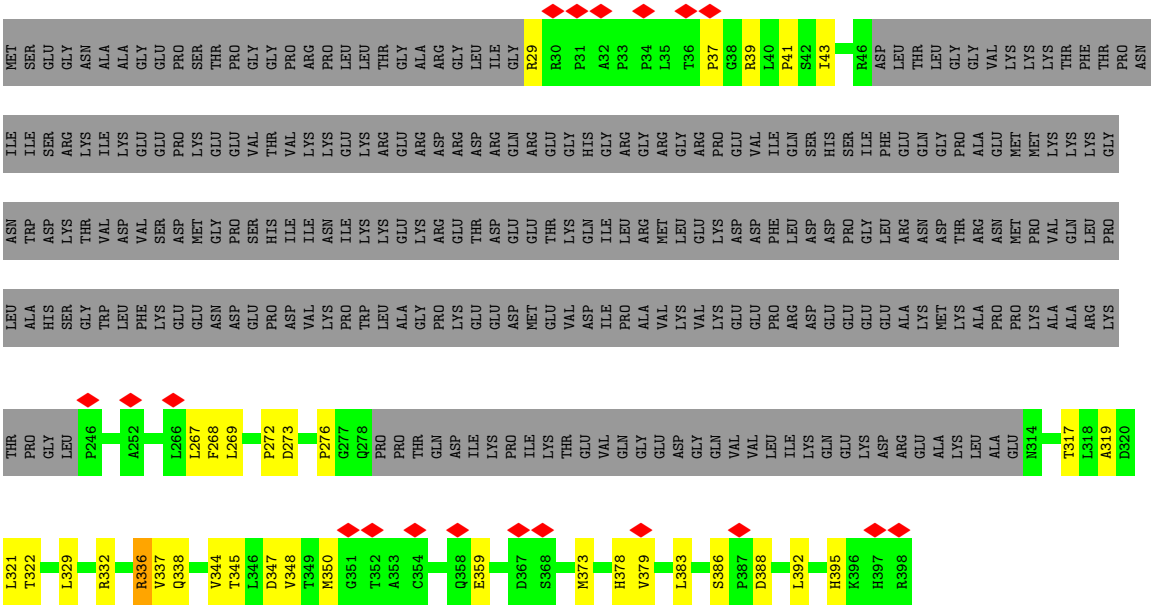


• Molecule 13: DNA-directed RNA polymerase III subunit RPC5

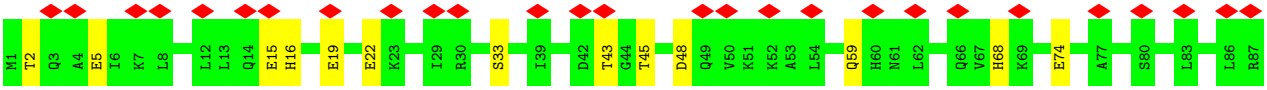


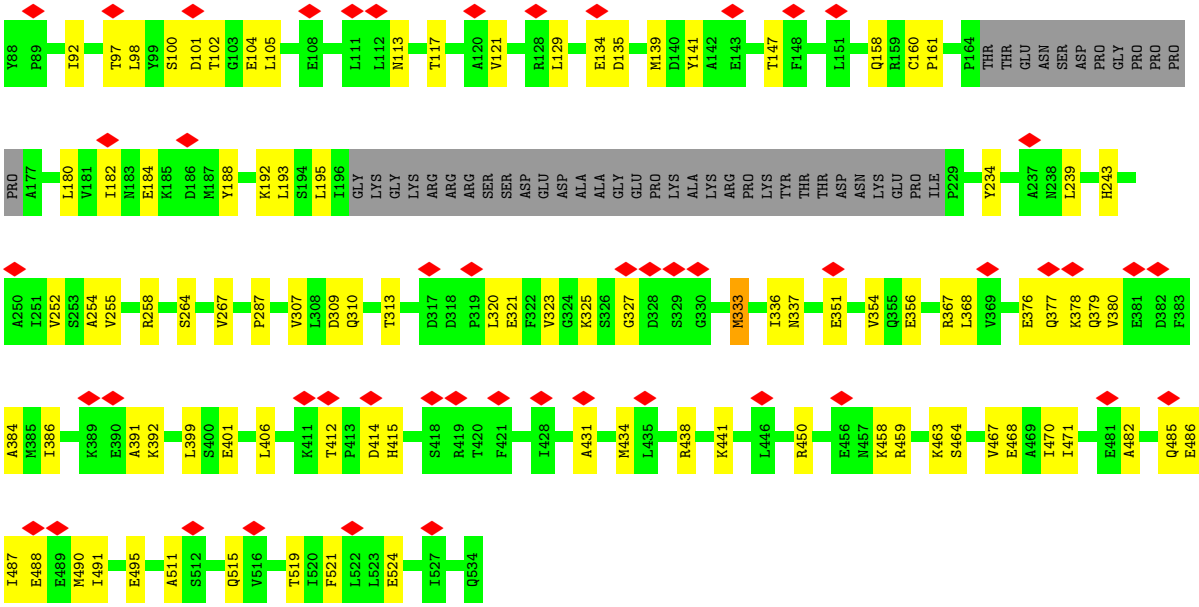


• Molecule 14: DNA-directed RNA polymerase III subunit RPC4



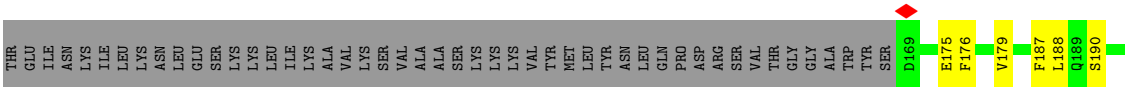
• Molecule 15: DNA-directed RNA polymerase III subunit RPC3

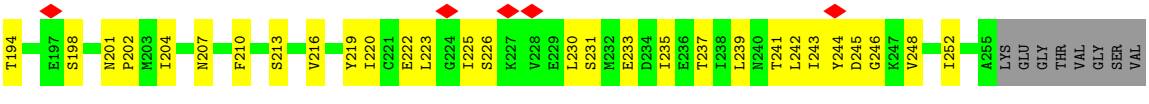


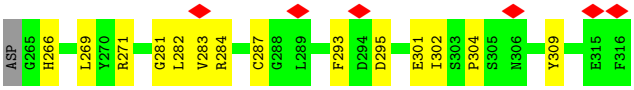


• Molecule 16: DNA-directed RNA polymerase III subunit RPC6

Chain P:

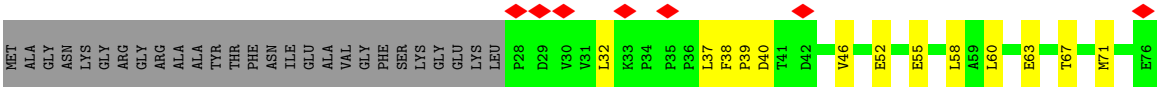


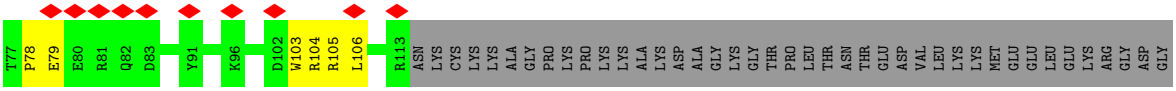


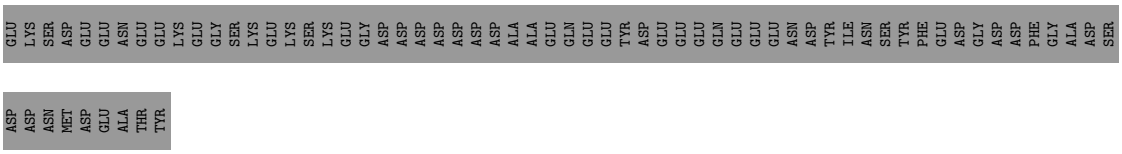


• Molecule 17: DNA-directed RNA polymerase III subunit RPC7

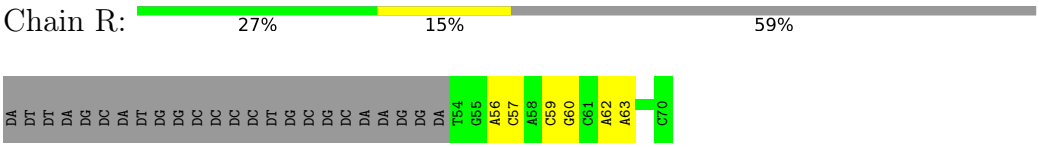
Chain Q:



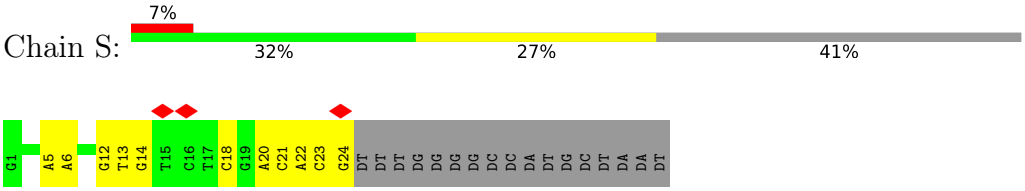




• Molecule 18: Non-template DNA



• Molecule 19: Template DNA



• Molecule 20: RNA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	155030	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.031	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	352.0, 352.0, 352.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SF4

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	0.24	0/11083	0.43	0/14946
2	B	0.24	0/8833	0.42	0/11912
3	C	0.24	0/2806	0.43	0/3803
4	D	0.23	0/1026	0.44	0/1384
5	E	0.24	0/1753	0.45	0/2368
6	F	0.23	0/646	0.39	0/873
7	G	0.25	0/1534	0.44	0/2087
8	H	0.24	0/1219	0.43	0/1644
9	I	0.25	0/878	0.46	0/1186
10	J	0.22	0/542	0.39	0/730
11	K	0.23	0/871	0.40	0/1174
12	L	0.23	0/403	0.40	0/536
13	M	0.24	0/1837	0.42	0/2481
14	N	0.25	0/1051	0.48	0/1417
15	O	0.24	0/3972	0.41	0/5359
16	P	0.26	0/1126	0.43	0/1522
17	Q	0.25	0/769	0.45	0/1038
18	R	0.46	0/387	0.88	0/594
19	S	0.48	0/552	0.86	0/850
20	T	0.11	0/117	0.68	0/180
All	All	0.25	0/41405	0.45	0/56084

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
4	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
15	O	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	589	LEU	Peptide
2	B	751	ILE	Peptide
4	D	77	LYS	Peptide
15	O	68	HIS	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	10886	0	11135	190	0
2	B	8668	0	8796	143	0
3	C	2752	0	2725	46	0
4	D	1013	0	1040	22	0
5	E	1723	0	1745	23	0
6	F	636	0	667	10	0
7	G	1493	0	1429	32	0
8	H	1197	0	1156	20	0
9	I	857	0	815	25	0
10	J	533	0	555	5	0
11	K	856	0	840	19	0
12	L	397	0	404	10	0
13	M	1797	0	1756	40	0
14	N	1038	0	1092	27	0
15	O	3913	0	3988	73	0
16	P	1103	0	1067	42	0
17	Q	746	0	749	15	0
18	R	346	0	192	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	S	493	0	271	12	0
20	T	106	0	54	4	0
21	A	2	0	0	0	0
21	B	1	0	0	0	0
21	I	2	0	0	0	0
21	J	1	0	0	0	0
21	L	1	0	0	0	0
22	P	8	0	0	3	0
All	All	40568	0	40476	653	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 8.

