



# Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 04:30 PM JST

PDB ID : 7D59  
EMDB ID : EMD-30578  
Title : cryo-EM structure of human RNA polymerase III in apo state  
Authors : Wang, Q.; Wan, F.; Lan, P.; Wu, J.; Lei, M.  
Deposited on : 2020-09-25  
Resolution : 3.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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The following versions of software and data (see [references ⓘ](#)) 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

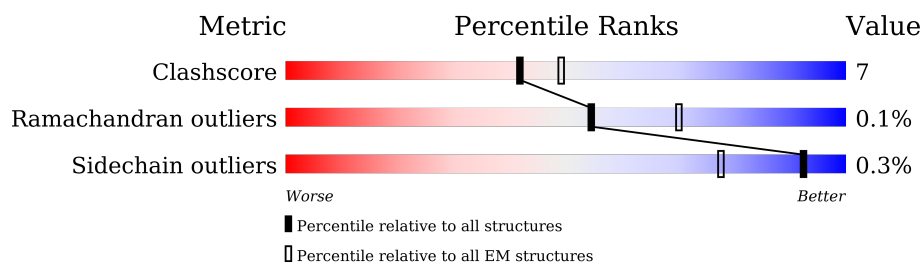
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1390	 80% 19%
2	B	1133	 81% 16%
3	C	346	 85% 15%
4	D	148	 13% 61% 23% 15%
5	E	210	 84% 16%
6	F	127	 50% 12% 38%
7	G	204	 9% 69% 21% 10%
8	H	150	 5% 81% 19%

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Mol	Chain	Length	Quality of chain
9	I	108	
10	J	67	
11	K	133	
12	L	58	
13	M	708	
14	N	398	
15	O	534	
16	P	316	
17	Q	223	

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
19	SF4	P	400	-	-	X	-

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 39898 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
1	A	1386	Total	C	N	O	S	0	0
			10881	6894	1897	2017	73		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1095	Total	C	N	O	S	0	0
			8668	5492	1513	1595	68		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	345	Total	C	N	O	S	0	0
			2752	1732	490	518	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	126	Total	C	N	O	S	0	0
			1013	634	176	200	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	210	Total	C	N	O	S	0	0
			1723	1088	301	325	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	79	Total	C	N	O	S	0	0
			636	407	108	116	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	183	Total	C	N	O	S	0	0
			1470	951	231	281	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		

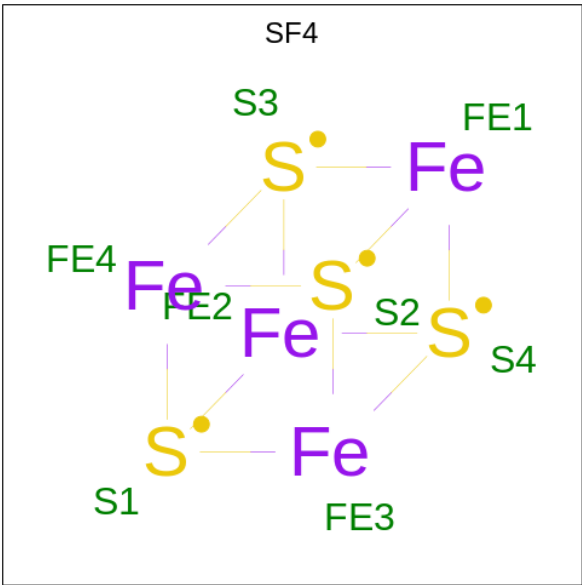
- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	121	Total	C	N	O	S	0	0
			1049	667	166	210	6		

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

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

- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).

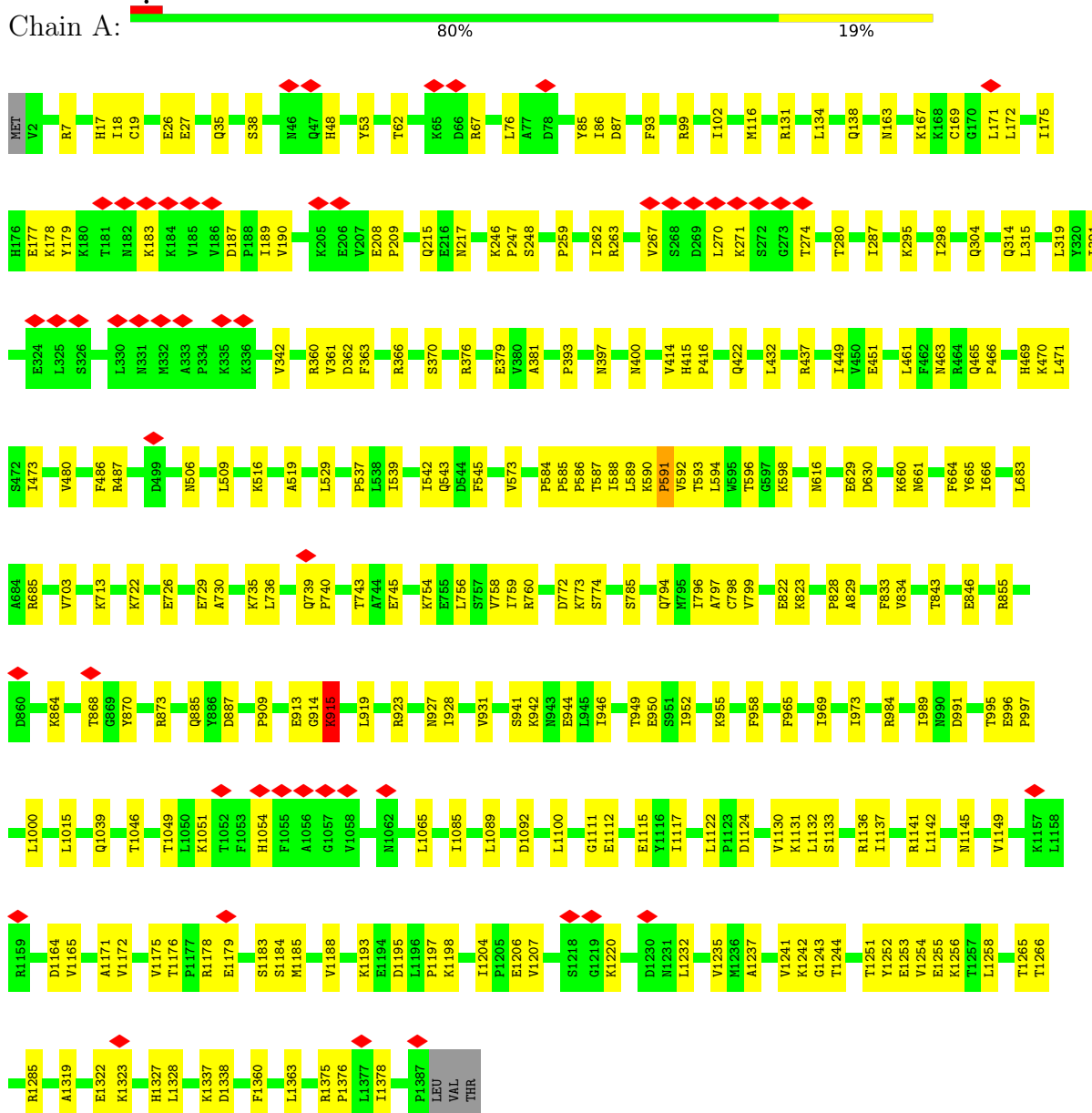


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
19	P	1	8	4	4	0

### 3 Residue-property plots

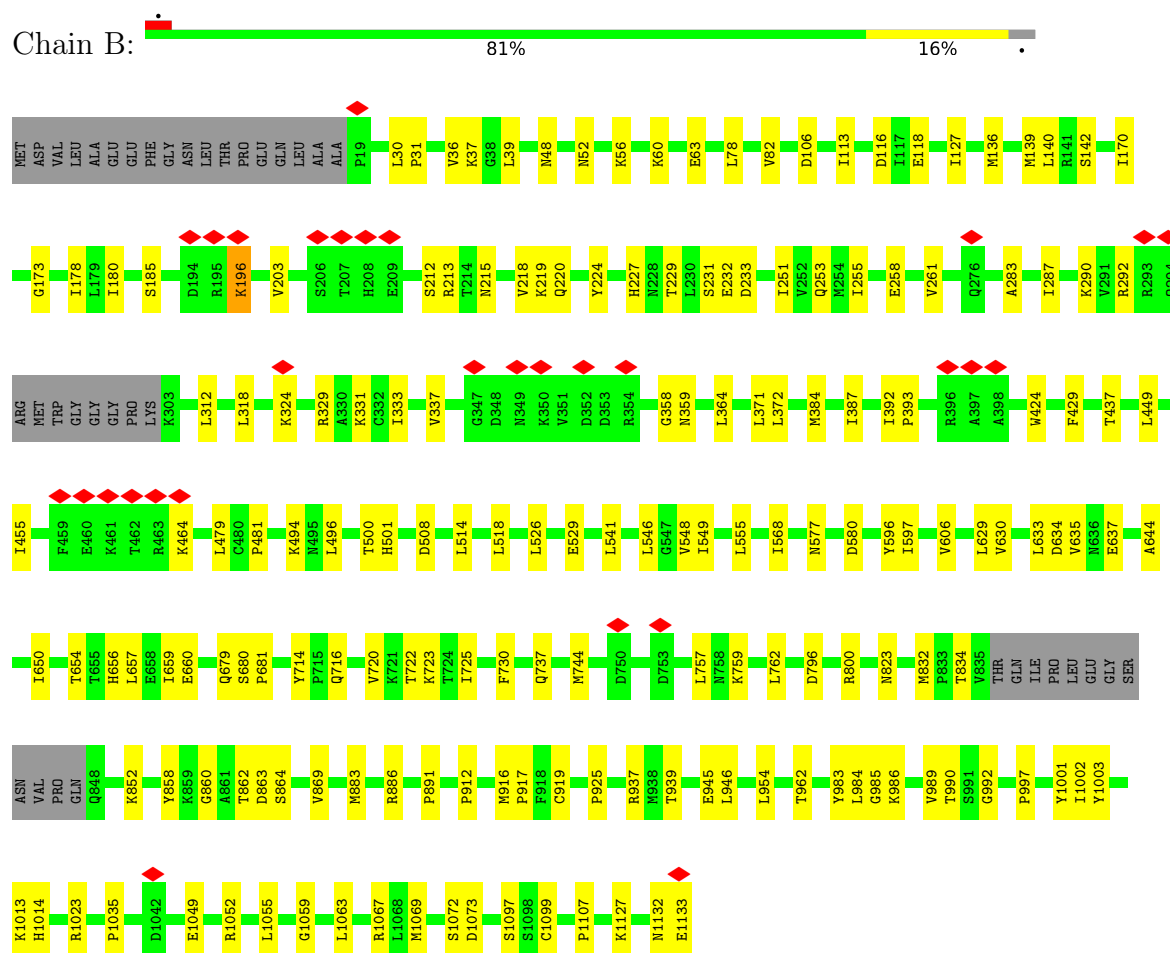
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

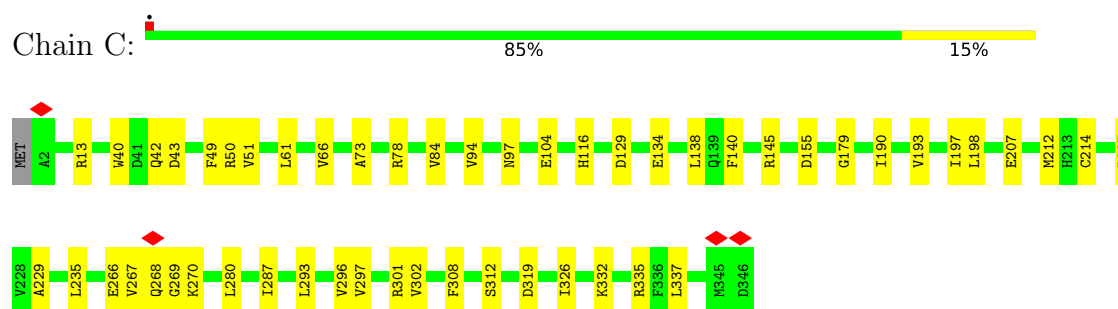




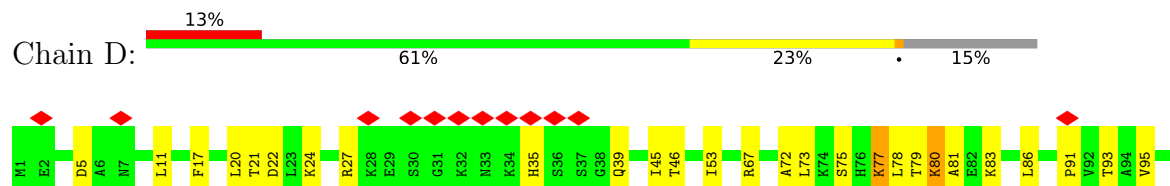
- Molecule 2: DNA-directed RNA polymerase III subunit RPC2

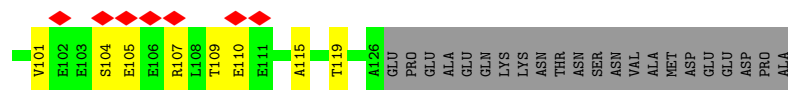


- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

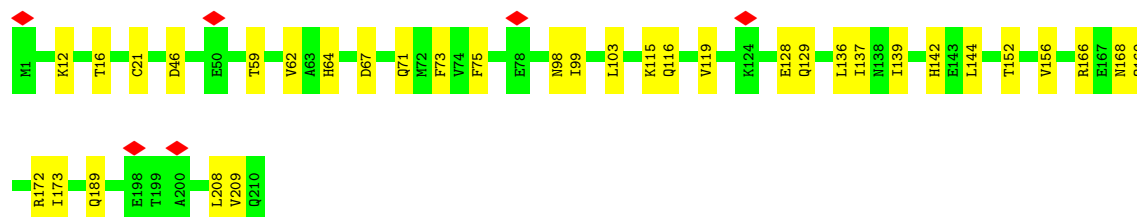
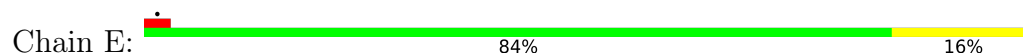


