



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 11:52 am GMT

PDB ID : 5M64
EMDB ID : EMD-3449
Title : RNA Polymerase I elongation complex with A49 tandem winged helix domain
Authors : Tafur, L.; Sadian, Y.; Hoffmann, N.A.; Jakobi, A.J.; Wetzel, R.; Hagen, W.J.H.; Sachse, C.; Muller, C.W.
Deposited on : 2016-10-24
Resolution : 4.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

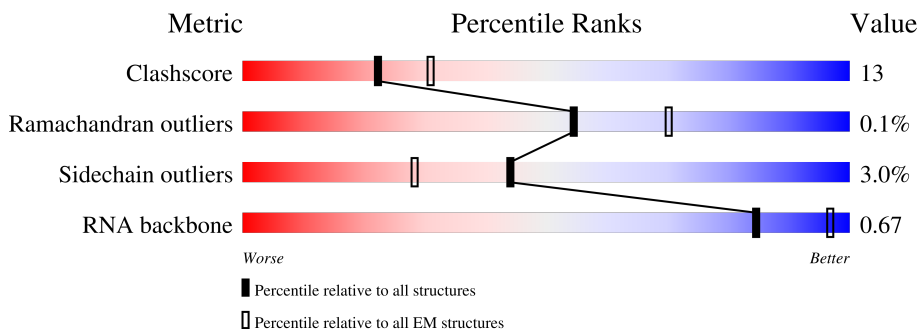
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.60 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1664	22% (red), 59% (green), 27% (yellow), 12% (grey)
2	B	1203	21% (red), 68% (green), 28% (yellow), 2% (grey)
3	C	335	20% (red), 64% (green), 26% (yellow), 9% (grey)
4	D	137	32% (red), 31% (green), 12% (yellow), 57% (grey)
5	E	215	25% (red), 72% (green), 26% (yellow), 1% (grey)
6	F	155	15% (red), 50% (green), 13% (yellow), 35% (grey)
7	G	326	41% (red), 41% (green), 20% (yellow), 38% (grey)

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Mol	Chain	Length	Quality of chain
8	H	146	
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	
15	S	70	
16	T	70	
17	R	10	

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 35876 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1466	11571	7309	2012	2188	62	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1170	9301	5888	1625	1737	51	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	304	2418	1536	414	460	8	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	59	467	293	80	94	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	214	1751	1111	309	320	11	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	202	1600	1026	276	293	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	134	1075	677	182	212	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	64	472	295	78	95	4	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	100	785	491	129	160	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	43	344	211	69	60	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	323	2573	1656	427	486	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	135	Total	C	N	O	S	0	0
			1070	685	175	206	4		

- Molecule 15 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	19	Total	C	N	O	P	0	0
			397	188	82	108	19		

- Molecule 16 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	25	Total	C	N	O	P	0	0
			509	244	86	154	25		

- Molecule 17 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	7	Total	C	N	O	P	0	0
			145	65	22	51	7		