All (653) 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:G:92:CYS:HB2	7:G:125:GLN:HB3	1.55	0.89
7:G:96:GLY:HA3	7:G:109:ILE:O	1.73	0.88
9:I:35:THR:HG21	14:N:29:ARG:HH22	1.41	0.85
1:A:995:THR:HG22	1:A:997:PRO:HD2	1.61	0.81
7:G:99:VAL:HG13	7:G:107:ILE:HG23	1.62	0.80
9:I:80:MET:HB2	9:I:95:TYR:HB2	1.65	0.79
1:A:1143:GLU:HB2	1:A:1202:GLN:HE22	1.50	0.77
2:B:725:ILE:HG23	2:B:730:PHE:HB3	1.66	0.77
7:G:97:VAL:HG12	7:G:109:ILE:HG12	1.66	0.77
15:O:486:GLU:O	15:O:490:MET:HB3	1.85	0.76
2:B:550:ARG:NH1	14:N:350:MET:SD	2.59	0.75
8:H:107:GLU:HG3	8:H:108:ALA:H	1.52	0.75
7:G:96:GLY:CA	7:G:109:ILE:O	2.35	0.75
1:A:591:PRO:HB2	1:A:592:VAL:HG23	1.70	0.74
5:E:173:ILE:HG22	5:E:209:VAL:HA	1.69	0.74
1:A:1254:VAL:HG11	1:A:1266:THR:HG21	1.70	0.73
13:M:120:ARG:HG2	13:M:121:GLN:H	1.53	0.73
1:A:397:ASN:HD21	6:F:74:ALA:HA	1.56	0.71
16:P:187:PHE:HE2	16:P:216:VAL:HG12	1.56	0.71
15:O:412:THR:HG22	15:O:414:ASP:H	1.54	0.71
1:A:1063:ILE:HA	1:A:1082:THR:HG21	1.72	0.71
1:A:362:ASP:OD1	2:B:1023:ARG:NH1	2.24	0.70
3:C:266:GLU:HG2	3:C:271:LYS:HG3	1.73	0.70
1:A:56:LEU:HD12	1:A:260:LEU:HD11	1.72	0.70
2:B:756:VAL:HB	2:B:928:ILE:HB	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ILE:HG22	1:A:543:GLN:H	1.56	0.70
13:M:53:GLN:HE22	13:M:200:HIS:HA	1.57	0.69
1:A:1043:GLU:HG2	1:A:1044:PRO:HD3	1.74	0.69
4:D:17:PHE:HB2	4:D:53:ILE:HG21	1.73	0.69
2:B:77:TYR:OH	2:B:381:ASN:ND2	2.25	0.69
1:A:105:LEU:O	1:A:110:LYS:NZ	2.25	0.67
1:A:1089:LEU:HD11	1:A:1101:VAL:HG11	1.76	0.67
15:O:43:THR:HG23	15:O:45:THR:H	1.59	0.67
1:A:1322:GLU:HG3	1:A:1323:LYS:H	1.58	0.67
13:M:246:LEU:HB2	14:N:392:LEU:HD23	1.76	0.67
2:B:919:CYS:HB3	2:B:1004:PHE:HE2	1.59	0.66
4:D:79:THR:HB	4:D:82:GLU:HB2	1.77	0.66
7:G:117:PRO:HB2	7:G:127:TRP:HZ3	1.60	0.66
14:N:272:PRO:HG3	14:N:386:SER:HA	1.78	0.66
9:I:36:ARG:NH2	9:I:37:LYS:O	2.29	0.66
5:E:153:LYS:HA	5:E:156:VAL:HG12	1.77	0.66
15:O:15:GLU:HG3	15:O:16:HIS:HD2	1.61	0.65
16:P:309:TYR:OH	17:Q:39:PRO:O	2.14	0.65
1:A:1137:ILE:HG23	1:A:1142:LEU:HB2	1.79	0.64
7:G:110:PRO:HD3	7:G:187:VAL:HB	1.80	0.64
16:P:225:ILE:HG13	16:P:226:SER:H	1.63	0.64
1:A:414:VAL:HG12	1:A:416:PRO:HD2	1.80	0.63
1:A:1217:GLN:HB2	1:A:1220:LYS:HB3	1.79	0.63
9:I:78:TYR:HB2	9:I:97:CYS:HB3	1.80	0.63
2:B:82:VAL:HG12	2:B:113:ILE:HG12	1.81	0.63
1:A:590:LYS:HB2	8:H:91:VAL:HG23	1.80	0.63
3:C:267:VAL:HG23	3:C:270:LYS:HE2	1.81	0.63
4:D:95:VAL:HG11	7:G:202:THR:HG21	1.81	0.63
1:A:670:ASP:OD2	1:A:923:ARG:NH2	2.32	0.62
14:N:337:VAL:HG23	14:N:348:VAL:HG13	1.81	0.62
3:C:202:LEU:HD11	3:C:208:ILE:HD12	1.81	0.62
1:A:703:VAL:HG23	1:A:796:ILE:HG12	1.80	0.62
1:A:165:THR:HG22	1:A:177:GLU:HB3	1.81	0.61
2:B:39:LEU:HD21	2:B:498:LEU:HD12	1.83	0.61
2:B:210:LYS:HG2	2:B:319:THR:HG21	1.82	0.61
7:G:131:TYR:HB3	7:G:137:ALA:HB3	1.82	0.61
15:O:264:SER:HA	15:O:267:VAL:HG12	1.82	0.61
2:B:204:THR:HG23	2:B:320:HIS:HB3	1.83	0.61
15:O:310:GLN:NE2	16:P:204:ILE:HG12	2.16	0.61
8:H:90:TYR:HB3	8:H:145:MET:HB3	1.83	0.61
2:B:329:ARG:NH1	2:B:524:ASN:O	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:2:THR:OG1	15:O:5:GLU:OE1	2.14	0.60
1:A:794:GLN:HG3	1:A:799:VAL:HA	1.84	0.60
15:O:287:PRO:HB3	15:O:333:MET:HG3	1.83	0.60
13:M:48:LYS:HB3	13:M:205:TRP:NE1	2.16	0.60
15:O:160:CYS:SG	17:Q:105:ARG:NH1	2.74	0.60
1:A:31:GLN:HE22	2:B:1118:GLN:HE22	1.47	0.60
16:P:304:PRO:HA	22:P:400:SF4:S1	2.41	0.60
1:A:266:VAL:HB	1:A:275:ASN:HB2	1.84	0.60
8:H:64:LEU:HB3	8:H:83:SER:HB2	1.83	0.60
7:G:115:GLN:NE2	7:G:130:GLU:O	2.35	0.60
1:A:461:LEU:HD23	1:A:473:ILE:HD11	1.84	0.59
5:E:104:ILE:HD11	5:E:127:LEU:HD12	1.83	0.59
1:A:464:ARG:NH1	20:T:8:C:O2'	2.35	0.59
3:C:40:TRP:NE1	11:K:102:GLU:OE1	2.35	0.59
7:G:39:VAL:HG12	7:G:40:TYR:H	1.66	0.59
2:B:659:ILE:HG22	2:B:660:GLU:HG2	1.85	0.59
1:A:1069:ARG:HH12	1:A:1249:ASN:HD21	1.50	0.59
10:J:40:LEU:HD11	10:J:49:LEU:HD12	1.84	0.59
13:M:6:ASP:HB3	14:N:332:ARG:HD2	1.83	0.59
1:A:864:LYS:HB3	1:A:1049:THR:HG21	1.84	0.59
1:A:996:GLU:HG3	1:A:997:PRO:HD3	1.84	0.59
2:B:178:ILE:HG12	2:B:437:THR:HG22	1.84	0.58
2:B:744:MET:HB3	2:B:1002:ILE:HG23	1.85	0.58
7:G:88:LYS:HG3	7:G:146:GLU:HG3	1.85	0.58
1:A:590:LYS:HB3	1:A:591:PRO:HD3	1.86	0.58
7:G:94:PRO:HA	7:G:119:LYS:HG2	1.84	0.58
1:A:509:LEU:O	2:B:1067:ARG:NH2	2.35	0.58
4:D:13:ASN:ND2	4:D:88:ASN:OD1	2.36	0.58
18:R:59:DC:H2'	18:R:60:DG:C8	2.39	0.58
13:M:113:ARG:HE	14:N:273:ASP:HB2	1.67	0.58
11:K:35:THR:HB	11:K:38:HIS:HB2	1.86	0.57
11:K:66:GLU:HB2	11:K:87:ARG:HG3	1.87	0.57
14:N:276:PRO:HG3	14:N:344:VAL:HG11	1.85	0.57
2:B:52:ASN:O	2:B:56:LYS:NZ	2.38	0.57
1:A:148:ASP:O	1:A:152:LYS:HG2	2.05	0.57
3:C:49:PHE:O	11:K:113:LYS:NZ	2.37	0.57
9:I:8:CYS:SG	9:I:9:GLY:N	2.78	0.57
15:O:399:LEU:HD11	15:O:406:LEU:HD23	1.87	0.57
1:A:381:ALA:HB3	1:A:487:ARG:HB2	1.86	0.57
1:A:490:GLU:HG2	2:B:751:ILE:HG13	1.85	0.57
9:I:20:CYS:SG	9:I:21:HIS:N	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:HIS:O	1:A:67:ARG:NH2	2.38	0.57
1:A:126:LEU:HG	1:A:237:LEU:HD12	1.87	0.57
2:B:751:ILE:HG22	2:B:752:GLU:H	1.69	0.57
19:S:23:DC:H2'	19:S:24:DG:C8	2.40	0.57
5:E:10:LEU:HD21	5:E:58:LEU:HD11	1.85	0.56
1:A:360:ARG:NH2	19:S:21:DC:OP1	2.39	0.56
2:B:596:TYR:HD2	2:B:633:LEU:HD12	1.70	0.56
4:D:115:ALA:HA	4:D:118:HIS:CE1	2.40	0.56
3:C:89:VAL:HB	3:C:111:GLY:HA2	1.87	0.56
16:P:237:THR:O	16:P:241:THR:HG23	2.06	0.56
1:A:863:VAL:HG13	2:B:463:ARG:HB2	1.86	0.56
2:B:186:LYS:HD3	2:B:205:SER:HB2	1.86	0.56
15:O:161:PRO:HB2	15:O:182:ILE:HG22	1.88	0.56
16:P:190:SER:O	16:P:194:THR:HG23	2.06	0.56
2:B:455:ILE:HD11	2:B:496:LEU:HG	1.87	0.56
2:B:501:HIS:N	2:B:593:CYS:O	2.38	0.55
1:A:1121:PHE:HE1	9:I:14:VAL:HG11	1.70	0.55
1:A:1136:ARG:HE	9:I:46:LEU:HD22	1.71	0.55
2:B:276:GLN:O	2:B:282:GLN:NE2	2.38	0.55
2:B:919:CYS:SG	2:B:920:ASP:N	2.79	0.55
13:M:108:THR:O	13:M:111:THR:OG1	2.24	0.55
17:Q:78:PRO:O	17:Q:79:GLU:HG2	2.06	0.55
16:P:302:ILE:HD11	17:Q:37:LEU:HB2	1.89	0.55
3:C:50:ARG:HG2	3:C:66:VAL:HB	1.86	0.55
13:M:31:PRO:O	14:N:39:ARG:NH2	2.39	0.55
13:M:53:GLN:OE1	13:M:200:HIS:ND1	2.40	0.55
13:M:192:SER:OG	13:M:193:TYR:N	2.39	0.55
1:A:13:LYS:HG2	2:B:1130:LYS:HD3	1.88	0.55
1:A:885:GLN:HE21	6:F:111:PRO:HG3	1.71	0.55
13:M:13:ILE:HB	14:N:329:LEU:HB2	1.87	0.55
14:N:336:ARG:HG3	14:N:347:ASP:OD2	2.07	0.55
15:O:463:LYS:NZ	15:O:495:GLU:OE2	2.38	0.55
1:A:1132:LEU:HB3	1:A:1171:ALA:HB1	1.88	0.55
3:C:40:TRP:CD1	3:C:42:GLN:HB2	2.41	0.55
3:C:145:ARG:HB3	3:C:207:GLU:HG3	1.88	0.55
3:C:197:ILE:HG12	10:J:16:ASN:HB3	1.87	0.55
18:R:59:DC:H2'	18:R:60:DG:H8	1.72	0.55
1:A:804:ILE:HD13	1:A:809:VAL:HG22	1.89	0.54
1:A:1308:LEU:HA	1:A:1311:MET:HG2	1.88	0.54
13:M:111:THR:HG23	13:M:114:TYR:HD2	1.72	0.54
1:A:490:GLU:HG2	2:B:751:ILE:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:208:LEU:HD12	14:N:373:MET:HB2	1.89	0.54
15:O:471:ILE:HG13	15:O:487:ILE:HD13	1.90	0.54
15:O:485:GLN:HA	15:O:488:GLU:HB3	1.90	0.54
2:B:503:THR:OG1	2:B:593:CYS:SG	2.65	0.54
1:A:191:SER:O	1:A:195:GLN:NE2	2.40	0.54
12:L:19:CYS:SG	12:L:20:GLY:N	2.81	0.54
1:A:23:LYS:NZ	1:A:31:GLN:OE1	2.41	0.54
2:B:522:ASP:HB3	2:B:525:LEU:HD13	1.90	0.54
1:A:227:PHE:HB3	1:A:248:SER:HA	1.89	0.54
1:A:869:GLY:HA3	19:S:18:DC:H1'	1.90	0.54
2:B:722:THR:HG23	2:B:962:THR:HA	1.90	0.54
13:M:48:LYS:HB3	13:M:205:TRP:HE1	1.72	0.54
6:F:66:LEU:HD11	6:F:97:LEU:HD22	1.90	0.53
1:A:905:ASP:HB2	1:A:1285:ARG:HH11	1.73	0.53
2:B:982:ASN:ND2	3:C:284:SER:O	2.38	0.53
15:O:386:ILE:HG22	15:O:391:ALA:HB2	1.91	0.53
2:B:986:LYS:HD2	2:B:1001:TYR:HB2	1.91	0.53
1:A:556:ASP:OD1	8:H:24:ARG:NH2	2.42	0.53
3:C:337:LEU:HG	11:K:100:LEU:HD23	1.90	0.53
16:P:231:SER:O	16:P:235:ILE:HG12	2.08	0.53
2:B:536:VAL:HG13	2:B:548:VAL:HG13	1.90	0.53
1:A:631:LEU:HD11	8:H:124:ARG:HD2	1.89	0.53
14:N:268:PHE:HB2	14:N:379:VAL:HG11	1.91	0.53
15:O:367:ARG:NH1	16:P:245:ASP:O	2.42	0.53
15:O:482:ALA:O	15:O:485:GLN:HG3	2.09	0.53
1:A:1284:ARG:HH12	5:E:199:THR:HG21	1.74	0.53
3:C:235:LEU:HB2	3:C:301:ARG:HE	1.74	0.53
5:E:122:ALA:N	5:E:123:PRO:HD3	2.24	0.53
14:N:317:THR:HG23	14:N:319:ALA:H	1.72	0.53
20:T:5:U:H2'	20:T:6:G:H8	1.73	0.53
1:A:90:LEU:HD12	1:A:221:LEU:HD11	1.90	0.53
1:A:396:VAL:HG22	1:A:448:ASP:H	1.74	0.53
2:B:620:ASN:ND2	2:B:622:GLU:OE2	2.42	0.53
11:K:120:ASP:HA	11:K:123:ASP:OD1	2.08	0.53
2:B:946:LEU:HD22	2:B:1003:TYR:CZ	2.44	0.52
3:C:146:CYS:HB2	3:C:202:LEU:HB3	1.90	0.52
2:B:124:GLN:HE22	2:B:399:GLN:HE22	1.57	0.52
3:C:73:ALA:HB1	3:C:308:PHE:HZ	1.74	0.52
7:G:97:VAL:O	7:G:108:LEU:HA	2.09	0.52
15:O:255:VAL:HG11	15:O:267:VAL:HG11	1.89	0.52
15:O:258:ARG:HG2	15:O:320:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:48:ASP:N	15:O:48:ASP:OD2	2.43	0.52
13:M:242:PRO:HG2	14:N:395:HIS:CD2	2.44	0.52
19:S:20:DA:H2'	19:S:21:DC:C6	2.43	0.52
13:M:45:LEU:HD23	13:M:61:ALA:HB2	1.91	0.52
3:C:304:ASP:OD1	3:C:305:HIS:ND1	2.43	0.52
7:G:86:ILE:HG22	7:G:149:ARG:HG2	1.90	0.52
1:A:713:LYS:NZ	1:A:797:ALA:O	2.39	0.52
3:C:246:GLU:OE1	3:C:249:ALA:N	2.42	0.52
2:B:142:SER:OG	2:B:143:SER:N	2.42	0.51
17:Q:32:LEU:HD23	17:Q:32:LEU:H	1.75	0.51
2:B:591:ARG:NH1	2:B:634:ASP:OD2	2.42	0.51
2:B:633:LEU:HD11	2:B:656:HIS:CE1	2.46	0.51
2:B:745:SER:HA	2:B:750:ASP:OD2	2.10	0.51
13:M:59:GLU:HA	13:M:100:GLN:O	2.09	0.51
1:A:984:ARG:HG3	1:A:989:ILE:HB	1.93	0.51
2:B:267:PRO:O	2:B:270:GLU:HG2	2.11	0.51
15:O:441:LYS:HE2	16:P:293:PHE:CZ	2.45	0.51
19:S:21:DC:H2'	19:S:22:DA:C8	2.44	0.51
1:A:742:CYS:SG	1:A:747:THR:OG1	2.69	0.51
15:O:351:GLU:HA	15:O:354:VAL:HG12	1.92	0.51
2:B:1073:ASP:OD1	2:B:1073:ASP:N	2.42	0.51
15:O:487:ILE:HA	15:O:490:MET:HG2	1.93	0.51
1:A:914:GLY:O	1:A:915:LYS:HG3	2.11	0.51
15:O:97:THR:HG23	15:O:98:LEU:HD12	1.93	0.51
15:O:309:ASP:O	15:O:313:THR:HG23	2.11	0.51
16:P:220:ILE:HD13	16:P:223:LEU:HD12	1.91	0.51
4:D:64:GLU:HG2	4:D:65:ILE:HD12	1.91	0.51
1:A:989:ILE:HD11	1:A:1000:LEU:HB3	1.92	0.51
2:B:113:ILE:HD11	2:B:136:MET:HB2	1.93	0.51
9:I:96:LYS:HD3	9:I:106:TRP:CE3	2.45	0.51
15:O:254:ALA:O	15:O:258:ARG:HB2	2.11	0.51
15:O:414:ASP:OD1	15:O:415:HIS:N	2.44	0.51
16:P:213:SER:HA	16:P:216:VAL:HG22	1.93	0.51
1:A:1244:THR:OG1	5:E:142:HIS:O	2.27	0.50
2:B:569:ASN:HD22	2:B:571:PHE:H	1.58	0.50