- Molecule 4: DNA-directed RNA polymerase III subunit RPC9

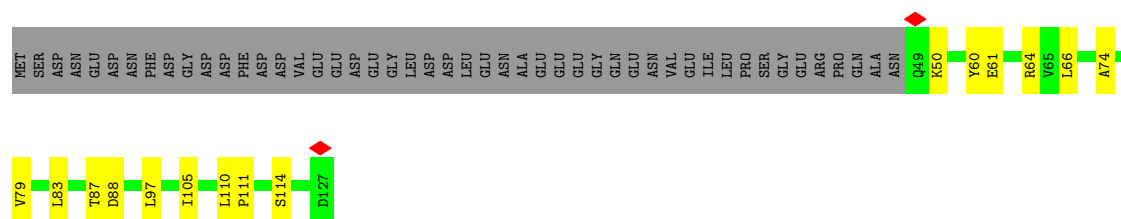




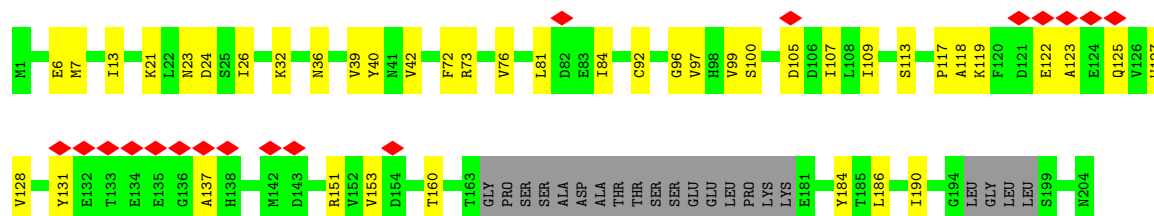
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



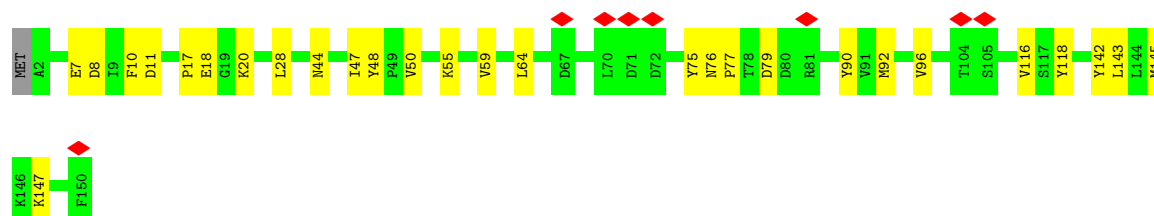
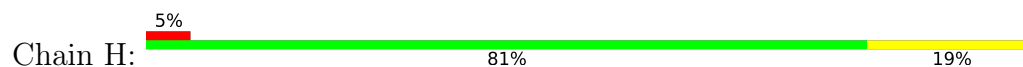
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



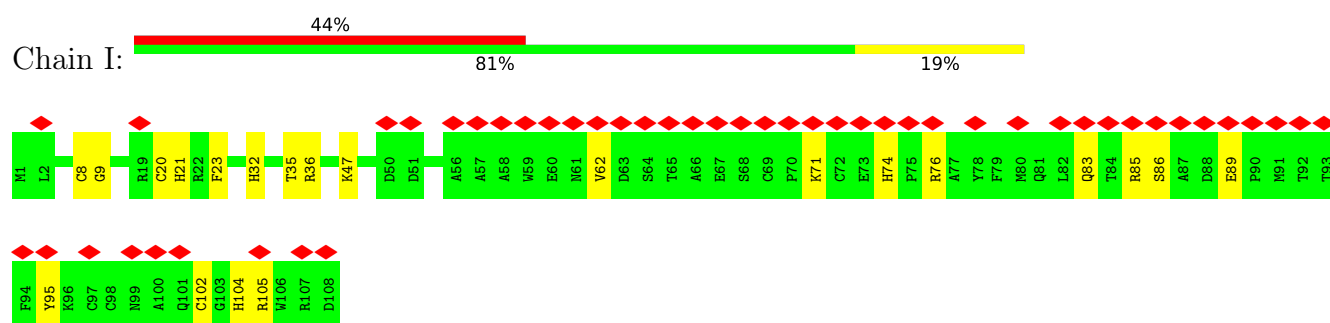
- Molecule 7: DNA-directed RNA polymerase III subunit RPC8



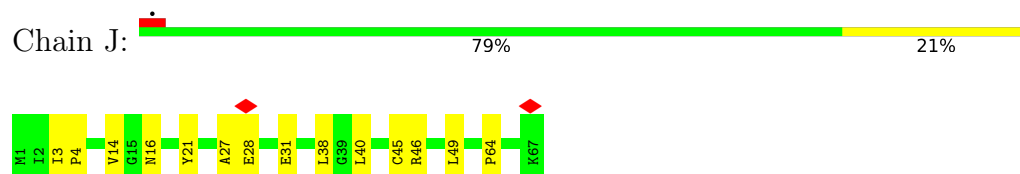
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



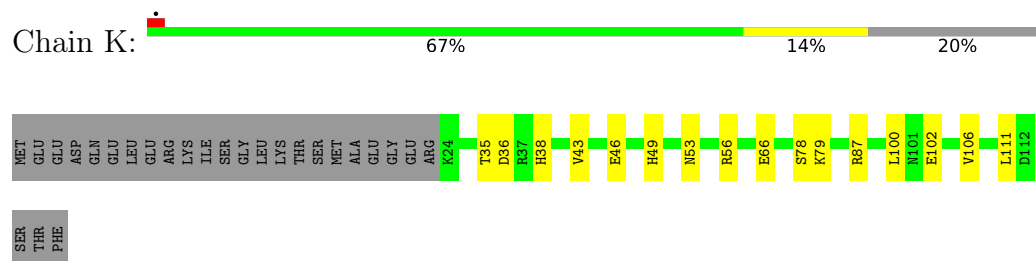
- Molecule 9: DNA-directed RNA polymerase III subunit RPC10



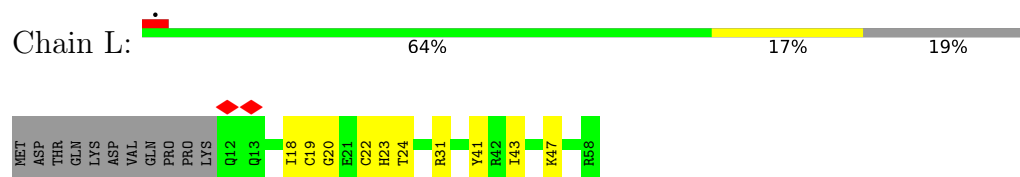
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



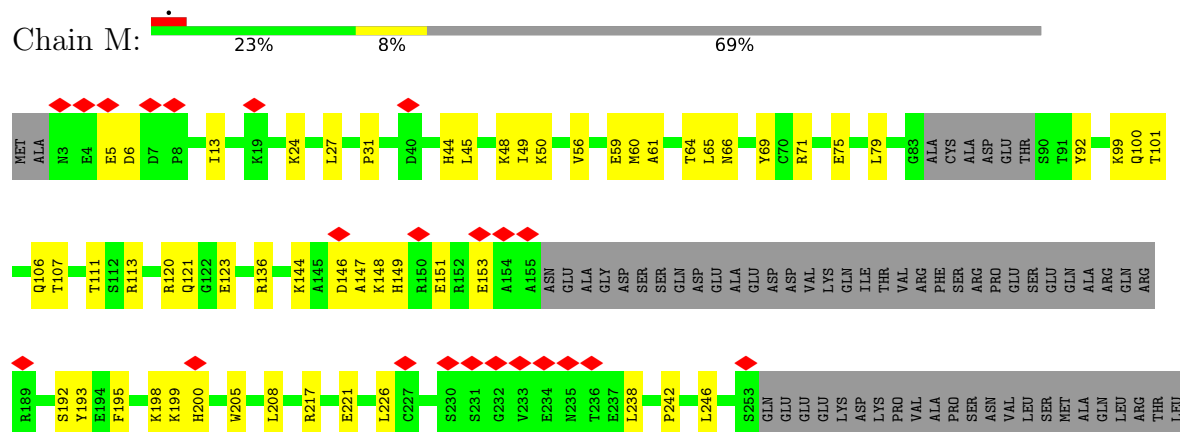
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