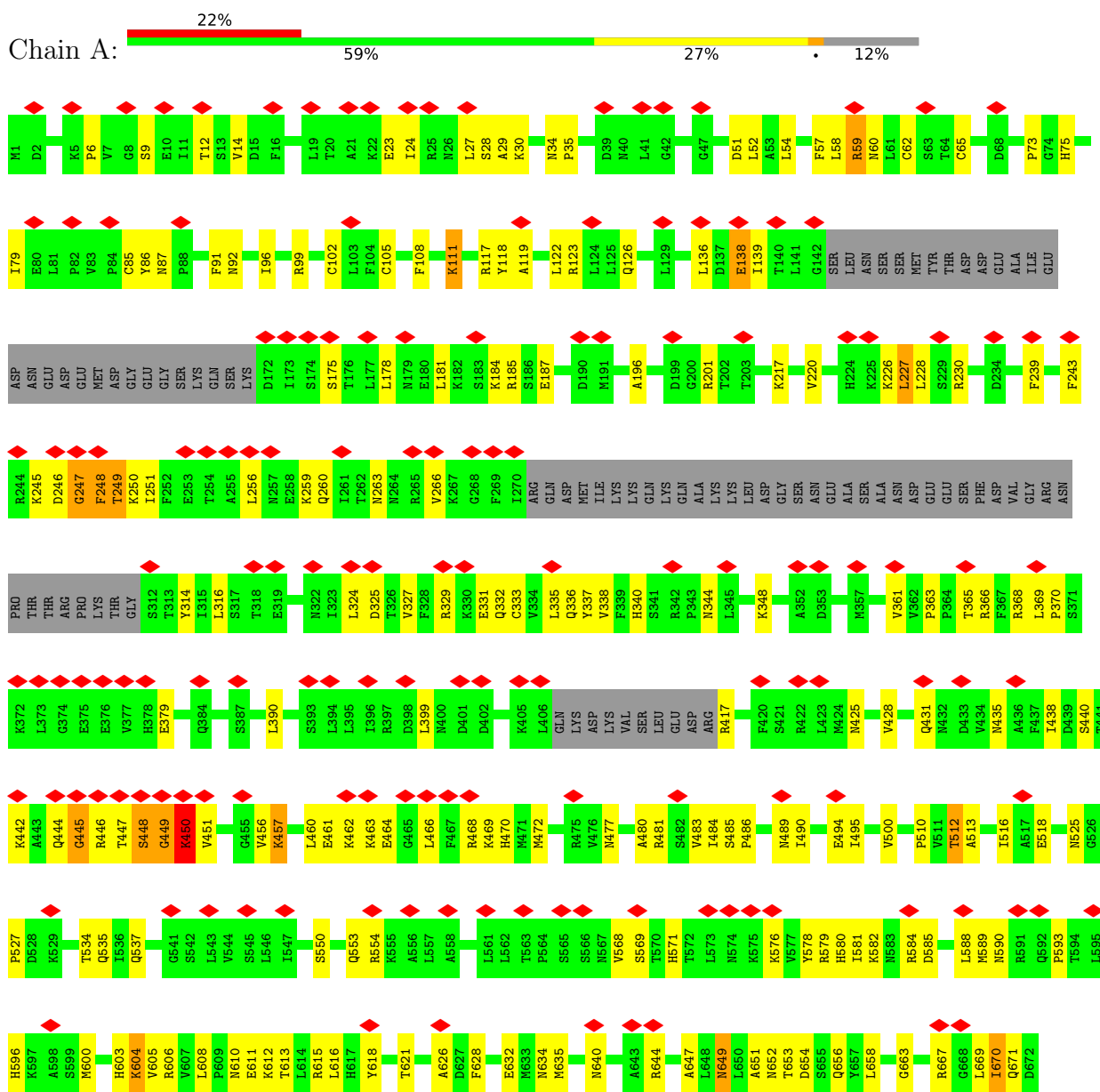
- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

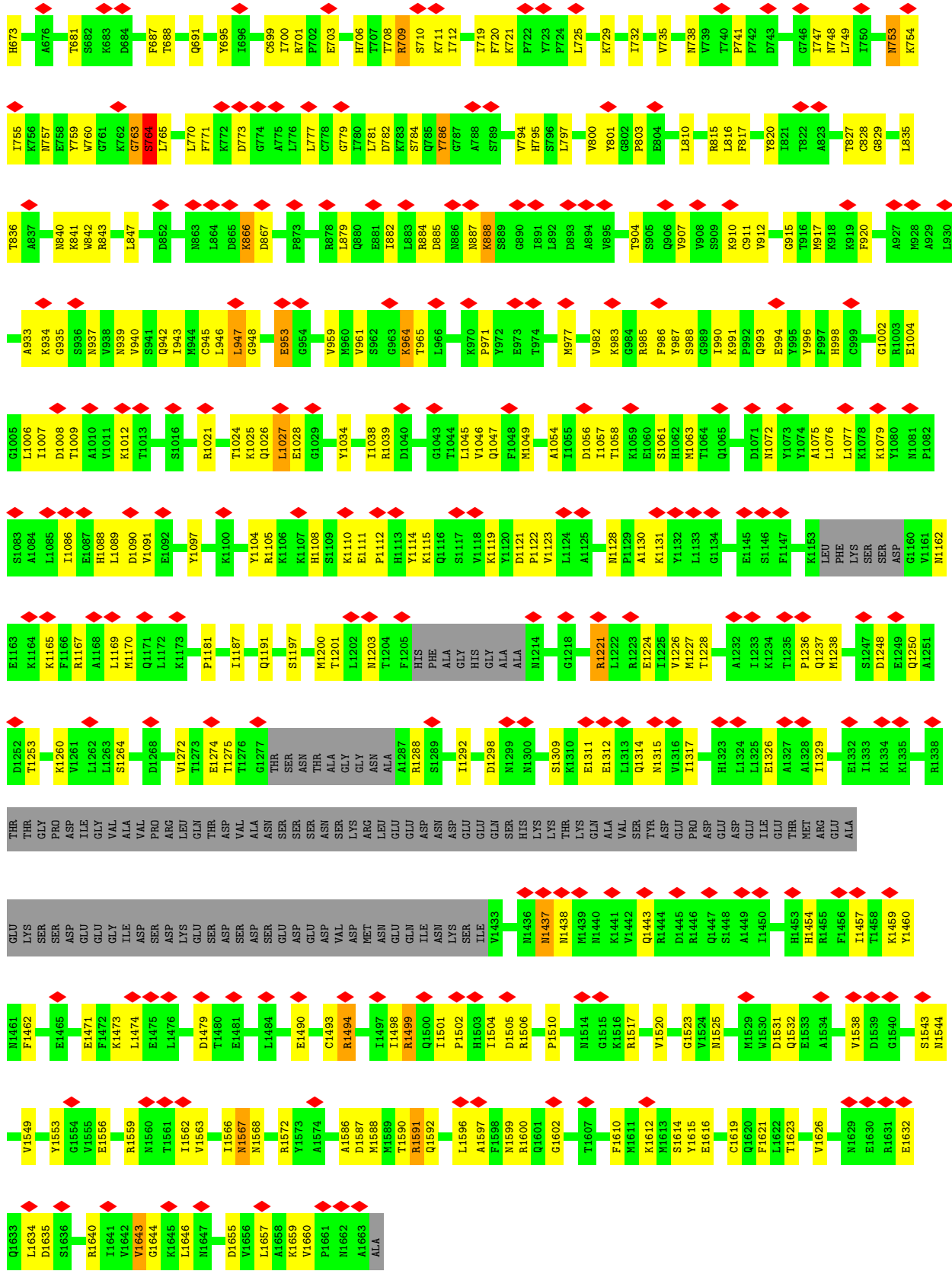
Mol	Chain	Residues	Atoms		AltConf
18	A	2	Total	Zn	0
			2	2	
18	B	1	Total	Zn	0
			1	1	
18	I	1	Total	Zn	0
			1	1	
18	J	1	Total	Zn	0
			1	1	
18	L	1	Total	Zn	0
			1	1	