3:C:83:GLU:HB3	3:C:328:VAL:HG11	1.92	0.50
11:K:53:ASN:HA	11:K:56:ARG:HG2	1.93	0.50
13:M:117:ALA:O	14:N:267:LEU:N	2.33	0.50
16:P:281:GLY:HA2	16:P:284:ARG:HD2	1.93	0.50
6:F:89:PRO:HA	6:F:92:ILE:HG12	1.93	0.50
1:A:1053:PHE:O	1:A:1055:PHE:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:919:CYS:HA	2:B:989:VAL:HA	1.92	0.50
8:H:92:MET:HB2	8:H:143:LEU:HB3	1.94	0.50
19:S:21:DC:H2'	19:S:22:DA:H8	1.76	0.50
1:A:356:LEU:HD22	1:A:1348:ILE:HG23	1.94	0.50
14:N:359:GLU:HA	14:N:378:HIS:HA	1.94	0.50
3:C:326:ILE:HG21	11:K:111:LEU:HB2	1.93	0.50
4:D:78:LEU:O	4:D:79:THR:OG1	2.24	0.50
1:A:287:ILE:HA	1:A:290:ASN:HD22	1.76	0.50
1:A:1220:LYS:HD3	1:A:1222:LYS:HG2	1.92	0.50
15:O:471:ILE:HG13	15:O:487:ILE:HG21	1.92	0.50
1:A:1028:GLU:HB2	6:F:58:THR:HG23	1.94	0.50
12:L:18:ILE:HD11	12:L:47:LYS:HG2	1.93	0.50
2:B:516:SER:HA	2:B:520:VAL:HG12	1.93	0.50
5:E:155:GLU:O	5:E:158:GLU:HG3	2.11	0.50
1:A:438:GLU:O	1:A:442:GLN:NE2	2.44	0.50
1:A:786:LYS:HG3	2:B:936:SER:HB2	1.93	0.50
3:C:149:ASN:HB3	3:C:152:ALA:HB2	1.93	0.50
4:D:69:PHE:CE1	4:D:120:VAL:HG22	2.47	0.50
7:G:122:GLU:HG2	7:G:123:ALA:H	1.75	0.50
16:P:252:ILE:HD11	16:P:266:HIS:HB3	1.94	0.50
13:M:53:GLN:O	13:M:106:GLN:NE2	2.45	0.49
2:B:182:GLU:HG2	2:B:457:SER:HA	1.94	0.49
8:H:75:TYR:CD2	8:H:77:PRO:HD2	2.47	0.49
2:B:367:GLN:O	2:B:371:LEU:HG	2.11	0.49
7:G:122:GLU:HG2	7:G:123:ALA:N	2.27	0.49
16:P:210:PHE:CE1	16:P:269:LEU:HD22	2.46	0.49
1:A:396:VAL:HG12	1:A:404:LEU:HD12	1.95	0.49
1:A:727:TYR:HD2	1:A:736:LEU:HD21	1.77	0.49
15:O:521:PHE:HA	15:O:524:GLU:HG2	1.93	0.49
10:J:64:PRO:HB3	12:L:23:HIS:CE1	2.48	0.49
1:A:990:ASN:OD1	1:A:995:THR:OG1	2.30	0.49
2:B:329:ARG:HH22	13:M:134:GLN:HE22	1.59	0.49
1:A:359:LYS:HD3	2:B:1068:LEU:O	2.12	0.49
1:A:913:GLU:HB2	1:A:919:LEU:HA	1.94	0.49
2:B:597:ILE:HA	2:B:630:VAL:HG12	1.95	0.49
4:D:82:GLU:HA	4:D:85:GLN:HB3	1.93	0.49
16:P:219:TYR:O	16:P:222:GLU:HG3	2.13	0.49
1:A:374:ASN:ND2	2:B:749:TYR:OH	2.46	0.49
7:G:149:ARG:HB2	7:G:192:GLU:HB2	1.95	0.49
8:H:75:TYR:HD2	8:H:77:PRO:HD2	1.78	0.49
8:H:96:VAL:HG22	8:H:116:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LYS:HD2	2:B:1025:ARG:HH12	1.78	0.48
1:A:615:ALA:H	1:A:643:SER:HB2	1.79	0.48
1:A:1074:ILE:HG23	1:A:1303:ILE:HD12	1.94	0.48
3:C:332:LYS:HA	3:C:335:ARG:HG2	1.96	0.48
7:G:147:GLU:OE2	7:G:149:ARG:NE	2.46	0.48
8:H:67:ASP:HB2	8:H:81:ARG:HG2	1.95	0.48
2:B:814:ILE:HG23	2:B:828:VAL:HG22	1.96	0.48
13:M:27:LEU:HD23	13:M:132:ILE:HG23	1.94	0.48
15:O:323:VAL:HG22	15:O:336:ILE:HG12	1.94	0.48
3:C:51:VAL:HG11	11:K:114:PHE:HD1	1.77	0.48
1:A:662:ASN:OD1	1:A:663:ILE:N	2.47	0.48
15:O:33:SER:HB2	15:O:74:GLU:HB3	1.94	0.48
15:O:100:SER:OG	15:O:101:ASP:N	2.46	0.48
1:A:17:HIS:CE1	1:A:1337:LYS:HD2	2.49	0.48
1:A:142:LEU:HD23	1:A:239:LEU:HD21	1.95	0.48
1:A:650:MET:HB3	1:A:655:LEU:HD22	1.96	0.48
1:A:986:LYS:O	8:H:108:ALA:HA	2.13	0.48
1:A:1101:VAL:HG21	1:A:1240:GLY:HA3	1.96	0.48
3:C:209:ASP:OD1	3:C:209:ASP:N	2.47	0.48
13:M:52:LYS:HE3	13:M:203:GLU:HB3	1.96	0.48
1:A:942:LYS:HB2	1:A:977:SER:HB3	1.94	0.48
1:A:1261:GLU:HG2	5:E:148:HIS:HE1	1.78	0.48
4:D:117:LEU:O	4:D:121:THR:HG23	2.14	0.48
15:O:15:GLU:OE2	15:O:450:ARG:NH2	2.46	0.48
15:O:519:THR:HG21	16:P:282:LEU:HB2	1.94	0.48
2:B:751:ILE:HG22	2:B:752:GLU:OE2	2.13	0.47
15:O:310:GLN:HE21	16:P:204:ILE:HG12	1.78	0.47
1:A:816:ARG:NH2	2:B:639:ASN:O	2.47	0.47
1:A:1384:PHE:CZ	4:D:70:LEU:HB3	2.49	0.47
4:D:77:LYS:HE2	4:D:107:ARG:HG2	1.96	0.47
11:K:120:ASP:OD2	11:K:121:TYR:N	2.47	0.47
1:A:207:VAL:HA	1:A:210:LEU:HB2	1.97	0.47
1:A:383:PRO:HB3	1:A:484:ARG:HA	1.95	0.47
1:A:955:LYS:HB2	1:A:958:PHE:HD2	1.78	0.47
2:B:250:GLU:HA	2:B:253:GLN:HE21	1.79	0.47
9:I:85:ARG:HG3	9:I:90:PRO:HB3	1.95	0.47
1:A:99:ARG:HA	1:A:102:ILE:HG12	1.97	0.47
2:B:257:THR:HB	14:N:37:PRO:HA	1.96	0.47
1:A:65:LYS:HZ2	1:A:76:LEU:H	1.61	0.47
1:A:533:ARG:HD3	1:A:534:ASN:ND2	2.30	0.47
1:A:887:ASP:OD1	1:A:887:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:916:MET:HB3	2:B:925:PRO:HD2	1.97	0.47
5:E:64:HIS:HD2	5:E:67:ASP:H	1.62	0.47
8:H:76:ASN:HB2	8:H:77:PRO:HD3	1.95	0.47
13:M:49:ILE:HG13	13:M:56:VAL:HG22	1.97	0.47
1:A:1360:PHE:CE1	6:F:64:ARG:HD3	2.50	0.47
7:G:100:SER:OG	7:G:105:ASP:HA	2.15	0.47
15:O:252:VAL:HA	15:O:255:VAL:HG12	1.97	0.47
12:L:31:ARG:HG3	13:M:700:TRP:H	1.80	0.47
15:O:234:TYR:OH	17:Q:104:ARG:NH1	2.46	0.47
2:B:444:SER:OG	2:B:445:TYR:N	2.47	0.47
1:A:1111:GLY:H	1:A:1197:PRO:HA	1.80	0.46
2:B:478:MET:HB3	2:B:592:LEU:HD13	1.97	0.46
16:P:188:LEU:HD23	16:P:248:VAL:HG11	1.96	0.46
19:S:20:DA:H2'	19:S:21:DC:H6	1.80	0.46
1:A:47:GLN:HE22	2:B:835:VAL:HG11	1.79	0.46
1:A:464:ARG:NH2	1:A:497:ASN:O	2.48	0.46
1:A:559:PHE:O	1:A:595:TRP:N	2.40	0.46
1:A:604:ILE:HD12	1:A:682:ARG:HB3	1.97	0.46
2:B:757:LEU:HD13	2:B:762:LEU:HD21	1.96	0.46
13:M:119:TYR:HD1	13:M:124:LEU:HG	1.80	0.46
14:N:388:ASP:OD1	14:N:388:ASP:N	2.41	0.46
1:A:11:VAL:HG21	2:B:1102:SER:HA	1.97	0.46
1:A:356:LEU:HA	1:A:359:LYS:HE3	1.97	0.46
1:A:1346:CYS:HB3	1:A:1351:ILE:O	2.14	0.46
2:B:496:LEU:HD22	2:B:500:THR:HG21	1.98	0.46
3:C:61:LEU:HD22	3:C:319:ASP:HA	1.95	0.46
9:I:96:LYS:HD3	9:I:106:TRP:HE3	1.80	0.46
1:A:65:LYS:NZ	1:A:76:LEU:H	2.13	0.46
1:A:883:CYS:SG	1:A:1355:ILE:HG13	2.54	0.46
1:A:1347:ILE:HD11	2:B:1064:LEU:HD21	1.97	0.46
8:H:79:ASP:OD1	8:H:79:ASP:N	2.46	0.46
10:J:41:LYS:O	10:J:46:ARG:NH2	2.48	0.46
1:A:393:PRO:HB3	1:A:451:GLU:HG2	1.96	0.46
8:H:18:GLU:O	8:H:21:LYS:NZ	2.45	0.46
15:O:161:PRO:HG3	15:O:184:GLU:HB2	1.98	0.46
16:P:239:LEU:O	16:P:243:ILE:HG23	2.16	0.46
2:B:792:GLY:HA2	2:B:813:GLY:HA2	1.98	0.46
3:C:193:VAL:HG23	3:C:194:HIS:HD2	1.80	0.46
11:K:68:CYS:HA	11:K:83:ARG:O	2.16	0.46
13:M:66:ASN:OD1	13:M:69:TYR:HB2	2.16	0.46
1:A:822:GLU:HB3	1:A:825:SER:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1098:ALA:HA	1:A:1101:VAL:HG12	1.98	0.46
7:G:39:VAL:HB	7:G:42:VAL:HG12	1.98	0.46
1:A:1384:PHE:HE1	4:D:74:LYS:HB2	1.80	0.46
2:B:812:ASP:HB2	12:L:15:MET:HG3	1.98	0.46
12:L:31:ARG:HG3	13:M:700:TRP:N	2.31	0.46
14:N:338:GLN:HE21	14:N:345:THR:CG2	2.29	0.46
16:P:219:TYR:O	16:P:223:LEU:HG	2.15	0.46
1:A:418:ALA:HA	1:A:452:ARG:HA	1.98	0.46
1:A:537:PRO:HG3	1:A:665:TYR:HB2	1.98	0.46
2:B:709:MET:HB3	2:B:772:TYR:HB2	1.98	0.46
7:G:38:VAL:HG22	7:G:44:LEU:HD13	1.97	0.46
15:O:59:GLN:NE2	15:O:113:ASN:O	2.48	0.46
15:O:401:GLU:OE1	15:O:438:ARG:NH2	2.48	0.46
19:S:13:DT:H2"	19:S:14:DG:C8	2.51	0.46
1:A:415:HIS:NE2	1:A:480:VAL:HG21	2.30	0.45
1:A:813:PHE:CE2	1:A:819:PRO:HD3	2.51	0.45
1:A:1063:ILE:HG23	1:A:1065:LEU:HD22	1.98	0.45
1:A:1206:GLU:OE2	1:A:1231:ASN:HB2	2.16	0.45
3:C:93:LEU:HB3	12:L:52:LEU:HD11	1.97	0.45
4:D:73:LEU:HD22	4:D:83:LYS:HG2	1.98	0.45
17:Q:60:LEU:O	17:Q:63:GLU:HG3	2.15	0.45
3:C:103:ASP:OD2	12:L:48:ARG:NH1	2.49	0.45
7:G:92:CYS:SG	7:G:127:TRP:HD1	2.39	0.45
15:O:104:GLU:HG2	15:O:105:LEU:HD12	1.97	0.45
1:A:1120:VAL:O	1:A:1126:CYS:HB2	2.17	0.45
16:P:207:ASN:OD1	16:P:271:ARG:NH2	2.50	0.45
2:B:810:ASP:OD2	2:B:811:ALA:N	2.49	0.45
4:D:61:GLN:HE21	4:D:65:ILE:HG22	1.82	0.45
16:P:304:PRO:CA	22:P:400:SF4:S1	3.04	0.45
1:A:666:ILE:HD12	1:A:923:ARG:HE	1.82	0.45
2:B:145:CYS:SG	2:B:146:VAL:N	2.89	0.45
2:B:526:LEU:H	2:B:526:LEU:HD23	1.80	0.45
15:O:368:LEU:HD13	15:O:384:ALA:HB2	1.99	0.45
15:O:376:GLU:OE2	15:O:379:GLN:HG2	2.17	0.45
19:S:12:DG:H2'	19:S:13:DT:H71	1.98	0.45
1:A:595:TRP:HE1	1:A:600:ILE:HG12	1.81	0.45
2:B:769:CYS:SG	2:B:770:LEU:N	2.89	0.45
3:C:118:ASP:OD1	3:C:120:ARG:NH2	2.49	0.45
7:G:119:LYS:HZ1	7:G:121:ASP:HB3	1.81	0.45
16:P:284:ARG:HG2	17:Q:46:VAL:HB	1.99	0.45
18:R:56:DA:H2"	18:R:57:DC:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:62:DA:H2"	18:R:63:DA:C8	2.51	0.45
1:A:967:GLN:HA	1:A:970:LYS:HE2	1.99	0.45
2:B:231:SER:OG	2:B:292:ARG:HD2	2.17	0.45
5:E:61:LEU:HD13	5:E:73:PHE:CZ	2.52	0.45
1:A:208:GLU:HA	1:A:211:LEU:HD22	1.98	0.45
1:A:1161:LYS:O	1:A:1163:GLY:N	2.48	0.45
3:C:55:HIS:CE1	3:C:57:ASP:HB2	2.52	0.45
15:O:134:GLU:HG2	15:O:135:ASP:H	1.82	0.45
16:P:301:GLU:HG3	16:P:302:ILE:H	1.80	0.45
13:M:108:THR:HG21	13:M:114:TYR:HE2	1.82	0.45
1:A:15:ILE:HD11	2:B:1126:LEU:HD22	1.99	0.45
1:A:586:PRO:HG2	1:A:589:LEU:HD22	1.98	0.45
1:A:1254:VAL:HG23	1:A:1258:LEU:HD12	1.98	0.45
3:C:280:LEU:H	3:C:280:LEU:HD23	1.82	0.45
19:S:5:DA:H2"	19:S:6:DA:C8	2.52	0.45
2:B:762:LEU:HG	2:B:891:PRO:HG2	1.99	0.44
3:C:82:ALA:HB1	3:C:220:LYS:HB2	1.98	0.44
5:E:173:ILE:N	5:E:208:LEU:O	2.50	0.44
8:H:58:LEU:HD11	8:H:123:MET:HE3	1.98	0.44
13:M:60:MET:O	13:M:99:LYS:HA	2.17	0.44
15:O:19:GLU:O	15:O:22:GLU:HG3	2.17	0.44
16:P:287:CYS:HA	22:P:400:SF4:S2	2.57	0.44
1:A:373:PRO:HD2	2:B:749:TYR:CZ	2.52	0.44
1:A:421:ILE:HD12	1:A:432:LEU:HD21	2.00	0.44
1:A:584:PRO:HB2	1:A:595:TRP:HH2	1.83	0.44
1:A:1044:PRO:O	1:A:1048:MET:HB2	2.17	0.44
1:A:1053:PHE:O	9:I:82:LEU:HD21	2.17	0.44
1:A:1118:GLU:OE2	9:I:41:ARG:HG2	2.17	0.44
7:G:6:GLU:HG2	7:G:73:ARG:HG2	1.99	0.44
9:I:97:CYS:SG	9:I:105:ARG:NE	2.90	0.44
10:J:40:LEU:HD13	10:J:46:ARG:HA	1.99	0.44
15:O:158:GLN:HB2	15:O:188:TYR:CE1	2.52	0.44
1:A:816:ARG:HD3	1:A:823:LYS:HG2	1.98	0.44
1:A:916:ASP:OD2	1:A:1284:ARG:NH2	2.45	0.44
1:A:924:VAL:O	1:A:928:ILE:HG12	2.17	0.44
1:A:967:GLN:O	1:A:971:LYS:HG2	2.18	0.44
2:B:105:ARG:HG3	12:L:43:ILE:HD11	1.98	0.44
2:B:723:LYS:H	2:B:962:THR:HG22	1.82	0.44
4:D:51:LYS:HD3	4:D:55:LYS:NZ	2.32	0.44
15:O:325:LYS:HZ3	15:O:327:GLY:HA3	1.82	0.44
15:O:431:ALA:O	15:O:434:MET:HG3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:511:ALA:HB2	17:Q:58:LEU:HD11	1.97	0.44
2:B:680:SER:OG	2:B:681:PRO:HD3	2.17	0.44
7:G:119:LYS:HD2	7:G:126:VAL:O	2.17	0.44
15:O:356:GLU:HG3	16:P:283:VAL:HG11	1.98	0.44
17:Q:67:THR:O	17:Q:71:MET:HG2	2.18	0.44
3:C:261:VAL:HG12	3:C:262:ILE:HG13	1.99	0.44
3:C:266:GLU:HA	3:C:270:LYS:O	2.18	0.44
5:E:185:ILE:HD12	5:E:209:VAL:HG21	1.98	0.44
15:O:367:ARG:NH1	16:P:246:GLY:HA3	2.33	0.44
15:O:368:LEU:HD12	16:P:244:TYR:CD2	2.52	0.44
1:A:47:GLN:NE2	2:B:835:VAL:HG11	2.32	0.44
1:A:743:THR:HG22	1:A:744:ALA:H	1.83	0.44
2:B:185:SER:HB2	2:B:359:ASN:O	2.18	0.44
2:B:673:PRO:HG2	2:B:945:GLU:HG3	1.99	0.44