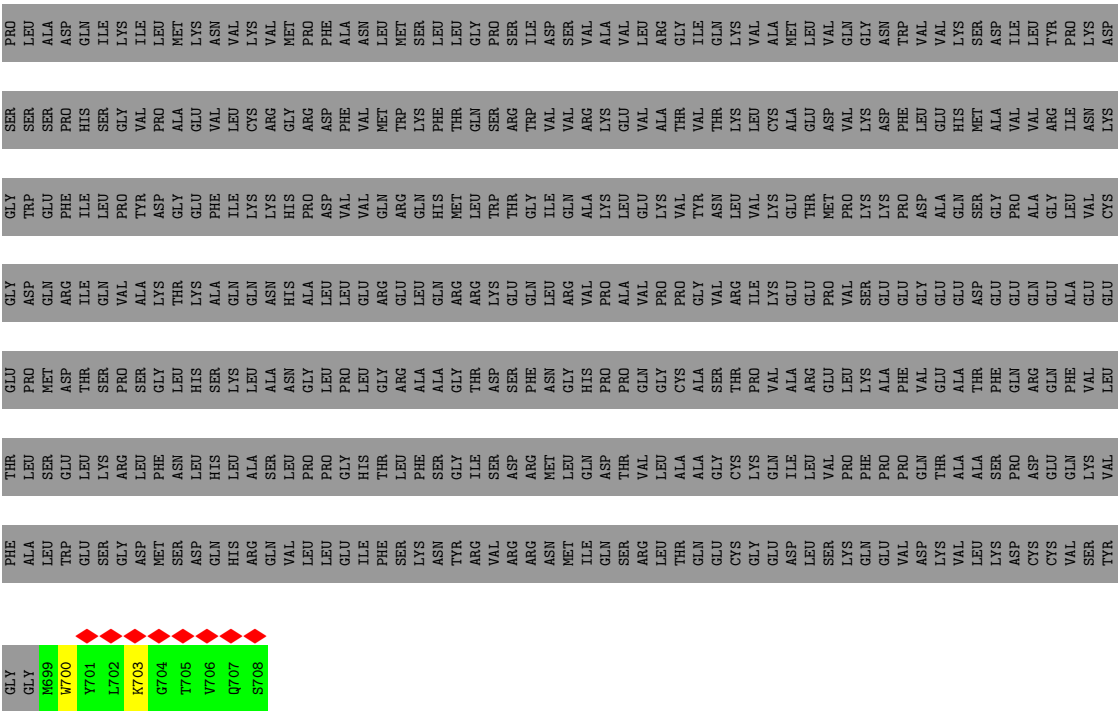


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

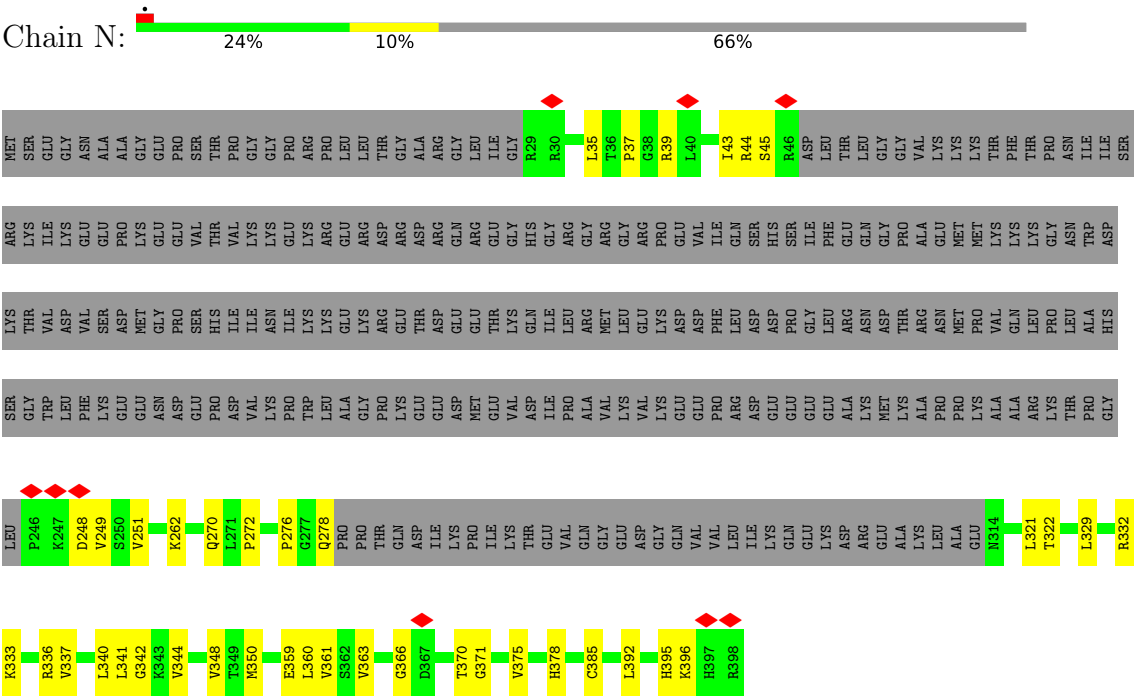


- Molecule 13: DNA-directed RNA polymerase III subunit RPC5

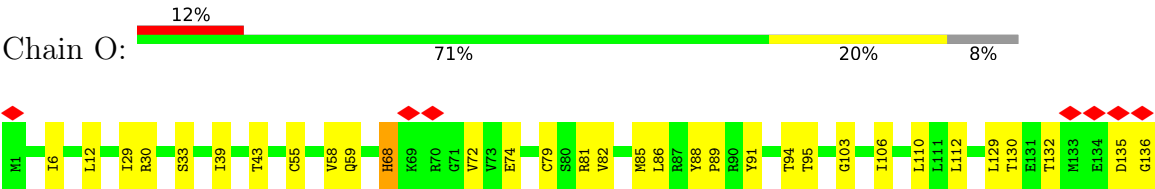


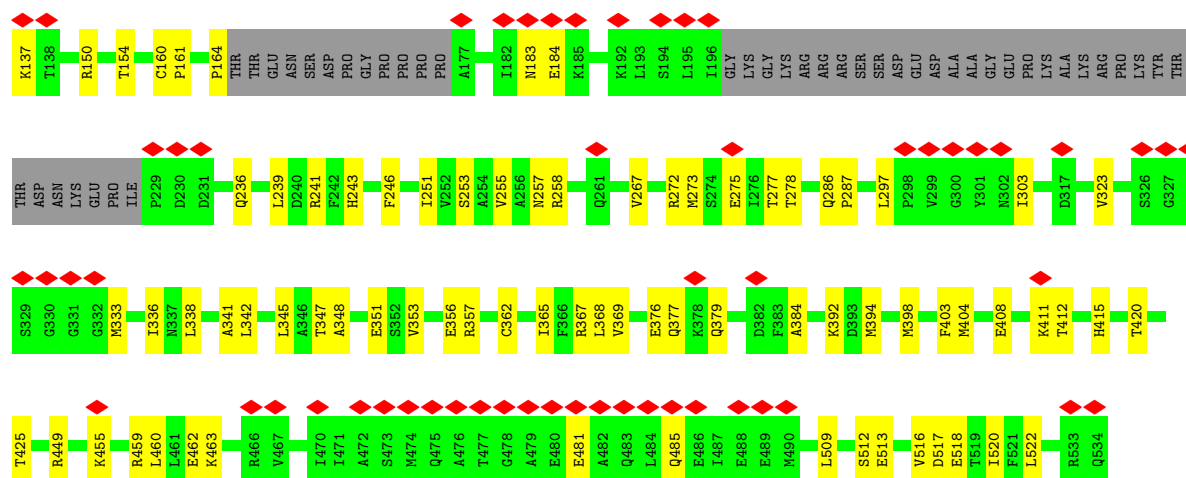


• Molecule 14: DNA-directed RNA polymerase III subunit RPC4

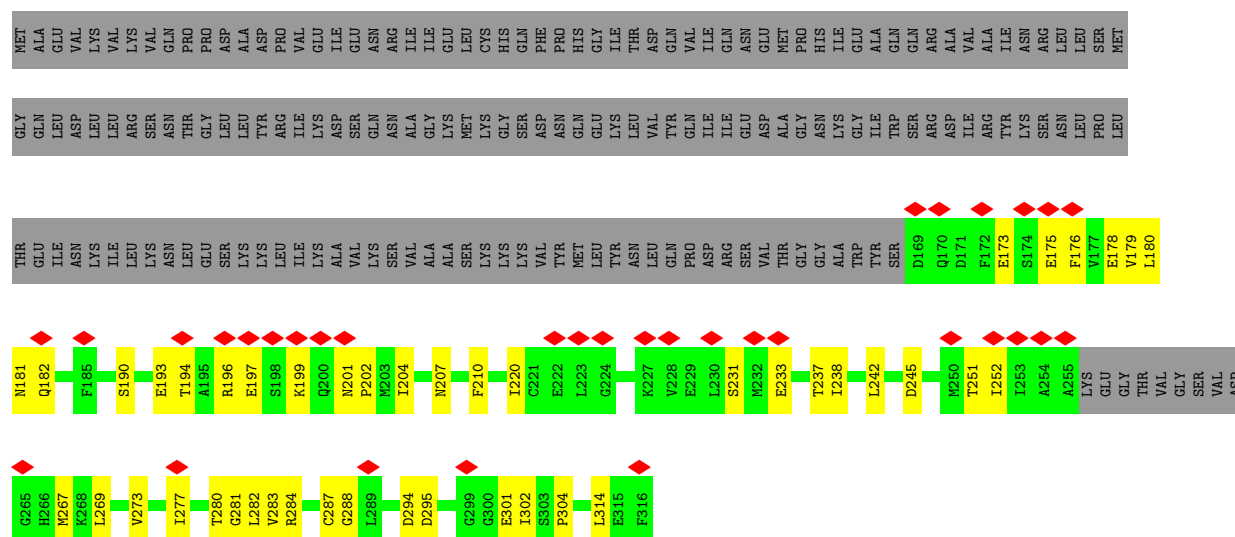
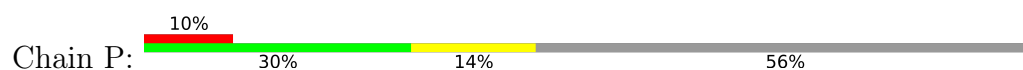


• Molecule 15: DNA-directed RNA polymerase III subunit RPC3

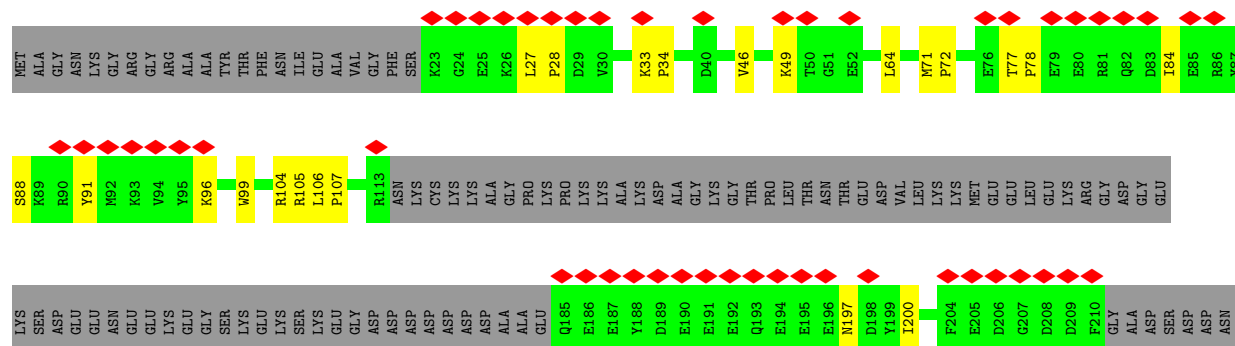
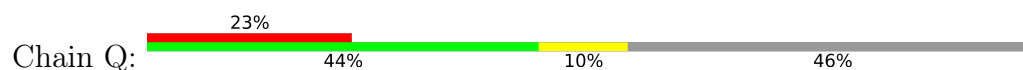


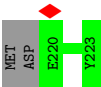


• Molecule 16: DNA-directed RNA polymerase III subunit RPC6



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





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	264514	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	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	0.057	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	366.24002, 366.24002, 366.24002	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.24	0/11078	0.41	0/14939
2	B	0.24	0/8833	0.41	0/11912
3	C	0.24	0/2806	0.42	0/3803
4	D	0.23	0/1026	0.41	0/1384
5	E	0.24	0/1753	0.42	0/2368
6	F	0.23	0/646	0.39	0/873
7	G	0.25	0/1510	0.45	0/2054
8	H	0.24	0/1219	0.43	0/1644
9	I	0.25	0/878	0.44	0/1186
10	J	0.23	0/542	0.39	0/730
11	K	0.23	0/871	0.39	0/1174
12	L	0.22	0/403	0.40	0/536
13	M	0.23	0/1837	0.42	0/2481
14	N	0.25	0/1051	0.46	0/1417
15	O	0.23	0/3972	0.41	0/5359
16	P	0.24	0/1126	0.42	0/1522
17	Q	0.25	0/1076	0.40	0/1449
All	All	0.24	0/40627	0.41	0/54831

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
4	D	0	1
15	O	0	1
All	All	0	2

There are no bond length outliers.



There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	77	LYS	Peptide
15	O	68	HIS	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10881	0	11126	181	0
2	B	8668	0	8794	113	0
3	C	2752	0	2725	34	0
4	D	1013	0	1040	21	0
5	E	1723	0	1745	22	0
6	F	636	0	667	13	0
7	G	1470	0	1409	28	0
8	H	1197	0	1156	17	0
9	I	857	0	817	15	0
10	J	533	0	555	9	0
11	K	856	0	840	13	0
12	L	397	0	401	6	0
13	M	1797	0	1756	44	0
14	N	1038	0	1092	28	0
15	O	3913	0	3988	67	0
16	P	1103	0	1066	38	0
17	Q	1049	0	985	17	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	I	2	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
19	P	8	0	0	3	0
All	All	39898	0	40162	585	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 7.