3 Residue-property plots

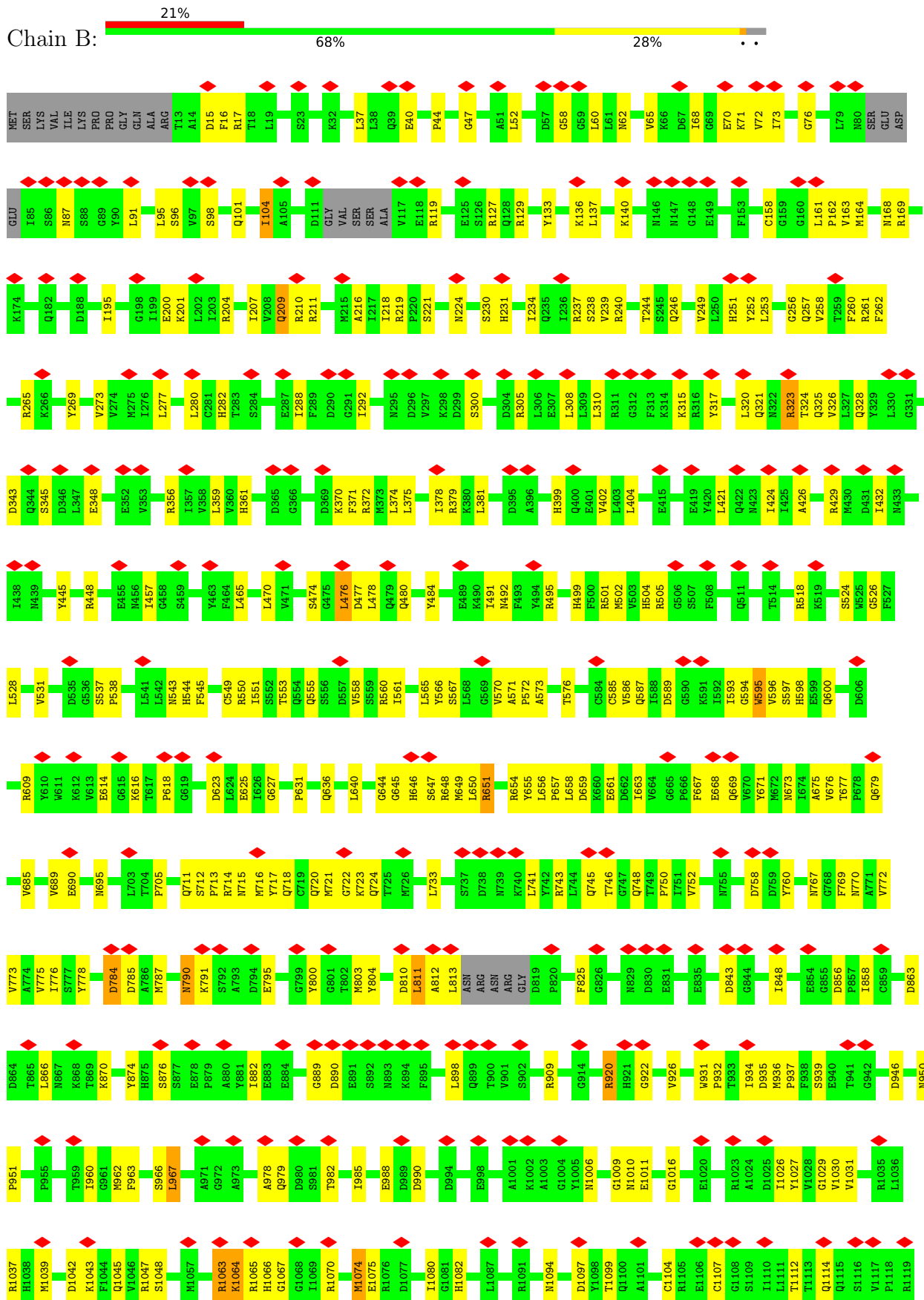
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