15:O:307:VAL:O	15:O:310:GLN:HB3	2.18	0.44
2:B:37:LYS:HD2	2:B:501:HIS:CD2	2.53	0.44
2:B:392:ILE:HB	2:B:393:PRO:HD3	1.98	0.44
7:G:107:ILE:HG13	7:G:186:LEU:O	2.18	0.44
12:L:41:TYR:CE2	12:L:43:ILE:HB	2.53	0.44
15:O:377:GLN:HE22	15:O:392:LYS:HE2	1.83	0.44
1:A:463:ASN:HB3	1:A:473:ILE:HG13	1.99	0.44
1:A:701:GLY:HA2	2:B:984:LEU:HD13	2.00	0.44
1:A:1314:SER:HB3	1:A:1317:MET:HB3	2.00	0.44
2:B:407:ARG:HD3	2:B:410:GLN:H	1.83	0.44
16:P:176:PHE:HE1	16:P:225:ILE:HD12	1.82	0.44
2:B:518:LEU:HD22	2:B:555:LEU:HD13	1.98	0.44
2:B:1078:ASP:N	2:B:1078:ASP:OD1	2.51	0.44
5:E:55:ARG:HB2	5:E:78:GLU:HA	2.00	0.44
15:O:141:TYR:HB2	15:O:195:LEU:HD22	1.99	0.44
17:Q:37:LEU:HG	17:Q:38:PHE:CD2	2.53	0.44
17:Q:52:GLU:HA	17:Q:55:GLU:OE2	2.18	0.44
20:T:5:U:H2'	20:T:6:G:C8	2.52	0.44
2:B:75:LEU:HD21	2:B:384:MET:HE3	2.00	0.43
2:B:357:TYR:HD2	2:B:475:GLN:HB3	1.83	0.43
15:O:92:ILE:HB	17:Q:60:LEU:HD21	1.99	0.43
16:P:194:THR:O	16:P:198:SER:OG	2.22	0.43
19:S:22:DA:H2'	19:S:23:DC:C6	2.53	0.43
1:A:116:MET:SD	1:A:163:ASN:ND2	2.91	0.43
1:A:499:ASP:N	1:A:503:ASP:OD2	2.36	0.43
1:A:1048:MET:HG3	1:A:1278:HIS:CD2	2.53	0.43
1:A:1184:SER:HB2	9:I:15:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:GLN:OE1	14:N:39:ARG:NH2	2.51	0.43
2:B:1013:LYS:HG3	2:B:1014:HIS:CD2	2.54	0.43
11:K:58:MET:HG3	11:K:103:LEU:HB2	1.99	0.43
15:O:367:ARG:HH11	16:P:246:GLY:HA3	1.82	0.43
15:O:467:VAL:HA	15:O:470:ILE:HD12	1.99	0.43
1:A:65:LYS:HZ2	1:A:75:ASN:HB2	1.83	0.43
1:A:1360:PHE:CZ	6:F:61:GLU:HA	2.52	0.43
2:B:750:ASP:HB2	2:B:930:ASN:HB2	1.99	0.43
2:B:1118:GLN:HG3	2:B:1123:ILE:HG13	1.99	0.43
5:E:64:HIS:NE2	5:E:66:ASP:OD1	2.52	0.43
15:O:376:GLU:OE2	15:O:378:LYS:HG2	2.18	0.43
2:B:679:GLN:HG2	2:B:681:PRO:HD2	2.01	0.43
2:B:716:GLN:HB2	2:B:737:GLN:HA	2.00	0.43
7:G:16:TRP:CD1	7:G:17:GLN:HG3	2.54	0.43
14:N:321:LEU:HG	14:N:322:THR:H	1.83	0.43
1:A:35:GLN:HB2	1:A:85:TYR:CE1	2.54	0.43
2:B:599:VAL:HG12	2:B:604:PRO:HA	2.00	0.43
1:A:279:LEU:HA	1:A:320:TYR:HE1	1.84	0.43
1:A:864:LYS:HA	1:A:867:GLU:OE2	2.18	0.43
2:B:423:ASN:ND2	2:B:434:GLN:HG3	2.33	0.43
2:B:757:LEU:HD23	2:B:927:ILE:HG12	2.01	0.43
5:E:51:GLY:O	5:E:54:ARG:HG2	2.19	0.43
13:M:113:ARG:NE	14:N:273:ASP:HB2	2.34	0.43
1:A:69:CYS:SG	1:A:70:GLU:N	2.92	0.43
1:A:982:LYS:O	1:A:986:LYS:HB2	2.19	0.43
2:B:714:TYR:O	2:B:737:GLN:NE2	2.52	0.43
9:I:1:MET:HB3	9:I:2:LEU:H	1.68	0.43
15:O:129:LEU:HB3	15:O:139:MET:HG3	2.01	0.43
3:C:193:VAL:HG23	3:C:194:HIS:CD2	2.54	0.43
1:A:6:PHE:HB2	7:G:37:LYS:HB3	2.00	0.43
2:B:751:ILE:O	2:B:753:ASP:N	2.52	0.43
3:C:293:LEU:O	3:C:295:LYS:N	2.52	0.43
3:C:94:VAL:HG21	3:C:97:ASN:HB2	2.00	0.42
1:A:280:THR:O	1:A:284:THR:HG23	2.19	0.42
1:A:464:ARG:HH11	20:T:8:C:HO2'	1.67	0.42
1:A:1107:LYS:HD3	1:A:1205:PRO:O	2.18	0.42
1:A:1379:PHE:HZ	4:D:84:LEU:HD22	1.85	0.42
2:B:66:THR:OG1	2:B:73:TRP:O	2.22	0.42
2:B:353:ASP:OD1	2:B:353:ASP:N	2.52	0.42
2:B:409:ASP:OD1	2:B:410:GLN:N	2.52	0.42
4:D:91:PRO:HB2	4:D:97:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:29:GLN:HB3	13:M:134:GLN:HA	2.00	0.42
13:M:114:TYR:HB3	14:N:268:PHE:CE1	2.54	0.42
15:O:180:LEU:HD23	15:O:180:LEU:H	1.84	0.42
1:A:175:ILE:HD11	15:O:415:HIS:CE1	2.53	0.42
7:G:114:LEU:HD13	7:G:129:TRP:CD2	2.54	0.42
13:M:15:VAL:HG13	13:M:126:LEU:HD13	2.01	0.42
1:A:19:CYS:HB2	1:A:1337:LYS:HG2	2.01	0.42
1:A:65:LYS:NZ	1:A:75:ASN:HB2	2.34	0.42
1:A:355:ASN:O	1:A:359:LYS:HG3	2.19	0.42
1:A:1119:GLU:O	1:A:1119:GLU:HG2	2.20	0.42
2:B:178:ILE:HG23	2:B:436:VAL:HG12	2.01	0.42
2:B:193:ALA:HA	2:B:198:ALA:HA	2.01	0.42
2:B:376:LEU:HG	2:B:410:GLN:HE22	1.84	0.42
2:B:759:LYS:HB3	2:B:912:PRO:HA	2.02	0.42
3:C:344:GLN:NE2	11:K:93:VAL:HG11	2.35	0.42
5:E:73:PHE:HD2	5:E:99:ILE:HG21	1.84	0.42
13:M:237:GLU:OE1	14:N:322:THR:HG21	2.20	0.42
11:K:123:ASP:OD2	11:K:124:GLN:N	2.53	0.42
14:N:41:PRO:HB2	14:N:43:ILE:HG13	2.01	0.42
1:A:583:LEU:HD23	1:A:583:LEU:HA	1.93	0.42
2:B:480:CYS:SG	2:B:666:GLY:N	2.92	0.42
5:E:12:LYS:O	5:E:16:THR:HG23	2.19	0.42
1:A:897:ILE:HG13	5:E:165:LEU:HD22	2.01	0.42
1:A:973:ILE:HD11	1:A:1015:LEU:HD21	2.02	0.42
1:A:1122:LEU:HG	1:A:1124:ASP:H	1.83	0.42
1:A:1239:HIS:HB2	5:E:5:GLU:OE1	2.19	0.42
8:H:51:ASP:OD1	8:H:51:ASP:N	2.52	0.42
11:K:46:GLU:HA	11:K:78:SER:HB3	2.02	0.42
1:A:283:LEU:HA	1:A:286:ILE:HG12	2.01	0.42
1:A:604:ILE:HD11	1:A:686:LEU:HD13	2.02	0.42
1:A:1347:ILE:HD13	2:B:1052:ARG:HD2	2.01	0.42
2:B:682:ARG:CZ	2:B:937:ARG:HG3	2.49	0.42
2:B:936:SER:OG	9:I:89:GLU:OE2	2.38	0.42
2:B:1078:ASP:HA	2:B:1103:SER:HA	2.02	0.42
2:B:1080:CYS:SG	2:B:1092:CYS:HB2	2.60	0.42
15:O:102:THR:OG1	15:O:147:THR:HG21	2.18	0.42
2:B:30:LEU:HB3	2:B:31:PRO:HD3	2.01	0.42
3:C:129:ASP:N	3:C:129:ASP:OD1	2.52	0.42
6:F:79:VAL:HG11	6:F:83:LEU:HD23	2.02	0.42
9:I:31:VAL:HG21	13:M:70:CYS:HB2	2.01	0.42
13:M:7:ASP:HB2	13:M:8:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:92:TYR:CE2	13:M:97:MET:HG3	2.54	0.42
15:O:117:THR:O	15:O:121:VAL:HG23	2.19	0.42
15:O:321:GLU:OE2	15:O:337:ASN:ND2	2.53	0.42
16:P:230:LEU:HB3	16:P:233:GLU:OE2	2.19	0.42
1:A:470:LYS:HB3	1:A:1039:GLN:HE22	1.84	0.42
1:A:1178:ARG:HB3	1:A:1180:ASN:ND2	2.35	0.42
5:E:61:LEU:HD11	5:E:71:GLN:HB3	2.00	0.42
1:A:506:ASN:OD1	1:A:506:ASN:N	2.53	0.41
2:B:569:ASN:HD21	2:B:571:PHE:HD2	1.66	0.41
2:B:623:ASP:HA	2:B:626:HIS:HB2	2.02	0.41
9:I:102:CYS:SG	9:I:103:GLY:N	2.93	0.41
1:A:368:VAL:HG22	1:A:504:GLU:HG2	2.01	0.41
1:A:1123:PRO:HA	9:I:20:CYS:SG	2.60	0.41
2:B:189:ILE:HG21	2:B:338:MET:HG3	2.02	0.41
2:B:772:TYR:HB3	2:B:884:LEU:HD11	2.01	0.41
8:H:8:ASP:HB3	8:H:10:PHE:CE2	2.55	0.41
9:I:63:ASP:OD2	9:I:63:ASP:N	2.48	0.41
16:P:187:PHE:CE2	16:P:216:VAL:HG12	2.44	0.41
2:B:1084:GLY:HA3	2:B:1126:LEU:H	1.85	0.41
4:D:110:GLU:O	4:D:113:ILE:HB	2.20	0.41
4:D:123:ILE:HD13	4:D:123:ILE:HA	1.94	0.41
5:E:82:VAL:HG11	5:E:110:MET:SD	2.60	0.41
1:A:1319:ALA:O	1:A:1324:THR:HG22	2.20	0.41
2:B:423:ASN:HD22	2:B:434:GLN:HG3	1.84	0.41
3:C:74:ASN:OD1	3:C:77:ARG:NH1	2.54	0.41
5:E:168:ASN:OD1	5:E:172:ARG:NH2	2.51	0.41
16:P:201:ASN:HB3	16:P:202:PRO:HD3	2.01	0.41
1:A:5:GLN:NE2	7:G:159:ASP:OD2	2.50	0.41
3:C:50:ARG:HE	3:C:66:VAL:HG21	1.86	0.41
6:F:112:ASP:OD1	6:F:113:GLY:N	2.54	0.41
15:O:491:ILE:HG23	15:O:495:GLU:HB3	2.03	0.41
17:Q:103:TRP:HD1	17:Q:106:LEU:HD23	1.86	0.41
1:A:643:SER:O	1:A:643:SER:OG	2.36	0.41
1:A:738:GLN:NE2	1:A:744:ALA:HA	2.36	0.41
1:A:1218:SER:HB2	9:I:101:GLN:HB3	2.03	0.41
1:A:1279:GLY:HA3	9:I:107:ARG:HH11	1.86	0.41
2:B:526:LEU:HD12	2:B:530:GLU:HB2	2.03	0.41
15:O:192:LYS:HD3	15:O:193:LEU:O	2.20	0.41
1:A:1137:ILE:O	1:A:1141:ARG:N	2.52	0.41
2:B:513:LYS:NZ	13:M:249:LEU:O	2.44	0.41
2:B:689:MET:SD	2:B:904:LYS:HD3	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:817:PRO:HB3	2:B:868:LYS:HA	2.01	0.41
2:B:914:GLU:HB3	3:C:78:ARG:HG2	2.01	0.41
16:P:175:GLU:H	16:P:175:GLU:CD	2.23	0.41
2:B:371:LEU:O	2:B:374:GLU:HG3	2.21	0.41
8:H:136:GLU:HB2	8:H:139:SER:OG	2.20	0.41
16:P:176:PHE:HA	16:P:179:VAL:HG22	2.03	0.41
1:A:178:LYS:HG2	1:A:179:TYR:H	1.85	0.41
1:A:290:ASN:OD1	1:A:313:LEU:HD11	2.21	0.41
1:A:635:ASP:O	1:A:648:GLY:HA2	2.21	0.41
1:A:738:GLN:HE22	1:A:744:ALA:HA	1.85	0.41
1:A:1086:THR:HG23	1:A:1224:LYS:HD3	2.02	0.41
2:B:36:VAL:HG12	2:B:37:LYS:HG2	2.02	0.41
2:B:58:ILE:HD13	2:B:374:GLU:HB3	2.01	0.41
2:B:171:VAL:O	2:B:174:VAL:HG22	2.19	0.41
2:B:946:LEU:HD22	2:B:1003:TYR:CE2	2.55	0.41
2:B:946:LEU:HD21	2:B:1005:GLY:HA3	2.02	0.41
3:C:75:ALA:O	3:C:79:ILE:HG12	2.21	0.41
4:D:5:ASP:OD2	4:D:8:SER:HB2	2.21	0.41
11:K:54:SER:O	11:K:58:MET:HG2	2.21	0.41
15:O:377:GLN:O	15:O:380:VAL:HG12	2.21	0.41
15:O:464:SER:O	15:O:468:GLU:HG2	2.21	0.41
2:B:70:ASP:HA	2:B:71:PRO:HD3	1.96	0.41
3:C:14:VAL:O	3:C:300:ALA:HA	2.21	0.41
15:O:239:LEU:O	15:O:243:HIS:ND1	2.54	0.41
15:O:515:GLN:HB3	16:P:281:GLY:HA3	2.02	0.41
15:O:519:THR:HG21	16:P:282:LEU:HD12	2.03	0.41
19:S:12:DG:H2'	19:S:13:DT:C6	2.56	0.41
2:B:407:ARG:HD3	2:B:409:ASP:OD1	2.20	0.40
2:B:1130:LYS:HB2	2:B:1133:GLU:HG3	2.01	0.40
9:I:98:CYS:O	9:I:103:GLY:HA2	2.21	0.40
14:N:269:LEU:HD11	14:N:383:LEU:HD12	2.02	0.40
17:Q:40:ASP:OD1	17:Q:40:ASP:N	2.52	0.40
2:B:528:GLY:O	2:B:531:LEU:HG	2.22	0.40
2:B:795:LEU:HB2	13:M:707:GLN:HE21	1.87	0.40
3:C:10:MET:SD	8:H:46:GLN:NE2	2.93	0.40
7:G:153:VAL:O	7:G:187:VAL:HG22	2.21	0.40
11:K:41:THR:OG1	11:K:83:ARG:HG2	2.20	0.40
11:K:66:GLU:HB2	11:K:87:ARG:CG	2.50	0.40
1:A:162:PHE:CZ	1:A:180:LYS:HE3	2.56	0.40
1:A:666:ILE:HG23	1:A:923:ARG:HH21	1.86	0.40
2:B:139:MET:HB2	2:B:142:SER:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:166:HIS:CD2	3:C:167:LYS:HG3	2.57	0.40
16:P:242:LEU:HB3	16:P:248:VAL:HG22	2.03	0.40
1:A:184:LYS:HG3	1:A:185:VAL:N	2.37	0.40
1:A:254:ARG:NH1	16:P:295:ASP:OD2	2.35	0.40
2:B:751:ILE:HD12	2:B:751:ILE:HG23	1.87	0.40
4:D:11:LEU:H	4:D:11:LEU:HD23	1.85	0.40
6:F:58:THR:HB	6:F:61:GLU:HG2	2.03	0.40
11:K:100:LEU:HD12	11:K:100:LEU:HA	1.89	0.40
2:B:706:ASP:O	2:B:774:ASN:HB2	2.21	0.40
3:C:13:ARG:HG3	3:C:302:VAL:HA	2.02	0.40
9:I:72:CYS:SG	9:I:74:HIS:HD2	2.44	0.40
13:M:33:ARG:HD2	13:M:34:PRO:HD2	2.03	0.40
15:O:458:LYS:HG3	15:O:459:ARG:H	1.86	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	1385/1390 (100%)	1304 (94%)	80 (6%)	1 (0%)	51	82
2	B	1089/1133 (96%)	1030 (95%)	59 (5%)	0	100	100
3	C	343/346 (99%)	316 (92%)	27 (8%)	0	100	100
4	D	124/148 (84%)	114 (92%)	9 (7%)	1 (1%)	19	51
5	E	208/210 (99%)	192 (92%)	16 (8%)	0	100	100
6	F	77/127 (61%)	73 (95%)	4 (5%)	0	100	100
7	G	181/204 (89%)	167 (92%)	14 (8%)	0	100	100
8	H	147/150 (98%)	138 (94%)	9 (6%)	0	100	100
9	I	106/108 (98%)	98 (92%)	8 (8%)	0	100	100
10	J	65/67 (97%)	63 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	105/133 (79%)	104 (99%)	1 (1%)	0	100	100
12	L	45/58 (78%)	42 (93%)	3 (7%)	0	100	100
13	M	214/708 (30%)	206 (96%)	8 (4%)	0	100	100
14	N	130/398 (33%)	117 (90%)	13 (10%)	0	100	100
15	O	484/534 (91%)	468 (97%)	16 (3%)	0	100	100
16	P	135/316 (43%)	127 (94%)	8 (6%)	0	100	100
17	Q	84/223 (38%)	77 (92%)	7 (8%)	0	100	100
All	All	4922/6253 (79%)	4636 (94%)	284 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	78	LEU
1	A	591	PRO