All (585) 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:96:GLY:HA3	7:G:109:ILE:O	1.52	1.07
7:G:99:VAL:O	7:G:107:ILE:HB	1.75	0.85
8:H:92:MET:HB2	8:H:143:LEU:HB3	1.59	0.84
1:A:913:GLU:HB2	1:A:919:LEU:HA	1.65	0.78
7:G:96:GLY:CA	7:G:109:ILE:O	2.34	0.75
13:M:120:ARG:HG2	13:M:121:GLN:H	1.51	0.75
1:A:246:LYS:HD2	1:A:248:SER:HB3	1.68	0.74
15:O:94:THR:HG21	15:O:246:PHE:HE1	1.50	0.74
15:O:255:VAL:HG21	15:O:267:VAL:HG21	1.69	0.73
7:G:131:TYR:HB3	7:G:137:ALA:HB3	1.71	0.72
13:M:49:ILE:HG13	13:M:56:VAL:HG12	1.70	0.72
2:B:725:ILE:HG23	2:B:730:PHE:HB3	1.69	0.72
14:N:251:VAL:HG22	14:N:350:MET:HG3	1.71	0.72
5:E:64:HIS:HD2	5:E:67:ASP:H	1.35	0.71
7:G:39:VAL:HG23	7:G:40:TYR:H	1.55	0.71
1:A:414:VAL:HG12	1:A:416:PRO:HD2	1.73	0.71
17:Q:72:PRO:HA	17:Q:96:LYS:HD2	1.73	0.70
1:A:735:LYS:HG3	1:A:736:LEU:H	1.55	0.70
1:A:995:THR:HG22	1:A:997:PRO:HD2	1.72	0.70
2:B:514:LEU:HD13	2:B:568:ILE:HD11	1.73	0.70
4:D:79:THR:HG22	4:D:81:ALA:H	1.57	0.69
16:P:281:GLY:HA2	16:P:284:ARG:HD2	1.74	0.69
5:E:73:PHE:HB2	5:E:99:ILE:HG21	1.75	0.68
2:B:139:MET:HB2	2:B:142:SER:HB2	1.75	0.68
7:G:97:VAL:HG22	7:G:109:ILE:HG12	1.76	0.68
1:A:703:VAL:HG23	1:A:796:ILE:HG12	1.76	0.68
2:B:496:LEU:HD22	2:B:500:THR:HG21	1.76	0.68
6:F:87:THR:HG22	6:F:88:ASP:H	1.59	0.68
1:A:376:ARG:HB2	1:A:379:GLU:HG3	1.76	0.68
5:E:173:ILE:HG22	5:E:209:VAL:HA	1.76	0.67
3:C:78:ARG:HH12	11:K:49:HIS:HB2	1.59	0.67
13:M:13:ILE:HB	14:N:329:LEU:HB2	1.77	0.67
1:A:397:ASN:HD21	6:F:74:ALA:HA	1.60	0.66
15:O:241:ARG:NH2	15:O:275:GLU:OE1	2.29	0.66
15:O:297:LEU:HD13	15:O:303:ILE:HD13	1.75	0.66
13:M:6:ASP:HB3	14:N:332:ARG:HD2	1.78	0.65
14:N:361:VAL:HG12	14:N:375:VAL:HA	1.78	0.65
5:E:115:LYS:HE2	5:E:129:GLN:HE22	1.61	0.65
7:G:100:SER:HB2	7:G:105:ASP:HA	1.78	0.64
7:G:92:CYS:HB2	7:G:125:GLN:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:357:ARG:NH1	16:P:288:GLY:O	2.30	0.64
13:M:31:PRO:O	14:N:39:ARG:NH2	2.30	0.64
14:N:43:ILE:HG13	14:N:44:ARG:H	1.62	0.64
1:A:1085:ILE:HD11	1:A:1232:LEU:HD13	1.79	0.63
1:A:864:LYS:HB2	1:A:1049:THR:HG21	1.80	0.63
15:O:517:ASP:HA	15:O:520:ILE:HD12	1.79	0.63
2:B:253:GLN:HE21	2:B:529:GLU:HB3	1.64	0.63
13:M:208:LEU:HG	14:N:371:GLY:HA3	1.79	0.63
2:B:633:LEU:HD22	2:B:637:GLU:HG2	1.81	0.62
15:O:277:THR:HG23	15:O:278:THR:HG23	1.82	0.62
15:O:348:ALA:HB3	16:P:277:ILE:HD12	1.81	0.62
1:A:955:LYS:HB2	1:A:958:PHE:HD2	1.65	0.62
1:A:1164:ASP:HB3	1:A:1176:THR:HB	1.81	0.62
15:O:164:PRO:HB3	15:O:183:ASN:HD21	1.66	0.61
4:D:73:LEU:HB3	4:D:83:LYS:HG2	1.81	0.61
1:A:885:GLN:HE21	6:F:111:PRO:HG3	1.65	0.61
5:E:168:ASN:O	5:E:172:ARG:NH2	2.32	0.61
1:A:363:PHE:O	2:B:1067:ARG:NH2	2.32	0.61
9:I:102:CYS:SG	9:I:104:HIS:NE2	2.74	0.61
1:A:1254:VAL:HG11	1:A:1266:THR:HG21	1.81	0.60
2:B:720:VAL:HG21	2:B:945:GLU:HG2	1.84	0.60
2:B:203:VAL:HG22	2:B:213:ARG:HG3	1.82	0.60
1:A:1112:GLU:HB2	9:I:47:LYS:HB2	1.82	0.60
2:B:178:ILE:HG12	2:B:437:THR:HG22	1.82	0.60
16:P:284:ARG:HH12	17:Q:49:LYS:HE3	1.67	0.60
1:A:989:ILE:HD11	1:A:1000:LEU:HB3	1.83	0.60
2:B:659:ILE:HG22	2:B:660:GLU:HG2	1.83	0.60
9:I:86:SER:OG	9:I:89:GLU:O	2.20	0.60
1:A:794:GLN:HG3	1:A:799:VAL:HA	1.84	0.59
13:M:246:LEU:HB3	14:N:392:LEU:HD23	1.84	0.59
1:A:1378:ILE:HG23	4:D:67:ARG:HE	1.68	0.59
2:B:212:SER:HB3	2:B:227:HIS:HE1	1.68	0.59
16:P:220:ILE:HD11	16:P:231:SER:HB2	1.84	0.59
1:A:175:ILE:HD11	15:O:415:HIS:HE1	1.67	0.59
5:E:64:HIS:CD2	5:E:67:ASP:H	2.18	0.59
15:O:130:THR:HG23	15:O:137:LYS:HB3	1.84	0.59
1:A:295:LYS:HD2	1:A:298:ILE:HD11	1.85	0.59
1:A:537:PRO:HG3	1:A:665:TYR:HB2	1.85	0.58
1:A:1243:GLY:O	5:E:142:HIS:NE2	2.37	0.58
3:C:13:ARG:HD2	3:C:302:VAL:HG22	1.85	0.58
16:P:180:LEU:HD11	16:P:238:ILE:HG13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:596:TYR:HD2	2:B:633:LEU:HD12	1.69	0.58
15:O:112:LEU:HD21	17:Q:64:LEU:HD11	1.86	0.58
4:D:72:ALA:O	4:D:75:SER:OG	2.22	0.57
2:B:253:GLN:NE2	2:B:529:GLU:OE1	2.36	0.57
2:B:886:ARG:NH1	3:C:104:GLU:OE2	2.36	0.57
4:D:17:PHE:HB2	4:D:53:ILE:HG12	1.87	0.57
14:N:366:GLY:HA3	14:N:370:THR:HG23	1.85	0.57
1:A:169:CYS:SG	15:O:415:HIS:NE2	2.74	0.57
3:C:51:VAL:HG11	11:K:114:PHE:HD1	1.68	0.57
15:O:509:LEU:O	15:O:513:GLU:HG3	2.04	0.57
6:F:66:LEU:HD11	6:F:97:LEU:HD22	1.86	0.57
1:A:1122:LEU:HG	1:A:1124:ASP:H	1.70	0.57
3:C:50:ARG:HG2	3:C:66:VAL:HB	1.86	0.57
7:G:118:ALA:HB3	7:G:128:VAL:HB	1.87	0.57
1:A:263:ARG:HD2	1:A:280:THR:HG22	1.87	0.57
3:C:337:LEU:HB2	11:K:100:LEU:HD23	1.87	0.57
1:A:713:LYS:NZ	1:A:797:ALA:O	2.38	0.57
1:A:984:ARG:HG3	1:A:989:ILE:HB	1.86	0.57
1:A:48:HIS:O	1:A:67:ARG:NH2	2.38	0.56
1:A:62:THR:HG23	1:A:76:LEU:HB3	1.87	0.56
15:O:367:ARG:NH1	16:P:245:ASP:O	2.38	0.56
7:G:113:SER:HB2	7:G:190:ILE:HD12	1.87	0.56
1:A:590:LYS:HB3	1:A:591:PRO:HD3	1.87	0.56
2:B:196:LYS:HZ1	2:B:218:VAL:H	1.53	0.56
3:C:73:ALA:HB1	3:C:308:PHE:HZ	1.70	0.56
2:B:577:ASN:ND2	2:B:580:ASP:OD2	2.38	0.56
16:P:301:GLU:HG3	16:P:302:ILE:H	1.71	0.56
1:A:909:PRO:HG3	1:A:1285:ARG:HH21	1.71	0.56
15:O:239:LEU:O	15:O:243:HIS:ND1	2.39	0.56
1:A:1243:GLY:HA3	5:E:137:ILE:HG21	1.87	0.56
8:H:90:TYR:HB3	8:H:145:MET:HB3	1.88	0.56
2:B:227:HIS:HD2	2:B:229:THR:HG22	1.71	0.56
15:O:253:SER:O	15:O:257:ASN:ND2	2.39	0.55
2:B:796:ASP:O	2:B:800:ARG:NH2	2.39	0.55
16:P:193:GLU:O	16:P:197:GLU:HG2	2.06	0.55
15:O:323:VAL:HG22	15:O:336:ILE:HG12	1.88	0.55
1:A:1115:GLU:HB2	1:A:1133:SER:HB3	1.87	0.55
2:B:39:LEU:HD21	2:B:449:LEU:HD21	1.89	0.55
8:H:7:GLU:HG2	8:H:59:VAL:HG22	1.88	0.55
2:B:834:THR:HG22	2:B:852:LYS:HD2	1.89	0.55
9:I:23:PHE:HB2	9:I:32:HIS:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:LYS:HG3	9:I:62:VAL:HA	1.89	0.54
2:B:180:ILE:HB	2:B:455:ILE:HG12	1.88	0.54
14:N:272:PRO:HD3	14:N:385:CYS:HB3	1.89	0.54
1:A:1204:ILE:HG22	1:A:1206:GLU:H	1.73	0.54
1:A:1183:SER:OG	1:A:1184:SER:N	2.41	0.54
16:P:181:ASN:HD21	16:P:242:LEU:HG	1.72	0.54
5:E:12:LYS:O	5:E:16:THR:HG23	2.08	0.54
12:L:19:CYS:SG	12:L:20:GLY:N	2.80	0.54
1:A:1195:ASP:HA	1:A:1198:LYS:HG2	1.89	0.54
2:B:333:ILE:O	2:B:337:VAL:HG23	2.07	0.54
15:O:129:LEU:HA	15:O:132:THR:HG22	1.90	0.54
1:A:1322:GLU:HG3	1:A:1323:LYS:H	1.73	0.54
2:B:990:THR:HA	2:B:997:PRO:HA	1.90	0.54
13:M:65:LEU:HD22	13:M:71:ARG:HE	1.73	0.54
9:I:20:CYS:SG	9:I:21:HIS:N	2.81	0.54
10:J:40:LEU:HD13	10:J:46:ARG:HA	1.89	0.54
17:Q:33:LYS:HD3	17:Q:34:PRO:HD2	1.90	0.53
1:A:93:PHE:HB2	1:A:314:GLN:HE21	1.73	0.53
2:B:744:MET:HB3	2:B:1002:ILE:HG23	1.91	0.53
14:N:340:LEU:HD23	14:N:342:GLY:H	1.73	0.53
15:O:411:LYS:HG3	15:O:412:THR:HG23	1.90	0.53
1:A:270:LEU:HD12	1:A:271:LYS:HG2	1.89	0.53
13:M:120:ARG:HD2	13:M:226:LEU:HD21	1.90	0.53
1:A:855:ARG:NH2	2:B:481:PRO:O	2.41	0.53
2:B:762:LEU:HG	2:B:891:PRO:HG2	1.90	0.53
1:A:629:GLU:HG3	1:A:630:ASP:H	1.73	0.53
5:E:59:THR:HG23	5:E:75:PHE:HB3	1.91	0.53
7:G:119:LYS:HD3	7:G:127:TRP:NE1	2.24	0.53
15:O:29:ILE:HD12	15:O:79:CYS:HB3	1.91	0.53
15:O:91:TYR:O	15:O:95:THR:HG23	2.09	0.53
1:A:175:ILE:HD11	15:O:415:HIS:CE1	2.44	0.53
5:E:71:GLN:NE2	5:E:98:ASN:O	2.42	0.53
5:E:166:ARG:H	5:E:169:GLN:HG3	1.74	0.53
15:O:160:CYS:HB2	17:Q:105:ARG:HH22	1.73	0.53
3:C:116:HIS:HB2	3:C:193:VAL:HG22	1.90	0.52
1:A:187:ASP:HB2	1:A:190:VAL:HG12	1.90	0.52
1:A:315:LEU:HD23	1:A:319:LEU:HD23	1.91	0.52
1:A:1100:LEU:HD12	1:A:1141:ARG:HH11	1.73	0.52
2:B:118:GLU:HG2	2:B:127:ILE:HG12	1.91	0.52
4:D:27:ARG:NH2	4:D:39:GLN:OE1	2.41	0.52
7:G:6:GLU:HG2	7:G:73:ARG:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1054:HIS:HE1	1:A:1065:LEU:HD12	1.74	0.52
12:L:31:ARG:HB3	13:M:700:TRP:HB2	1.90	0.52
15:O:516:VAL:HG12	16:P:282:LEU:HA	1.91	0.52
1:A:381:ALA:HB3	1:A:487:ARG:HB2	1.92	0.52
3:C:197:ILE:HG12	10:J:16:ASN:HB3	1.91	0.52
13:M:50:LYS:NZ	13:M:200:HIS:O	2.42	0.52
2:B:1059:GLY:HA3	6:F:60:TYR:HE1	1.75	0.52
1:A:473:ILE:HD13	2:B:1055:LEU:HD21	1.90	0.52
3:C:235:LEU:HB2	3:C:301:ARG:HE	1.74	0.52
1:A:941:SER:N	1:A:944:GLU:OE2	2.33	0.52
9:I:95:TYR:OH	9:I:105:ARG:NE	2.39	0.52
1:A:393:PRO:HB3	1:A:451:GLU:HG2	1.91	0.52
16:P:190:SER:O	16:P:194:THR:HG23	2.10	0.52
13:M:113:ARG:HD3	14:N:270:GLN:HE21	1.75	0.52
13:M:246:LEU:HD11	14:N:396:LYS:HD2	1.91	0.52
7:G:122:GLU:HG2	7:G:123:ALA:H	1.75	0.51
1:A:914:GLY:O	1:A:915:LYS:HG3	2.10	0.51
2:B:518:LEU:HD13	2:B:555:LEU:HD12	1.92	0.51
2:B:283:ALA:O	2:B:287:ILE:HG12	2.10	0.51
1:A:1132:LEU:HD11	1:A:1137:ILE:HD11	1.92	0.51
3:C:49:PHE:O	11:K:113:LYS:NZ	2.37	0.51
5:E:103:LEU:HD13	5:E:128:GLU:HG2	1.91	0.51
4:D:98:GLN:NE2	4:D:105:GLU:OE2	2.43	0.51
1:A:189:ILE:HD12	1:A:189:ILE:H	1.75	0.51
1:A:461:LEU:HD23	1:A:473:ILE:HD11	1.92	0.51
1:A:743:THR:HG22	1:A:745:GLU:H	1.76	0.51
1:A:1117:ILE:HG12	1:A:1130:VAL:HG23	1.93	0.51
3:C:138:LEU:HD21	3:C:190:ILE:HG21	1.92	0.51
13:M:60:MET:HG3	13:M:100:GLN:HB2	1.93	0.51
1:A:1165:VAL:HG22	1:A:1175:VAL:HG13	1.92	0.51
2:B:140:LEU:HD21	2:B:170:ILE:HG13	1.93	0.51
9:I:83:GLN:HB3	9:I:85:ARG:HH22	1.76	0.51
10:J:40:LEU:HD11	10:J:49:LEU:HD12	1.92	0.51
13:M:48:LYS:HB2	13:M:205:TRP:HE1	1.75	0.51
15:O:161:PRO:HG3	15:O:184:GLU:HB2	1.92	0.51
1:A:175:ILE:HD12	1:A:217:ASN:ND2	2.25	0.51
1:A:666:ILE:HG23	1:A:923:ARG:HH21	1.76	0.51
2:B:1097:SER:HG	2:B:1099:CYS:HG	1.59	0.51
15:O:347:THR:O	15:O:351:GLU:HG2	2.10	0.51
15:O:376:GLU:HB3	15:O:379:GLN:HG2	1.93	0.51
1:A:773:LYS:NZ	8:H:20:LYS:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:81:LEU:HD21	15:O:459:ARG:HH22	1.76	0.51
1:A:463:ASN:HB3	1:A:473:ILE:HA	1.92	0.50
1:A:1375:ARG:HG3	1:A:1376:PRO:HD2	1.93	0.50
5:E:189:GLN:O	5:E:209:VAL:HG12	2.11	0.50
2:B:526:LEU:HD11	2:B:548:VAL:HG21	1.94	0.50
4:D:5:ASP:OD2	4:D:5:ASP:N	2.44	0.50
2:B:196:LYS:NZ	2:B:218:VAL:H	2.09	0.50
2:B:869:VAL:HG22	2:B:883:MET:HG2	1.92	0.50
4:D:20:LEU:HD21	4:D:46:THR:HA	1.93	0.50
1:A:756:LEU:HD11	1:A:828:PRO:HB3	1.92	0.50
1:A:928:ILE:HA	1:A:931:VAL:HG12	1.94	0.50
1:A:1252:TYR:O	1:A:1255:GLU:HG3	2.11	0.50
3:C:140:PHE:HB2	3:C:212:MET:HG2	1.93	0.50
15:O:377:GLN:HE22	15:O:392:LYS:HE2	1.76	0.50
14:N:276:PRO:HG3	14:N:344:VAL:HG11	1.94	0.50
1:A:7:ARG:NH2	7:G:160:THR:OG1	2.45	0.50
1:A:1237:ALA:HB1	5:E:136:LEU:HD12	1.93	0.50
3:C:145:ARG:HB2	3:C:207:GLU:HG3	1.93	0.50
13:M:66:ASN:OD1	13:M:69:TYR:HB2	2.11	0.50
2:B:258:GLU:HB3	2:B:261:VAL:HG22	1.92	0.50
1:A:543:GLN:HB2	1:A:785:SER:HB3	1.93	0.50
1:A:873:ARG:CZ	17:Q:197:ASN:HD21	2.25	0.50
2:B:479:LEU:HD13	2:B:494:LYS:HD2	1.94	0.50
1:A:772:ASP:OD2	1:A:774:SER:OG	2.30	0.50
1:A:829:ALA:HA	1:A:833:PHE:HB3	1.94	0.50
1:A:592:VAL:HG23	1:A:594:LEU:HG	1.94	0.49
1:A:1322:GLU:HB3	1:A:1327:HIS:CE1	2.46	0.49
3:C:40:TRP:NE1	11:K:102:GLU:OE1	2.45	0.49
15:O:135:ASP:OD1	15:O:136:GLY:N	2.44	0.49
17:Q:106:LEU:HG	17:Q:107:PRO:HD2	1.94	0.49
1:A:1137:ILE:HG23	1:A:1142:LEU:HB2	1.94	0.49
3:C:84:VAL:HB	3:C:227:PRO:HG3	1.93	0.49
1:A:35:GLN:NE2	1:A:87:ASP:OD1	2.45	0.49
1:A:509:LEU:O	2:B:1067:ARG:NH2	2.44	0.49
1:A:1165:VAL:HG13	1:A:1175:VAL:HG22	1.93	0.49
2:B:597:ILE:HA	2:B:630:VAL:HG12	1.93	0.49
3:C:138:LEU:HB3	3:C:214:CYS:HB3	1.93	0.49
9:I:35:THR:OG1	9:I:36:ARG:N	2.45	0.49
1:A:509:LEU:H	2:B:1067:ARG:NH2	2.09	0.49
2:B:36:VAL:HG23	2:B:37:LYS:HG2	1.94	0.49
2:B:722:THR:HG23	2:B:962:THR:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:326:ILE:HG21	11:K:111:LEU:HB2	1.94	0.49
8:H:96:VAL:HG22	8:H:116:VAL:HG22	1.93	0.49
10:J:14:VAL:HG11	10:J:45:CYS:HB2	1.93	0.49
1:A:596:THR:HG22	1:A:598:LYS:H	1.77	0.49
1:A:965:PHE:O	1:A:969:ILE:HG12	2.12	0.49
2:B:82:VAL:HG22	2:B:113:ILE:HG12	1.95	0.49
10:J:27:ALA:O	10:J:28:GLU:HG3	2.12	0.49
13:M:192:SER:OG	13:M:193:TYR:N	2.45	0.49
9:I:102:CYS:HG	9:I:104:HIS:CD2	2.30	0.49
11:K:35:THR:HB	11:K:38:HIS:HB2	1.94	0.49
2:B:862:THR:HG22	2:B:863:ASP:H	1.77	0.49
15:O:341:ALA:O	15:O:345:LEU:HG	2.11	0.49
1:A:86:ILE:HD13	1:A:287:ILE:HD11	1.94	0.49
12:L:22:CYS:SG	12:L:24:THR:OG1	2.65	0.49
1:A:1092:ASP:OD1	1:A:1220:LYS:NZ	2.46	0.48
7:G:81:LEU:HD11	7:G:153:VAL:HG13	1.95	0.48
15:O:6:ILE:HG21	15:O:30:ARG:HE	1.78	0.48
1:A:19:CYS:HB3	1:A:1337:LYS:HG2	1.95	0.48
11:K:36:ASP:OD1	11:K:36:ASP:N	2.40	0.48
16:P:196:ARG:O	16:P:199:LYS:HG2	2.13	0.48
1:A:131:ARG:NH1	1:A:138:GLN:HE22	2.11	0.48
2:B:916:MET:HB3	2:B:925:PRO:HD2	1.95	0.48
2:B:1073:ASP:OD1	2:B:1073:ASP:N	2.44	0.48
4:D:45:ILE:HD11	7:G:36:ASN:HD22	1.77	0.48
15:O:449:ARG:HH21	16:P:314:LEU:HD21	1.78	0.48
15:O:518:GLU:O	15:O:522:LEU:HG	2.13	0.48
2:B:508:ASP:OD2	2:B:508:ASP:N	2.46	0.48
1:A:259:PRO:O	1:A:262:ILE:HG22	2.14	0.48
2:B:113:ILE:HD11	2:B:136:MET:HB2	1.96	0.48
2:B:723:LYS:H	2:B:962:THR:HG22	1.78	0.48
2:B:78:LEU:HB2	2:B:116:ASP:HB3	1.95	0.48
4:D:17:PHE:O	4:D:21:THR:HG23	2.12	0.48
1:A:739:GLN:HB3	1:A:740:PRO:HD3	1.96	0.48
2:B:63:GLU:OE1	2:B:63:GLU:N	2.47	0.48
2:B:372:LEU:HB2	2:B:424:TRP:HZ3	1.78	0.48
4:D:86:LEU:HD11	4:D:91:PRO:HB3	1.96	0.48
8:H:79:ASP:OD1	8:H:79:ASP:N	2.46	0.48
11:K:53:ASN:HA	11:K:56:ARG:HG2	1.95	0.48
17:Q:77:THR:N	17:Q:78:PRO:HD3	2.28	0.48
1:A:397:ASN:H	1:A:400:ASN:HB2	1.79	0.48
5:E:173:ILE:N	5:E:208:LEU:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:64:PRO:HB3	12:L:23:HIS:CE1	2.48	0.48
1:A:1132:LEU:HB3	1:A:1171:ALA:HB1	1.96	0.47
7:G:13:ILE:HD11	7:G:26:ILE:HD11	1.96	0.47
13:M:238:LEU:HA	14:N:278:GLN:HE22	1.78	0.47
1:A:834:VAL:HG13	1:A:846:GLU:HB3	1.96	0.47
1:A:1089:LEU:HD23	1:A:1241:VAL:HA	1.96	0.47
2:B:1132:ASN:ND2	2:B:1133:GLU:OE1	2.47	0.47
15:O:82:VAL:O	15:O:85:MET:HG3	2.14	0.47
16:P:173:GLU:HG3	16:P:176:PHE:HB3	1.96	0.47
16:P:201:ASN:HB3	16:P:202:PRO:HD3	1.95	0.47
1:A:469:HIS:HD2	1:A:471:LEU:HB2	1.78	0.47
1:A:1360:PHE:CZ	6:F:64:ARG:HD3	2.50	0.47
1:A:246:LYS:HG2	1:A:247:PRO:HD2	1.97	0.47
1:A:1111:GLY:H	1:A:1197:PRO:HA	1.80	0.47
2:B:986:LYS:HD2	2:B:1001:TYR:HB2	1.96	0.47
3:C:43:ASP:OD1	3:C:43:ASP:N	2.47	0.47
15:O:12:LEU:HD11	15:O:86:LEU:HD21	1.96	0.47
15:O:33:SER:HB3	15:O:74:GLU:HB3	1.97	0.47
15:O:258:ARG:NH1	16:P:273:VAL:HB	2.30	0.47
16:P:175:GLU:O	16:P:178:GLU:HG3	2.15	0.47
2:B:633:LEU:HD11	2:B:656:HIS:CE1	2.50	0.47
15:O:356:GLU:HG3	16:P:283:VAL:HG21	1.97	0.47
1:A:941:SER:OG	1:A:942:LYS:N	2.47	0.47
15:O:86:LEU:HB2	15:O:517:ASP:OD1	2.14	0.47
16:P:181:ASN:HD22	16:P:238:ILE:HG23	1.79	0.47
1:A:177:GLU:OE1	1:A:215:GLN:NE2	2.48	0.47
2:B:823:ASN:ND2	2:B:860:GLY:O	2.45	0.47
15:O:460:LEU:HA	15:O:463:LYS:HG2	1.97	0.47
16:P:280:THR:HG22	16:P:282:LEU:H	1.80	0.47
17:Q:27:LEU:N	17:Q:28:PRO:HD3	2.30	0.47
3:C:94:VAL:HG21	3:C:97:ASN:HB2	1.96	0.46
3:C:267:VAL:O	3:C:269:GLY:N	2.46	0.46
3:C:129:ASP:OD1	3:C:129:ASP:N	2.47	0.46
9:I:74:HIS:CE1	9:I:76:ARG:HH11	2.33	0.46
13:M:242:PRO:HG2	14:N:395:HIS:CD2	2.50	0.46
16:P:233:GLU:O	16:P:237:THR:HG23	2.16	0.46
1:A:422:GLN:HB3	1:A:449:ILE:HB	1.97	0.46
1:A:1179:GLU:OE1	1:A:1185:MET:N	2.48	0.46
2:B:224:TYR:HB3	2:B:233:ASP:HB3	1.97	0.46
1:A:794:GLN:HE21	1:A:799:VAL:HG13	1.80	0.46
1:A:1363:LEU:HB3	6:F:105:ILE:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:304:PRO:HA	19:P:400:SF4:S1	2.55	0.46
1:A:1232:LEU:HB3	1:A:1253:GLU:OE1	2.16	0.46
3:C:134:GLU:HG3	3:C:179:GLY:HA3	1.97	0.46
3:C:287:ILE:HG21	3:C:297:VAL:HG11	1.98	0.46
7:G:21:LYS:HB3	7:G:24:ASP:OD1	2.16	0.46
13:M:59:GLU:HG2	13:M:101:THR:HG22	1.97	0.46
13:M:121:GLN:HG2	14:N:262:LYS:NZ	2.31	0.46
17:Q:71:MET:SD	17:Q:72:PRO:HD2	2.56	0.46
2:B:985:GLY:HA3	2:B:1003:TYR:HE1	1.81	0.46
2:B:1013:LYS:HG3	2:B:1014:HIS:CD2	2.50	0.46
1:A:529:LEU:HD23	1:A:539:ILE:HD13	1.96	0.46
16:P:204:ILE:HA	16:P:207:ASN:HD21	1.80	0.46
1:A:587:THR:HG22	1:A:588:ILE:HG23	1.96	0.46
1:A:1258:LEU:HA	5:E:139:ILE:HD11	1.98	0.46
1:A:1319:ALA:HA	1:A:1327:HIS:NE2	2.30	0.46
6:F:87:THR:HG22	6:F:88:ASP:N	2.29	0.46
3:C:155:ASP:OD2	3:C:155:ASP:N	2.48	0.45
15:O:338:LEU:O	15:O:342:LEU:HG	2.16	0.45
15:O:512:SER:O	15:O:516:VAL:HG22	2.15	0.45
1:A:361:VAL:HG11	2:B:1067:ARG:O	2.16	0.45
2:B:329:ARG:NH1	13:M:136:ARG:HH22	2.14	0.45
16:P:284:ARG:HG2	17:Q:46:VAL:HG13	1.97	0.45
1:A:660:LYS:HG3	1:A:661:ASN:H	1.81	0.45
2:B:757:LEU:HD13	2:B:762:LEU:HD21	1.97	0.45
5:E:152:THR:O	5:E:156:VAL:HG23	2.16	0.45
13:M:146:ASP:OD2	13:M:147:ALA:N	2.50	0.45
13:M:106:GLN:OE1	13:M:107:THR:N	2.49	0.45
16:P:251:THR:HB	16:P:269:LEU:HG	1.99	0.45
1:A:949:THR:HA	1:A:952:ILE:HG22	1.99	0.45
2:B:56:LYS:O	2:B:60:LYS:HG2	2.16	0.45
2:B:716:GLN:HB2	2:B:737:GLN:HA	1.98	0.45
2:B:232:GLU:HB2	2:B:290:LYS:HE3	1.99	0.45
16:P:190:SER:O	16:P:193:GLU:HG2	2.17	0.45
1:A:542:ILE:HB	1:A:545:PHE:HD2	1.80	0.45
2:B:371:LEU:HD22	2:B:429:PHE:CZ	2.52	0.45
13:M:48:LYS:HB2	13:M:205:TRP:NE1	2.32	0.45
15:O:251:ILE:O	15:O:255:VAL:HG22	2.17	0.45
1:A:629:GLU:HG3	1:A:630:ASP:N	2.31	0.45
3:C:280:LEU:H	3:C:280:LEU:HD23	1.82	0.45
1:A:730:ALA:HB1	1:A:735:LYS:HB3	1.98	0.45
4:D:80:LYS:HE3	17:Q:84:ILE:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:321:LEU:HG	14:N:322:THR:H	1.81	0.45
1:A:664:PHE:HZ	1:A:683:LEU:HD21	1.81	0.45
1:A:1145:ASN:O	1:A:1149:VAL:HG23	2.17	0.45
8:H:48:TYR:OH	8:H:147:LYS:HG3	2.17	0.45
15:O:459:ARG:O	15:O:462:GLU:HG3	2.17	0.45
1:A:26:GLU:HG2	1:A:27:GLU:N	2.32	0.44
1:A:722:LYS:HE3	1:A:722:LYS:HB3	1.86	0.44
8:H:17:PRO:HG2	8:H:18:GLU:OE2	2.17	0.44
2:B:48:ASN:O	2:B:52:ASN:ND2	2.50	0.44
13:M:71:ARG:O	13:M:75:GLU:HG2	2.17	0.44
1:A:1265:THR:HB	5:E:144:LEU:HD13	1.99	0.44
14:N:359:GLU:HA	14:N:378:HIS:HA	1.99	0.44
16:P:304:PRO:CA	19:P:400:SF4:S1	3.05	0.44
1:A:996:GLU:HB3	1:A:997:PRO:HD3	1.98	0.44
12:L:41:TYR:CE2	12:L:43:ILE:HB	2.52	0.44
15:O:150:ARG:O	15:O:154:THR:HG22	2.18	0.44
1:A:116:MET:SD	1:A:163:ASN:ND2	2.91	0.44
2:B:917:PRO:HB3	2:B:992:GLY:N	2.32	0.44
8:H:28:LEU:HD11	8:H:50:VAL:HG11	1.98	0.44
14:N:337:VAL:HG23	14:N:348:VAL:HG23	1.98	0.44
1:A:470:LYS:HB3	1:A:1039:GLN:HE22	1.83	0.44
1:A:616:ASN:HB2	1:A:927:ASN:ND2	2.33	0.44
1:A:726:GLU:O	1:A:729:GLU:HG3	2.17	0.44
1:A:1179:GLU:OE2	1:A:1184:SER:HA	2.17	0.44
1:A:1252:TYR:CZ	1:A:1256:LYS:HD3	2.53	0.44
2:B:679:GLN:HG2	2:B:681:PRO:HD2	1.98	0.44
1:A:99:ARG:HA	1:A:102:ILE:HG12	1.99	0.44
1:A:941:SER:HB2	1:A:991:ASP:OD1	2.16	0.44
2:B:185:SER:HB2	2:B:359:ASN:O	2.17	0.44
2:B:983:TYR:CD2	2:B:984:LEU:HG	2.53	0.44
13:M:238:LEU:HD21	14:N:341:LEU:HD23	2.00	0.44
1:A:415:HIS:CE1	1:A:480:VAL:HG21	2.53	0.44
1:A:586:PRO:HG2	1:A:589:LEU:HD22	2.00	0.44
1:A:465:GLN:HB3	1:A:466:PRO:HD3	1.99	0.44
13:M:27:LEU:HD12	14:N:360:LEU:HB3	2.00	0.44
1:A:516:LYS:NZ	6:F:88:ASP:OD1	2.50	0.43
1:A:1322:GLU:CG	1:A:1323:LYS:H	2.31	0.43
2:B:541:LEU:HD13	2:B:546:LEU:HD11	2.00	0.43
2:B:919:CYS:HB3	2:B:989:VAL:HG22	2.00	0.43
2:B:937:ARG:HB3	2:B:939:THR:HG23	2.00	0.43
2:B:650:ILE:HD11	2:B:657:LEU:HD13	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:71:LYS:HG2	9:I:104:HIS:CD2	2.53	0.43
13:M:149:HIS:O	13:M:153:GLU:HG2	2.18	0.43
16:P:199:LYS:HA	16:P:199:LYS:HD2	1.74	0.43
2:B:606:VAL:HG22	2:B:629:LEU:HD12	2.00	0.43
6:F:50:LYS:HA	6:F:50:LYS:HD2	1.77	0.43
13:M:75:GLU:O	13:M:79:LEU:HG	2.18	0.43
15:O:481:GLU:O	15:O:485:GLN:HG2	2.18	0.43
3:C:40:TRP:CD1	3:C:42:GLN:HB2	2.54	0.43
6:F:110:LEU:HD13	6:F:114:SER:HB2	2.00	0.43
2:B:37:LYS:HD2	2:B:501:HIS:CD2	2.53	0.43
8:H:76:ASN:HB2	8:H:77:PRO:HD3	2.01	0.43
15:O:404:MET:HB2	15:O:425:THR:O	2.19	0.43
1:A:267:VAL:HG12	1:A:274:THR:HG23	2.01	0.43
1:A:1360:PHE:CZ	6:F:61:GLU:HA	2.54	0.43
2:B:384:MET:HA	2:B:387:ILE:HG22	1.99	0.43
10:J:21:TYR:OH	10:J:31:GLU:OE1	2.29	0.43
11:K:46:GLU:HA	11:K:78:SER:HB3	2.00	0.43
1:A:584:PRO:HA	1:A:585:PRO:HD3	1.96	0.43
15:O:103:GLY:HA2	15:O:106:ILE:HG22	2.01	0.43
1:A:169:CYS:SG	1:A:175:ILE:HG12	2.59	0.43
1:A:868:THR:HG21	1:A:1046:THR:HA	2.01	0.43
2:B:644:ALA:HB2	2:B:654:THR:HG21	2.01	0.43
2:B:858:TYR:HH	2:B:864:SER:HG	1.66	0.43
2:B:954:LEU:HD23	2:B:954:LEU:HA	1.89	0.43
16:P:252:ILE:HD12	16:P:267:MET:O	2.19	0.43
1:A:1232:LEU:HA	1:A:1235:VAL:HG12	2.00	0.43
2:B:714:TYR:O	2:B:737:GLN:NE2	2.52	0.43
13:M:24:LYS:HB3	14:N:363:VAL:O	2.19	0.43
14:N:43:ILE:C	14:N:45:SER:H	2.23	0.43
2:B:759:LYS:HB3	2:B:912:PRO:HA	2.01	0.42
4:D:11:LEU:HD23	4:D:11:LEU:H	1.84	0.42
11:K:66:GLU:HB2	11:K:87:ARG:HG3	2.01	0.42
13:M:64:THR:O	13:M:65:LEU:HD23	2.19	0.42
15:O:368:LEU:HD13	15:O:384:ALA:HB2	2.00	0.42
16:P:294:ASP:OD1	16:P:295:ASP:N	2.51	0.42
1:A:1204:ILE:HB	1:A:1207:VAL:HG12	2.01	0.42
2:B:526:LEU:H	2:B:526:LEU:HD23	1.84	0.42
2:B:680:SER:OG	2:B:681:PRO:HD3	2.19	0.42
4:D:93:THR:HG22	4:D:95:VAL:HG12	2.01	0.42
5:E:116:GLN:HA	5:E:119:VAL:HG12	2.01	0.42
8:H:64:LEU:HD23	8:H:64:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:195:PHE:HA	13:M:198:LYS:HE2	2.00	0.42
15:O:272:ARG:HG3	15:O:273:MET:SD	2.59	0.42
2:B:229:THR:HG21	2:B:312:LEU:HD11	2.01	0.42
2:B:231:SER:HB3	2:B:292:ARG:HG2	2.00	0.42
4:D:109:THR:OG1	4:D:110:GLU:N	2.52	0.42
15:O:365:ILE:O	15:O:369:VAL:HG22	2.19	0.42
1:A:178:LYS:HG2	1:A:179:TYR:H	1.84	0.42
1:A:1251:THR:HA	1:A:1254:VAL:HG12	2.00	0.42
3:C:266:GLU:HA	3:C:270:LYS:O	2.19	0.42
3:C:293:LEU:HD13	3:C:296:VAL:HG21	2.00	0.42
7:G:42:VAL:HG22	7:G:76:VAL:HG11	2.01	0.42
13:M:92:TYR:HE1	13:M:99:LYS:HG2	1.84	0.42
2:B:549:ILE:HG21	2:B:555:LEU:HD22	2.02	0.42
4:D:115:ALA:O	4:D:119:THR:HG23	2.20	0.42
13:M:44:HIS:HA	13:M:60:MET:HA	2.01	0.42
2:B:215:ASN:N	2:B:215:ASN:OD1	2.51	0.42
3:C:138:LEU:HD12	3:C:138:LEU:HA	1.94	0.42
3:C:229:ALA:H	3:C:312:SER:HA	1.85	0.42
3:C:332:LYS:HA	3:C:335:ARG:HG2	2.00	0.42
5:E:21:CYS:SG	5:E:62:VAL:HG21	2.59	0.42
6:F:79:VAL:HG11	6:F:83:LEU:HD23	2.02	0.42
16:P:179:VAL:O	16:P:182:GLN:HG3	2.20	0.42
8:H:44:ASN:HD22	8:H:47:ILE:HD12	1.84	0.42
8:H:75:TYR:CD2	8:H:77:PRO:HD2	2.55	0.42
14:N:35:LEU:HB3	14:N:37:PRO:HD2	2.02	0.42
1:A:18:ILE:HG23	1:A:1338:ASP:HB3	2.02	0.42
1:A:134:LEU:HD23	1:A:134:LEU:HA	1.87	0.42
1:A:217:ASN:OD1	15:O:408:GLU:HB3	2.19	0.42
1:A:754:LYS:O	1:A:758:VAL:HG23	2.20	0.42
1:A:1136:ARG:NH1	9:I:47:LYS:O	2.39	0.42
13:M:148:LYS:O	13:M:151:GLU:HG3	2.20	0.42
15:O:258:ARG:HH12	16:P:273:VAL:HB	1.85	0.42
15:O:353:VAL:HG12	16:P:283:VAL:HG13	2.02	0.42
1:A:360:ARG:HD2	2:B:1035:PRO:O	2.19	0.42
1:A:370:SER:N	1:A:486:PHE:O	2.52	0.42
1:A:870:TYR:CD1	17:Q:200:ILE:HD11	2.54	0.42
7:G:97:VAL:HG22	7:G:109:ILE:CG1	2.47	0.42
14:N:248:ASP:OD1	14:N:249:VAL:N	2.53	0.42
1:A:35:GLN:HB2	1:A:85:TYR:CE1	2.55	0.42
1:A:38:SER:OG	1:A:53:TYR:O	2.36	0.42
1:A:183:LYS:HD3	1:A:183:LYS:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HG	1:A:172:LEU:HG	2.02	0.41
1:A:542:ILE:HB	1:A:545:PHE:CD2	2.55	0.41
1:A:843:THR:HB	1:A:846:GLU:HG3	2.01	0.41
2:B:832:MET:O	2:B:852:LYS:HG2	2.20	0.41
10:J:3:ILE:HD12	10:J:4:PRO:HD2	2.01	0.41
2:B:251:ILE:O	2:B:255:ILE:HG12	2.19	0.41
8:H:11:ASP:HB3	8:H:55:LYS:HG2	2.01	0.41
13:M:195:PHE:O	13:M:199:LYS:HG2	2.20	0.41
13:M:703:LYS:HE3	13:M:703:LYS:HB3	1.85	0.41
1:A:909:PRO:HG3	1:A:1285:ARG:HD2	2.01	0.41
1:A:973:ILE:HD11	1:A:1015:LEU:HD21	2.01	0.41
1:A:1185:MET:HA	1:A:1188:VAL:HG22	2.02	0.41
2:B:30:LEU:HB3	2:B:31:PRO:HD3	2.01	0.41
2:B:464:LYS:HE3	2:B:464:LYS:HB3	1.92	0.41
4:D:22:ASP:OD2	4:D:22:ASP:N	2.52	0.41
7:G:117:PRO:HB2	7:G:127:TRP:HZ3	1.85	0.41
9:I:8:CYS:SG	9:I:9:GLY:N	2.93	0.41
1:A:295:LYS:HB3	17:Q:27:LEU:HD21	2.02	0.41
1:A:362:ASP:HB3	2:B:1023:ARG:HH11	1.84	0.41
4:D:77:LYS:HE3	4:D:107:ARG:HH21	1.84	0.41
9:I:71:LYS:HG2	9:I:104:HIS:HD2	1.85	0.41
16:P:287:CYS:HA	19:P:400:SF4:S2	2.60	0.41
1:A:208:GLU:HB3	1:A:209:PRO:HD3	2.03	0.41
1:A:304:GLN:NE2	15:O:420:THR:O	2.53	0.41
1:A:759:ILE:HG13	1:A:760:ARG:N	2.36	0.41
2:B:358:GLY:HA2	2:B:635:VAL:HB	2.03	0.41
7:G:21:LYS:HG3	7:G:23:ASN:H	1.84	0.41
11:K:43:VAL:HG11	11:K:79:LYS:HE2	2.02	0.41
13:M:217:ARG:O	13:M:221:GLU:HG2	2.21	0.41
15:O:110:LEU:HD11	15:O:236:GLN:HA	2.02	0.41
1:A:321:ILE:HG22	1:A:342:VAL:HG23	2.03	0.41
1:A:1131:LYS:HD2	1:A:1172:VAL:HG22	2.03	0.41
2:B:318:LEU:HB2	2:B:331:LYS:NZ	2.36	0.41
2:B:634:ASP:H	2:B:637:GLU:HB3	1.86	0.41
3:C:61:LEU:HD22	3:C:319:ASP:HA	2.01	0.41
7:G:39:VAL:HG23	7:G:40:TYR:N	2.30	0.41
16:P:210:PHE:CE1	16:P:269:LEU:HD22	2.55	0.41
16:P:242:LEU:HD23	16:P:242:LEU:HA	1.92	0.41
1:A:361:VAL:HG12	2:B:1072:SER:HB2	2.02	0.41
1:A:822:GLU:HG2	1:A:823:LYS:H	1.85	0.41
1:A:887:ASP:OD1	1:A:887:ASP:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1069:MET:HG3	2:B:1107:PRO:HG3	2.02	0.41
4:D:35:HIS:ND1	7:G:32:LYS:HD2	2.35	0.41
5:E:46:ASP:OD1	5:E:46:ASP:N	2.50	0.41
10:J:38:LEU:HD23	10:J:38:LEU:HA	1.88	0.41
13:M:121:GLN:HG2	14:N:262:LYS:HZ3	1.85	0.41
15:O:362:CYS:HB2	15:O:394:MET:CE	2.51	0.41
1:A:798:CYS:SG	1:A:799:VAL:N	2.93	0.41
2:B:180:ILE:HG12	2:B:364:LEU:HD23	2.02	0.41
2:B:919:CYS:HA	2:B:989:VAL:HA	2.03	0.41
4:D:101:VAL:HB	4:D:104:SER:HB3	2.03	0.41
16:P:176:PHE:HA	16:P:179:VAL:HG22	2.02	0.41
1:A:17:HIS:HB2	2:B:1127:LYS:HD3	2.02	0.41
1:A:519:ALA:HB2	2:B:1063:LEU:HD22	2.03	0.41
1:A:794:GLN:HA	1:A:798:CYS:O	2.20	0.41
2:B:219:LYS:O	2:B:220:GLN:HG2	2.20	0.41
8:H:8:ASP:HB3	8:H:10:PHE:CE2	2.56	0.41
13:M:120:ARG:HD3	13:M:123:GLU:OE2	2.20	0.41
15:O:39:ILE:O	15:O:43:THR:HG23	2.21	0.41
15:O:68:HIS:HB2	15:O:72:VAL:HG23	2.03	0.41
15:O:278:THR:HG21	15:O:286:GLN:H	1.86	0.41
15:O:398:MET:SD	15:O:403:PHE:HD2	2.44	0.41
1:A:432:LEU:HD22	1:A:437:ARG:HG2	2.02	0.41
1:A:573:VAL:HG11	1:A:685:ARG:CZ	2.51	0.41
1:A:1242:LYS:HG2	1:A:1244:THR:H	1.85	0.41
2:B:392:ILE:HB	2:B:393:PRO:HD3	2.03	0.41
7:G:7:MET:HB2	7:G:72:PHE:CE1	2.56	0.41
13:M:5:GLU:HB2	14:N:333:LYS:NZ	2.36	0.41
15:O:55:CYS:HA	15:O:58:VAL:HG12	2.02	0.41
15:O:287:PRO:HB3	15:O:333:MET:HB3	2.02	0.41
1:A:1328:LEU:HD23	1:A:1328:LEU:HA	1.86	0.40
2:B:596:TYR:CD2	2:B:633:LEU:HD12	2.53	0.40
7:G:84:ILE:HG12	7:G:151:ARG:HG2	2.03	0.40
8:H:92:MET:O	8:H:142:TYR:HA	2.21	0.40
13:M:45:LEU:HG	13:M:61:ALA:HB2	2.03	0.40
17:Q:96:LYS:HA	17:Q:96:LYS:HD3	1.67	0.40
1:A:589:LEU:HB3	1:A:593:THR:HG23	2.02	0.40
11:K:102:GLU:O	11:K:106:VAL:HG23	2.22	0.40
1:A:660:LYS:HG3	1:A:661:ASN:N	2.36	0.40
7:G:184:TYR:CZ	7:G:186:LEU:HD21	2.57	0.40
8:H:92:MET:HB3	8:H:118:TYR:CD1	2.57	0.40
13:M:111:THR:O	13:M:111:THR:OG1	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:59:GLN:OE1	17:Q:99:TRP:NE1	2.54	0.40
17:Q:88:SER:HB2	17:Q:91:TYR:CD2	2.57	0.40
1:A:366:ARG:HA	1:A:506:ASN:HA	2.04	0.40
1:A:946:ILE:O	1:A:950:GLU:HG2	2.21	0.40
1:A:1178:ARG:HD2	1:A:1178:ARG:HA	1.96	0.40
2:B:985:GLY:HA3	2:B:1003:TYR:CE1	2.56	0.40
12:L:18:ILE:HD11	12:L:47:LYS:HG2	2.03	0.40
2:B:106:ASP:HA	2:B:173:GLY:HA3	2.03	0.40
2:B:946:LEU:HD22	2:B:1003:TYR:CE2	2.56	0.40
2:B:1049:GLU:HA	2:B:1052:ARG:HB3	2.04	0.40
3:C:198:LEU:HD12	3:C:198:LEU:HA	1.96	0.40
15:O:88:TYR:HB2	15:O:89:PRO:HD3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1384/1390 (100%)	1316 (95%)	66 (5%)	2 (0%)	51	83
2	B	1089/1133 (96%)	1043 (96%)	46 (4%)	0	100	100
3	C	343/346 (99%)	314 (92%)	28 (8%)	1 (0%)	41	73
4	D	124/148 (84%)	117 (94%)	6 (5%)	1 (1%)	19	54
5	E	208/210 (99%)	196 (94%)	12 (6%)	0	100	100
6	F	77/127 (61%)	75 (97%)	2 (3%)	0	100	100
7	G	177/204 (87%)	167 (94%)	10 (6%)	0	100	100
8	H	147/150 (98%)	144 (98%)	3 (2%)	0	100	100
9	I	106/108 (98%)	100 (94%)	6 (6%)	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%)	41 (91%)	4 (9%)	0	100	100
13	M	214/708 (30%)	210 (98%)	4 (2%)	0	100	100
14	N	130/398 (33%)	120 (92%)	10 (8%)	0	100	100
15	O	484/534 (91%)	472 (98%)	12 (2%)	0	100	100
16	P	135/316 (43%)	127 (94%)	8 (6%)	0	100	100
17	Q	115/223 (52%)	112 (97%)	3 (3%)	0	100	100
All	All	4948/6253 (79%)	4721 (95%)	223 (4%)	4 (0%)	54	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	268	GLN
4	D	78	LEU
1	A	591	PRO
1	A	915	LYS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1208/1212 (100%)	1204 (100%)	4 (0%)	92	96
2	B	958/988 (97%)	956 (100%)	2 (0%)	93	97
3	C	301/302 (100%)	301 (100%)	0	100	100
4	D	117/136 (86%)	115 (98%)	2 (2%)	60	83
5	E	192/192 (100%)	192 (100%)	0	100	100
6	F	69/111 (62%)	69 (100%)	0	100	100
7	G	164/181 (91%)	164 (100%)	0	100	100
8	H	130/131 (99%)	130 (100%)	0	100	100
9	I	94/94 (100%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	96/119 (81%)	96 (100%)	0	100	100
12	L	44/55 (80%)	44 (100%)	0	100	100
13	M	200/622 (32%)	199 (100%)	1 (0%)	88	94
14	N	119/347 (34%)	118 (99%)	1 (1%)	81	92
15	O	439/476 (92%)	437 (100%)	2 (0%)	88	94
16	P	125/280 (45%)	125 (100%)	0	100	100
17	Q	115/195 (59%)	114 (99%)	1 (1%)	78	91
All	All	4427/5497 (80%)	4414 (100%)	13 (0%)	92	96