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	1208/1212 (100%)	1204 (100%)	4 (0%)	92	98
2	B	958/988 (97%)	953 (100%)	5 (0%)	88	96
3	C	301/302 (100%)	301 (100%)	0	100	100
4	D	117/136 (86%)	115 (98%)	2 (2%)	60	86
5	E	192/192 (100%)	189 (98%)	3 (2%)	62	86
6	F	69/111 (62%)	69 (100%)	0	100	100
7	G	167/181 (92%)	166 (99%)	1 (1%)	86	96
8	H	130/131 (99%)	129 (99%)	1 (1%)	81	94
9	I	94/94 (100%)	93 (99%)	1 (1%)	73	92
10	J	56/56 (100%)	55 (98%)	1 (2%)	59	85
11	K	96/119 (81%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	L	44/55 (80%)	44 (100%)	0	100 100
13	M	200/622 (32%)	200 (100%)	0	100 100
14	N	119/347 (34%)	118 (99%)	1 (1%)	81 94
15	O	439/476 (92%)	438 (100%)	1 (0%)	93 98
16	P	125/280 (45%)	125 (100%)	0	100 100
17	Q	83/195 (43%)	83 (100%)	0	100 100
All	All	4398/5497 (80%)	4378 (100%)	20 (0%)	89 96