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	LYS
1	A	915	LYS
1	A	1051	LYS
1	A	1193	LYS
2	B	196	LYS
2	B	324	LYS
4	D	24	LYS
4	D	80	LYS
13	M	144	LYS
14	N	336	ARG
15	O	81	ARG
15	O	455	LYS
17	Q	104	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	138	GLN
1	A	157	HIS
1	A	215	GLN
1	A	217	ASN
1	A	314	GLN
1	A	397	ASN
1	A	419	ASN

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Mol	Chain	Res	Type
1	A	469	HIS
1	A	534	ASN
1	A	599	GLN
1	A	616	ASN
1	A	623	GLN
1	A	737	GLN
1	A	794	GLN
1	A	815	ASN
1	A	885	GLN
1	A	927	ASN
1	A	1039	GLN
1	A	1231	ASN
2	B	92	ASN
2	B	208	HIS
2	B	227	HIS
2	B	253	GLN
2	B	280	GLN
2	B	349	ASN
2	B	381	ASN
2	B	410	GLN
2	B	413	ASN
2	B	423	ASN
2	B	683	ASN
2	B	758	ASN
2	B	829	ASN
2	B	1010	GLN
2	B	1034	GLN
2	B	1082	GLN
2	B	1132	ASN
3	C	32	ASN
3	C	55	HIS
3	C	127	GLN
3	C	172	HIS
3	C	344	GLN
4	D	60	HIS
4	D	76	HIS
4	D	98	GLN
5	E	71	GLN
5	E	129	GLN
7	G	17	GLN
7	G	36	ASN
14	N	270	GLN

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Mol	Chain	Res	Type
14	N	278	GLN
14	N	338	GLN
14	N	395	HIS
15	O	60	HIS
15	O	302	ASN
15	O	377	GLN
15	O	515	GLN
15	O	534	GLN
16	P	181	ASN
17	Q	197	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
19	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
19	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
19	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.