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	452	ARG
1	A	754	LYS
1	A	915	LYS
1	A	1161	LYS
2	B	195	ARG
2	B	292	ARG
2	B	396	ARG
2	B	404	LYS
2	B	801	LYS
4	D	28	LYS
4	D	77	LYS
5	E	93	ARG
5	E	153	LYS
5	E	202	ARG
7	G	97	VAL
8	H	81	ARG
9	I	36	ARG
10	J	47	ARG
14	N	336	ARG
15	O	333	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	40	ASN
1	A	47	GLN
1	A	157	HIS

Continued on next page...

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Mol	Chain	Res	Type
1	A	163	ASN
1	A	192	ASN
1	A	195	GLN
1	A	343	GLN
1	A	355	ASN
1	A	374	ASN
1	A	397	ASN
1	A	419	ASN
1	A	465	GLN
1	A	599	GLN
1	A	616	ASN
1	A	623	GLN
1	A	693	ASN
1	A	738	GLN
1	A	775	ASN
1	A	794	GLN
1	A	802	GLN
1	A	885	GLN
1	A	1039	GLN
1	A	1180	ASN
1	A	1202	GLN
1	A	1385	HIS
2	B	181	GLN
2	B	227	HIS
2	B	280	GLN
2	B	381	ASN
2	B	405	HIS
2	B	413	ASN
2	B	423	ASN
2	B	569	ASN
2	B	683	ASN
2	B	758	ASN
2	B	829	ASN
2	B	1034	GLN
2	B	1100	HIS
3	C	55	HIS
3	C	172	HIS
3	C	213	HIS
3	C	344	GLN
4	D	13	ASN
4	D	60	HIS
4	D	61	GLN

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Mol	Chain	Res	Type
4	D	76	HIS
4	D	88	ASN
4	D	118	HIS
7	G	17	GLN
8	H	46	GLN
9	I	74	HIS
9	I	99	ASN
11	K	45	HIS
11	K	85	GLN
12	L	23	HIS
13	M	106	GLN
13	M	125	HIS
13	M	130	HIS
13	M	197	GLN
13	M	235	ASN
13	M	707	GLN
14	N	338	GLN
14	N	395	HIS
15	O	113	ASN
15	O	377	GLN
15	O	379	GLN
15	O	402	ASN
15	O	415	HIS
15	O	515	GLN
17	Q	62	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	T	4/20 (20%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
22	SF4	P	400	16	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
22	SF4	P	400	16	-	-	0/6/5/5

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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	P	400	SF4	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

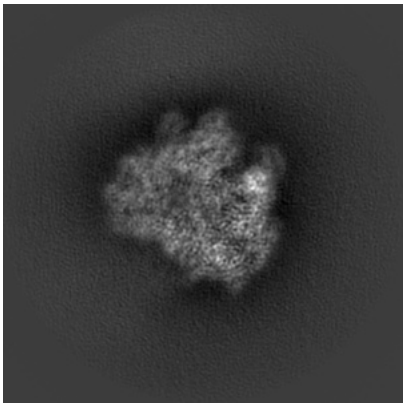
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30577. These allow visual inspection of the internal detail of the map and identification of artifacts.

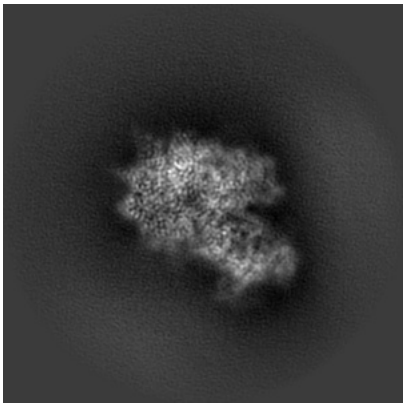
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

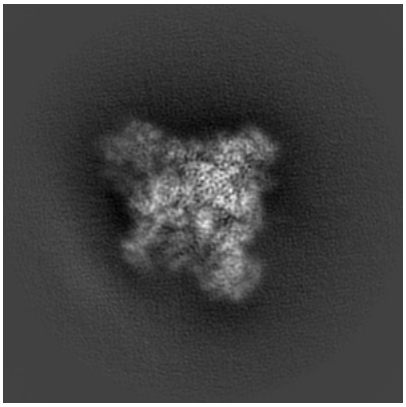
6.1.1 Primary map



X



Y

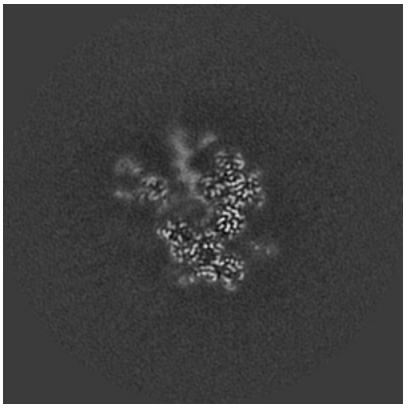


Z

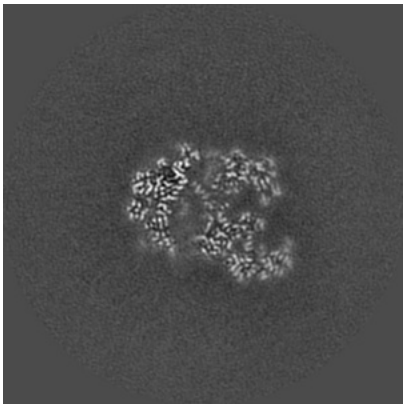
The images above show the map projected in three orthogonal directions.