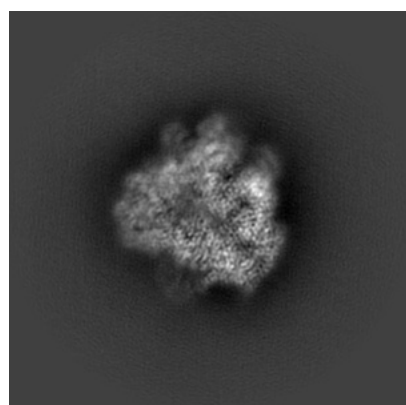
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30578. These allow visual inspection of the internal detail of the map and identification of artifacts.

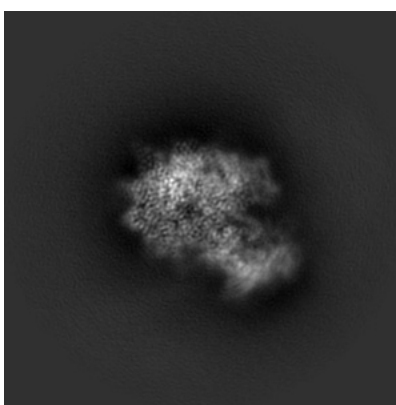
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

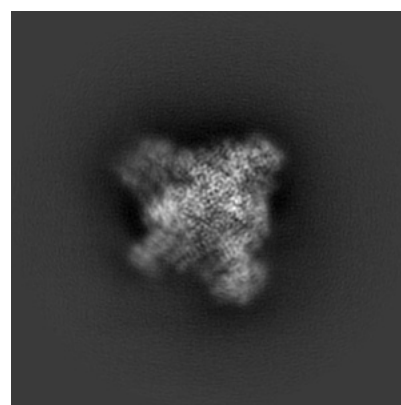
#### 6.1.1 Primary map



X



Y

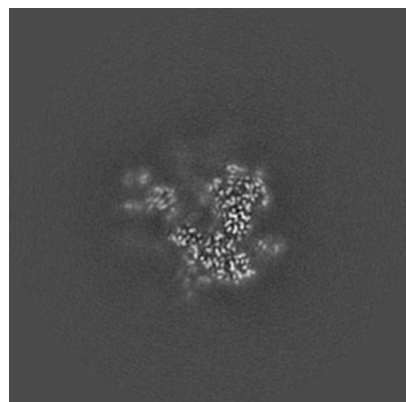


Z

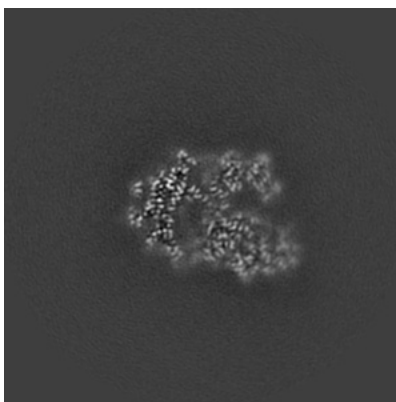
The images above show the map projected in three orthogonal directions.

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

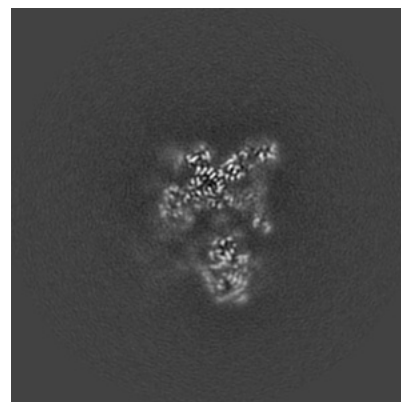
#### 6.2.1 Primary map



X Index: 168



Y Index: 168

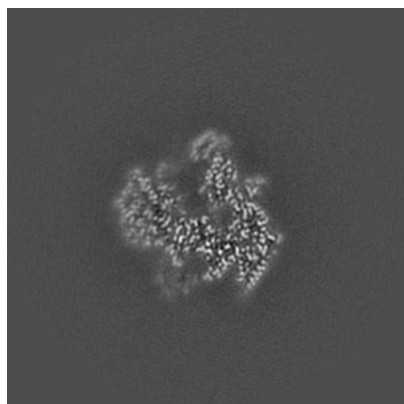


Z Index: 168

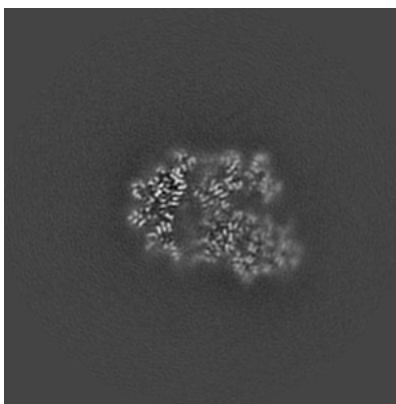
The images above show central slices of the map in three orthogonal directions.

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

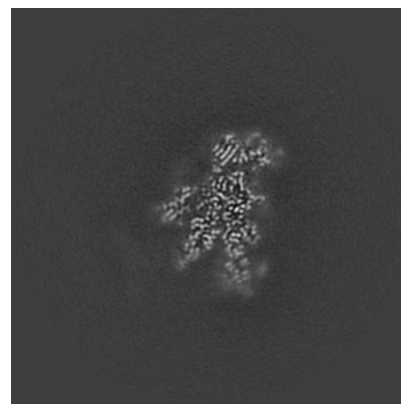
### 6.3.1 Primary map



X Index: 186



Y Index: 170

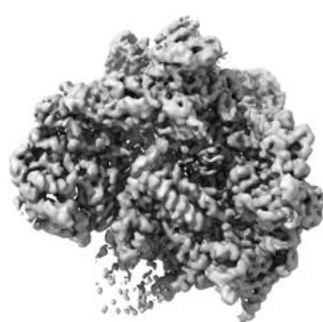


Z Index: 141

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

## 6.4 Orthogonal surface views [i](#)

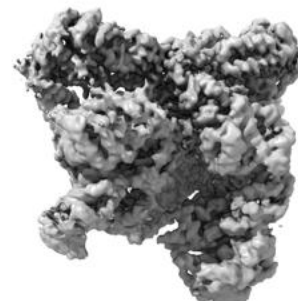
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

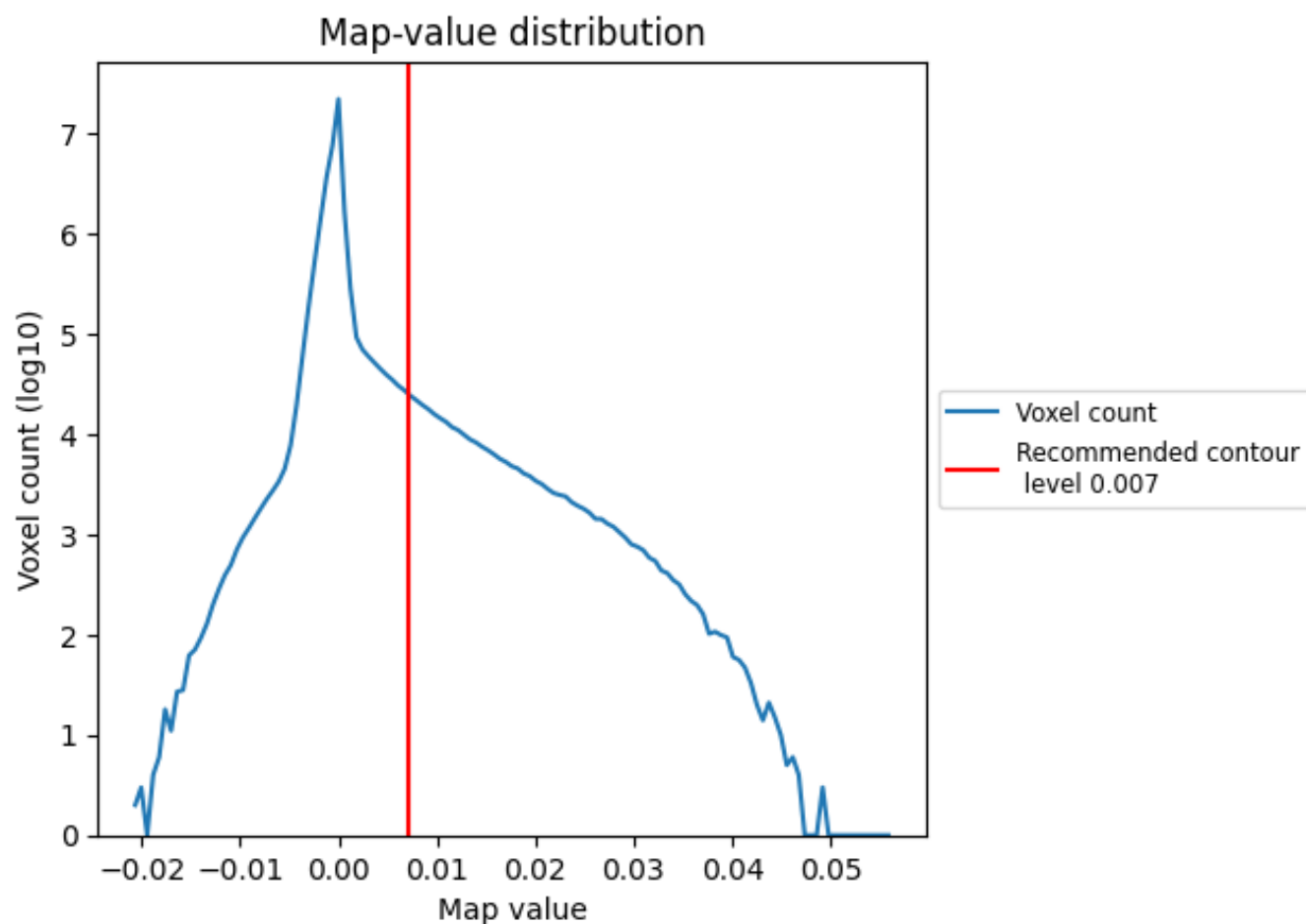
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

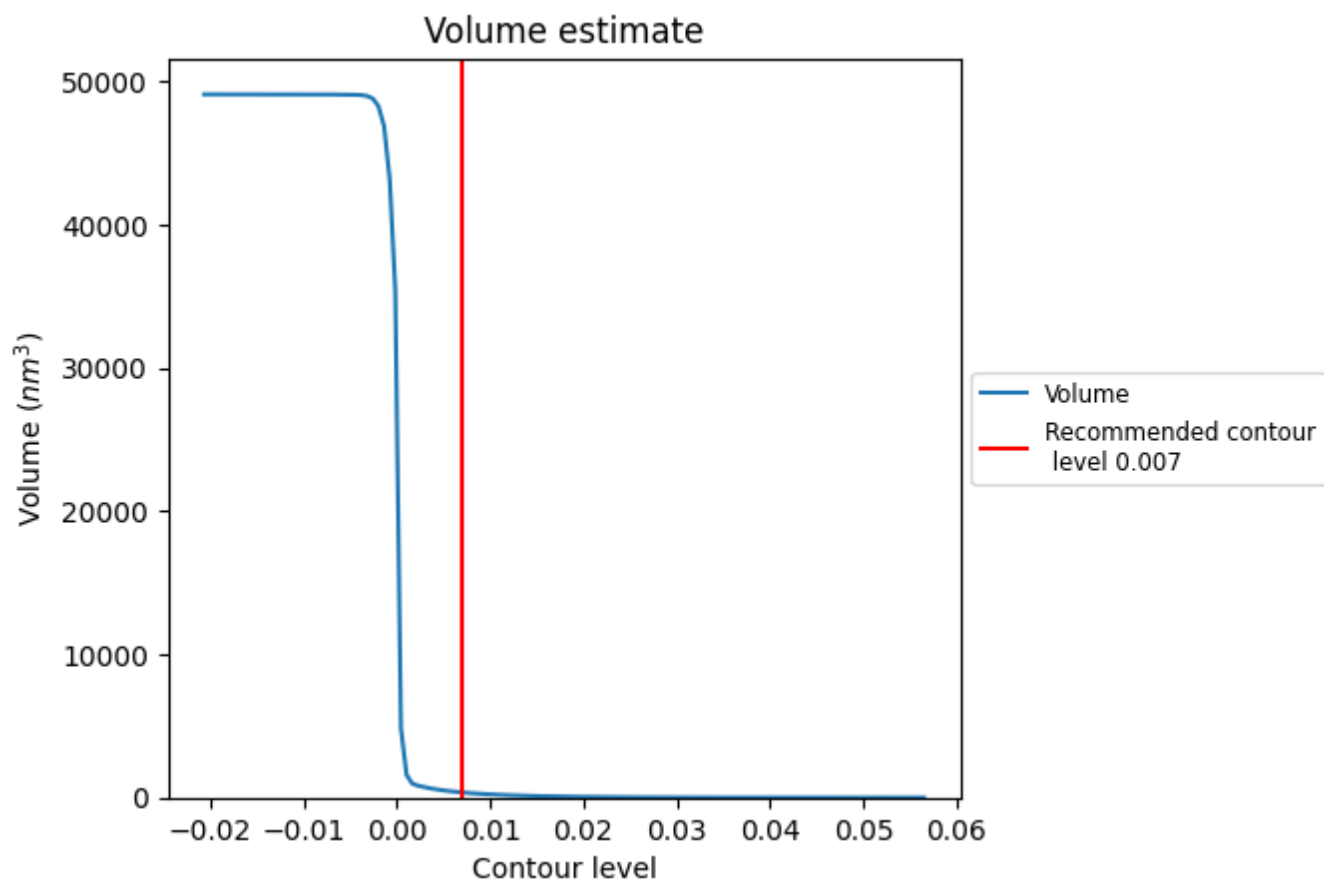
This section contains the results of statistical analysis of the map.