6.2 Central slices

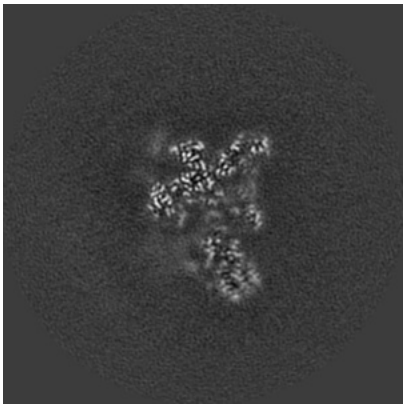
6.2.1 Primary map



X Index: 160



Y Index: 160

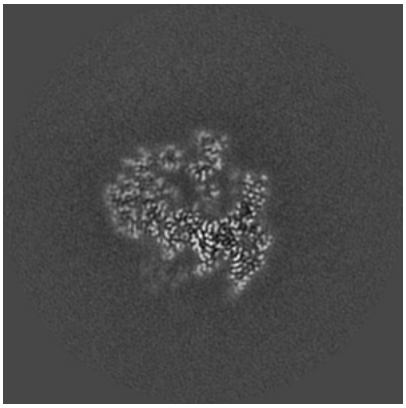


Z Index: 160

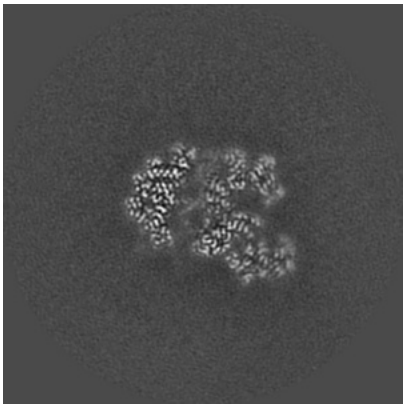
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

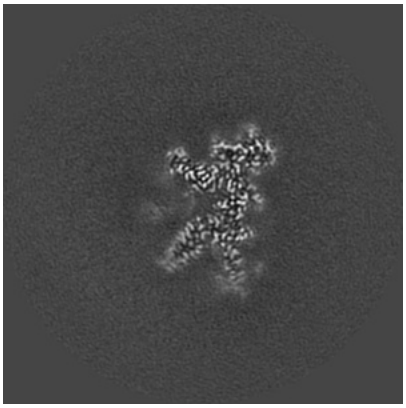
6.3.1 Primary map



X Index: 183



Y Index: 164



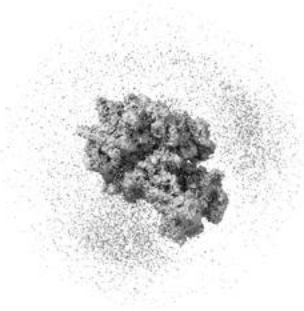
Z Index: 141

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

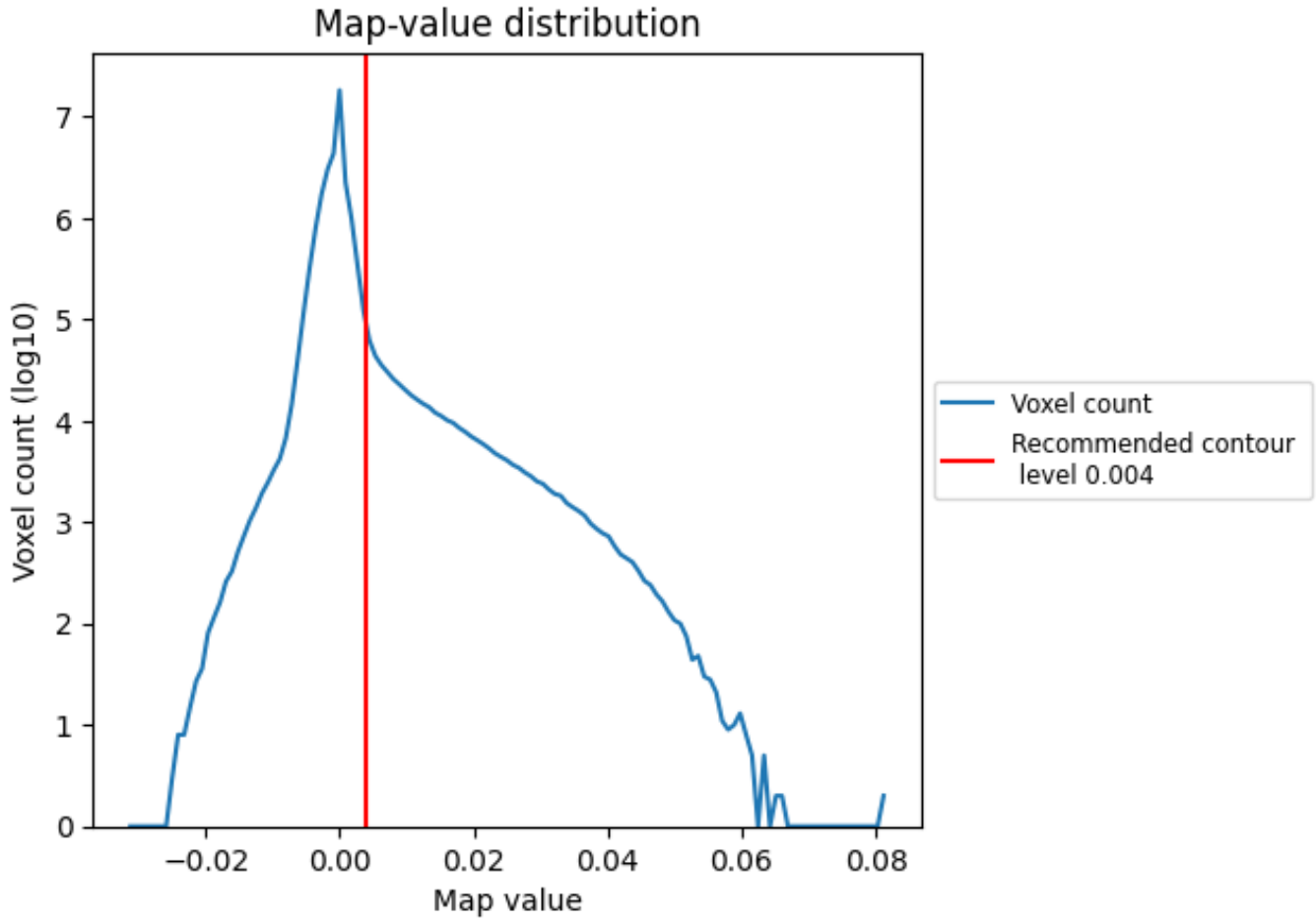
6.5 Mask visualisation (i)

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

7 Map analysis

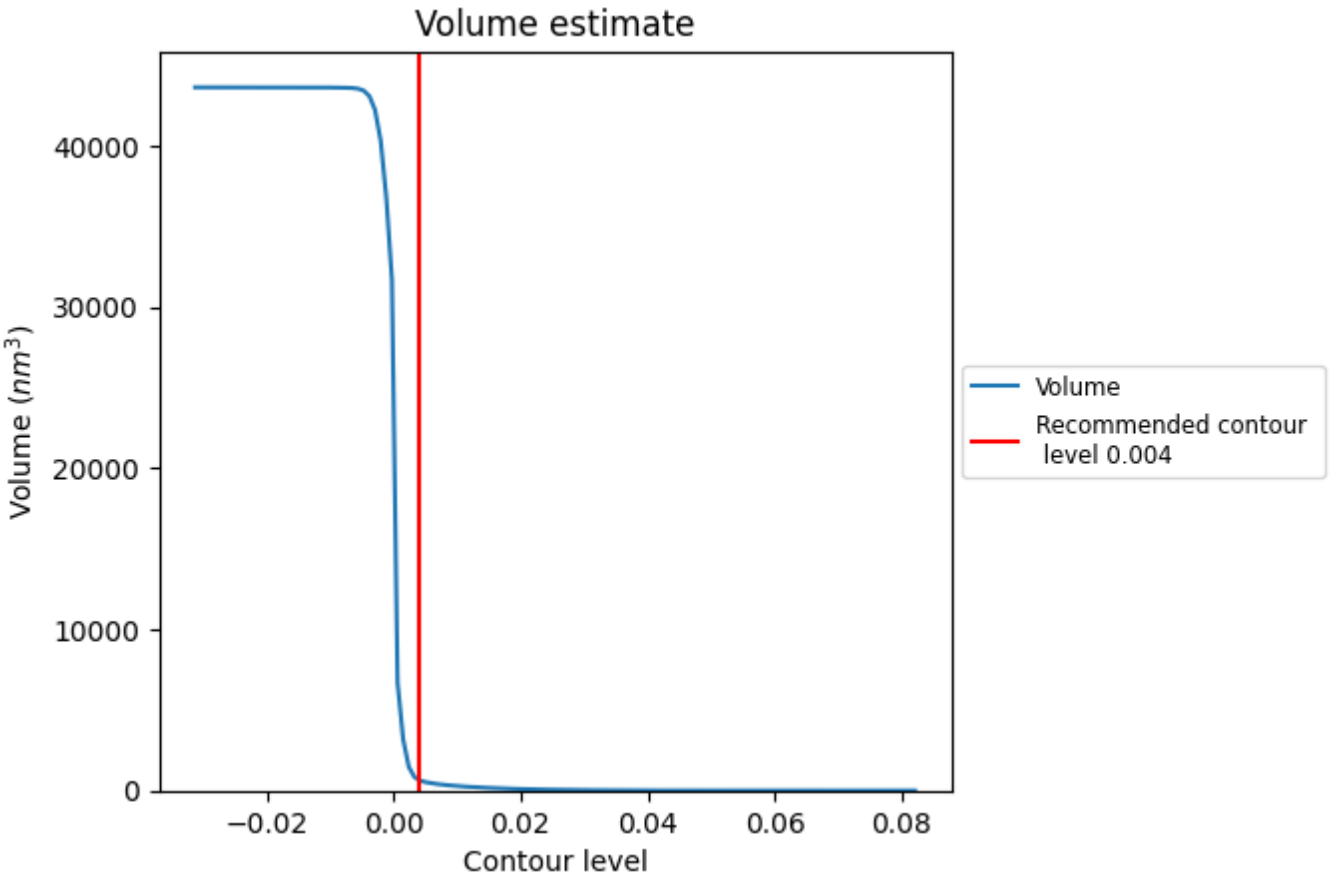
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

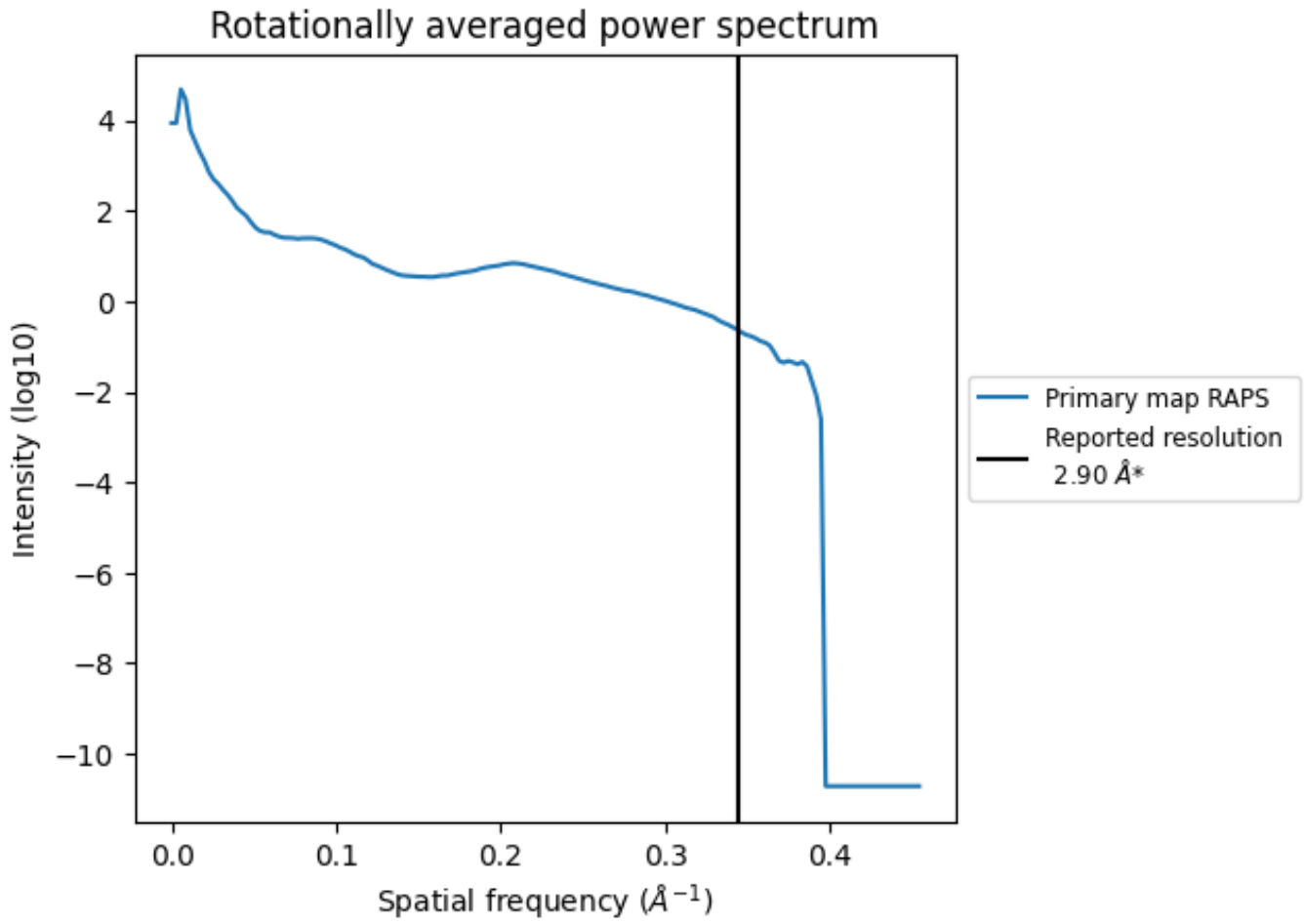
7.2 Volume estimate



The volume at the recommended contour level is 658 nm^3; this corresponds to an approximate mass of 594 kDa.

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

7.3 Rotationally averaged power spectrum (i)



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

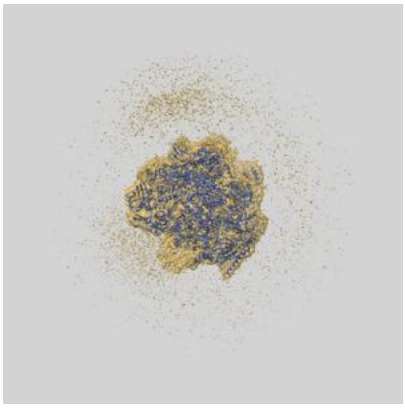
8 Fourier-Shell correlation (i)

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

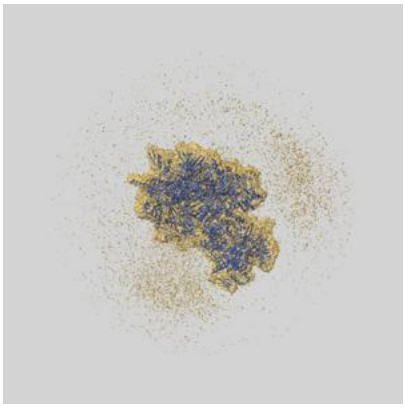
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30577 and PDB model 7D58. Per-residue inclusion information can be found in section 3 on page 8.

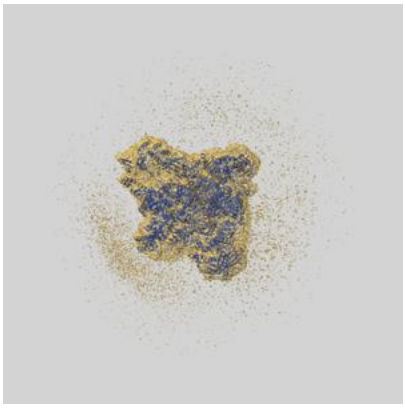
9.1 Map-model overlay



X



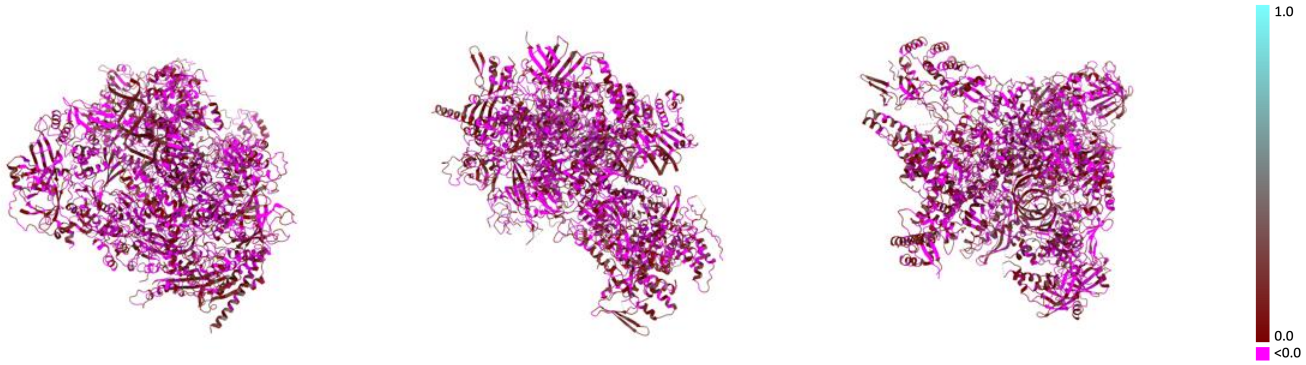
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.004 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.

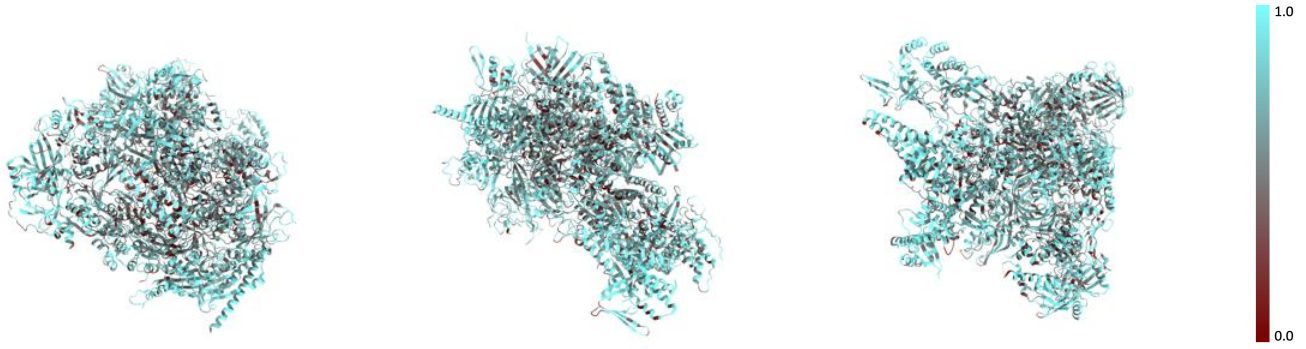
9.2 Q-score mapped to coordinate model



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.

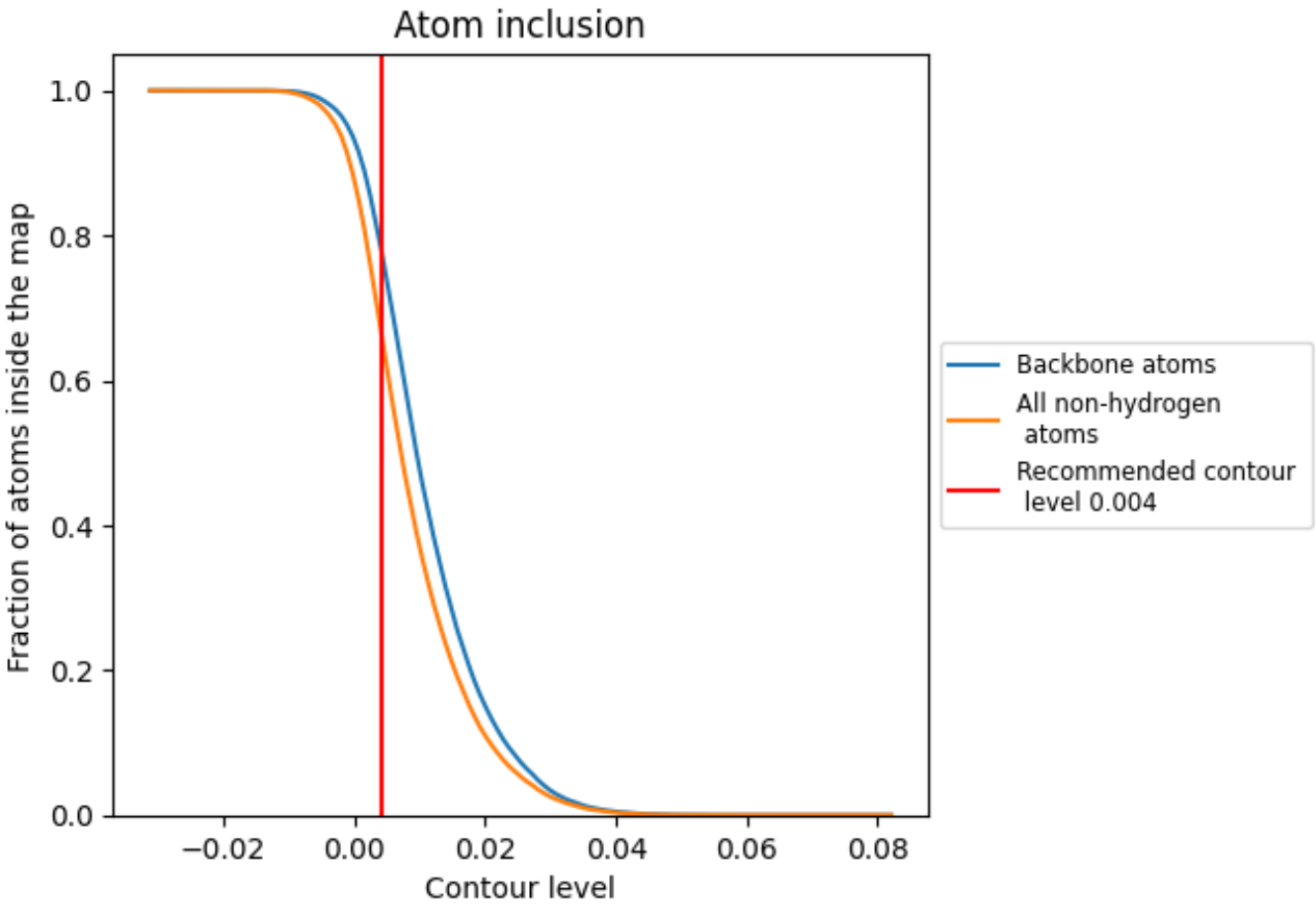
9.3 Atom inclusion mapped to coordinate model



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 (0.004).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 67% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6714	0.0140
A	0.6109	-0.0100
B	0.6326	0.0030
C	0.7693	0.0600
D	0.7950	0.0590
E	0.6683	-0.0180
F	0.6434	-0.0020
G	0.7563	0.0490
H	0.6726	-0.0020
I	0.6177	0.0040
J	0.6910	0.0220
K	0.7337	0.0670
L	0.7769	0.0640
M	0.7327	0.0330
N	0.7338	0.0040
O	0.7059	0.0240
P	0.7593	0.0380
Q	0.6403	0.0300
R	0.8555	0.1390
S	0.6897	0.0700
T	0.4434	0.0250