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



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

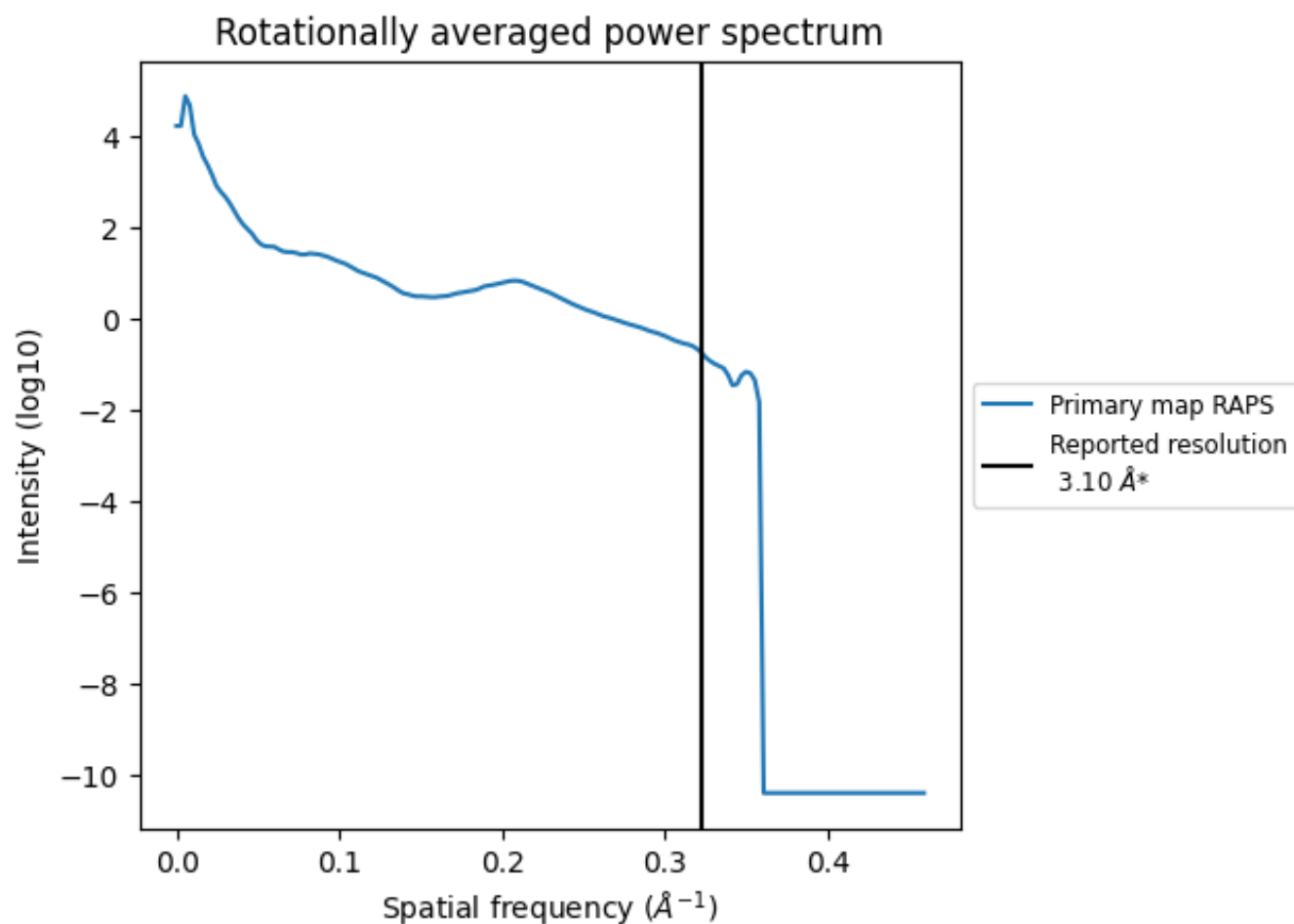
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 357  $\text{nm}^3$ ; this corresponds to an approximate mass of 323 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

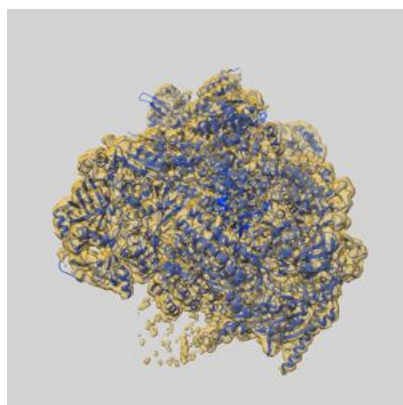
## 8 Fourier-Shell correlation ⓘ

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

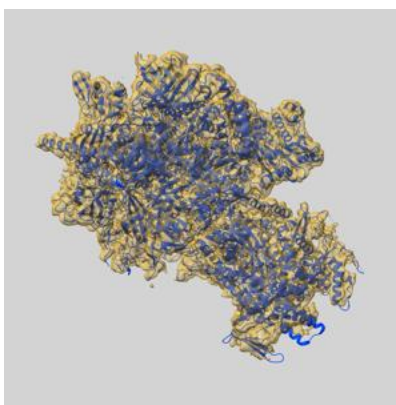
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30578 and PDB model 7D59. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

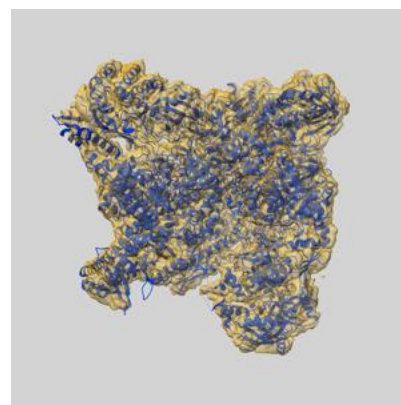
### 9.1 Map-model overlay [i](#)



X



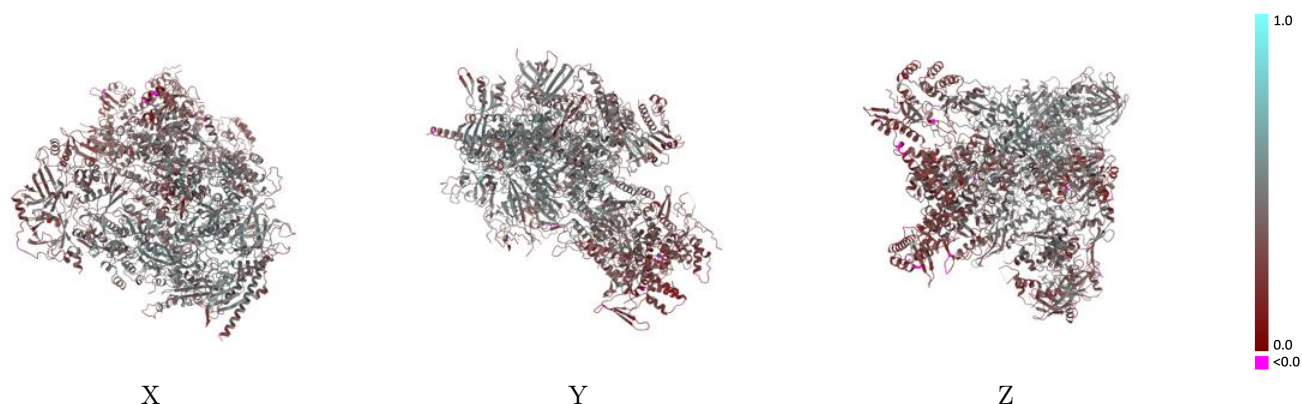
Y



Z

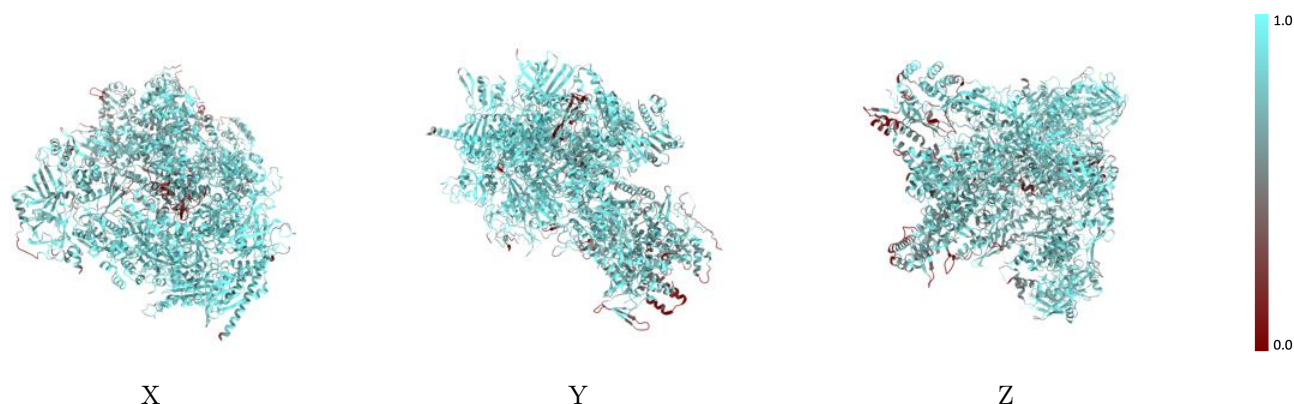
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



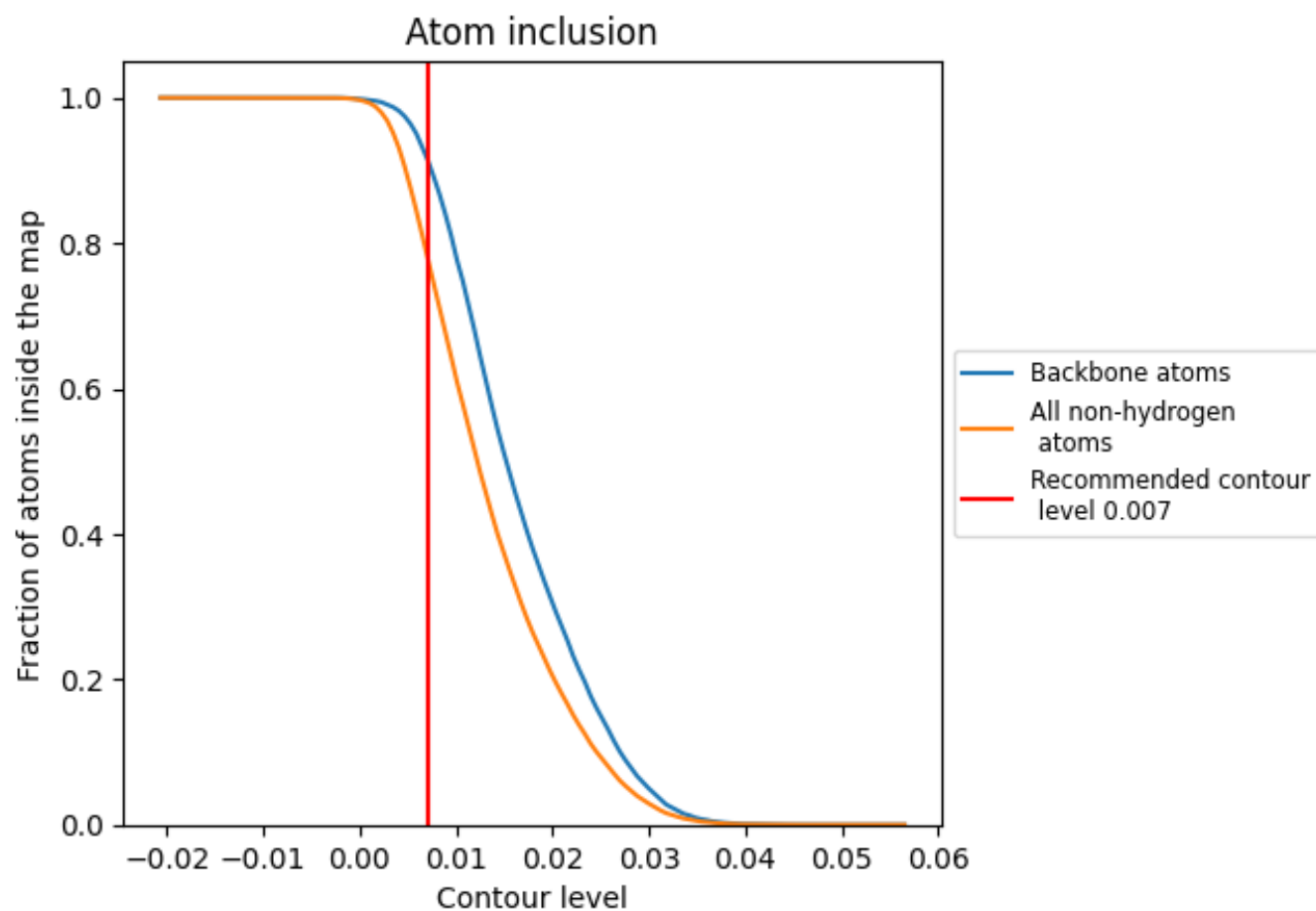
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).





































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 78% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7824	 0.3910
A	 0.8174	 0.4260
B	 0.8349	 0.4390
C	 0.8754	 0.4430
D	 0.6980	 0.2680
E	 0.7985	 0.3340
F	 0.8817	 0.4630
G	 0.7462	 0.3510
H	 0.8385	 0.4270
I	 0.4958	 0.2940
J	 0.8810	 0.4840
K	 0.8835	 0.4390
L	 0.8556	 0.4320
M	 0.7133	 0.3070
N	 0.7819	 0.3700
O	 0.6754	 0.2960
P	 0.6117	 0.2650
Q	 0.4975	 0.3050