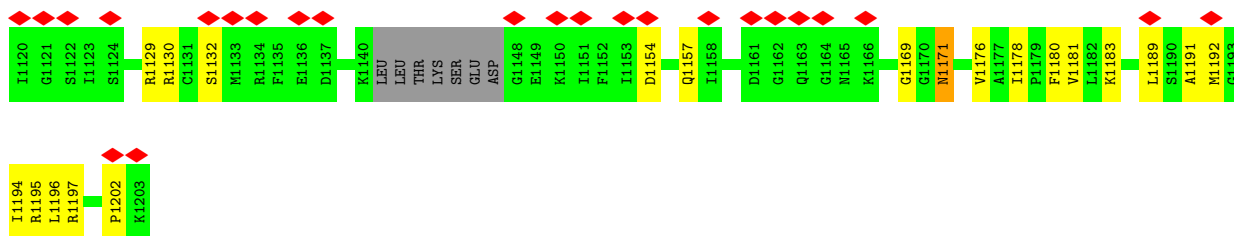
• Molecule 1: DNA-directed RNA polymerase I subunit RPA190



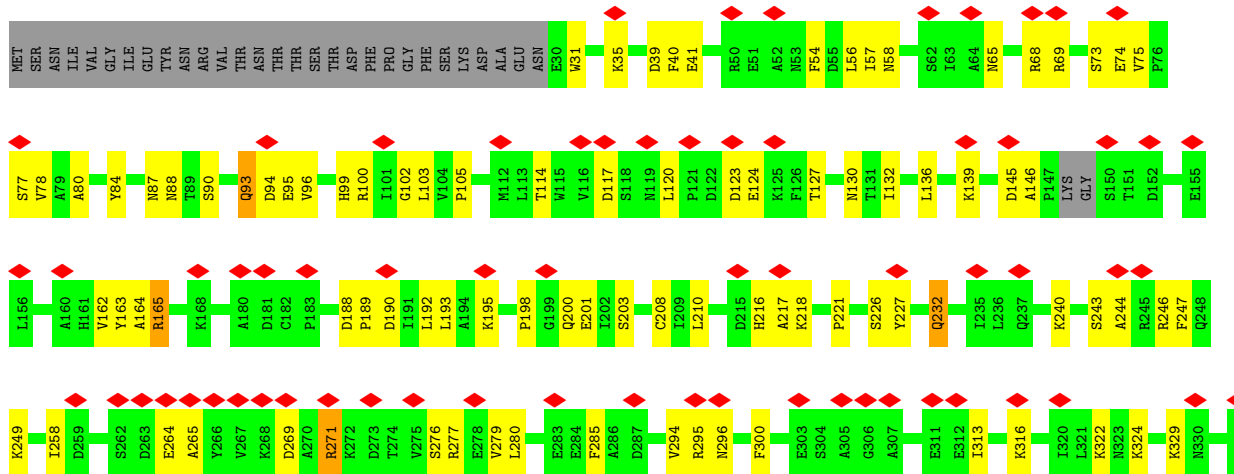


● Molecule 2: DNA-directed RNA polymerase I subunit RPA135

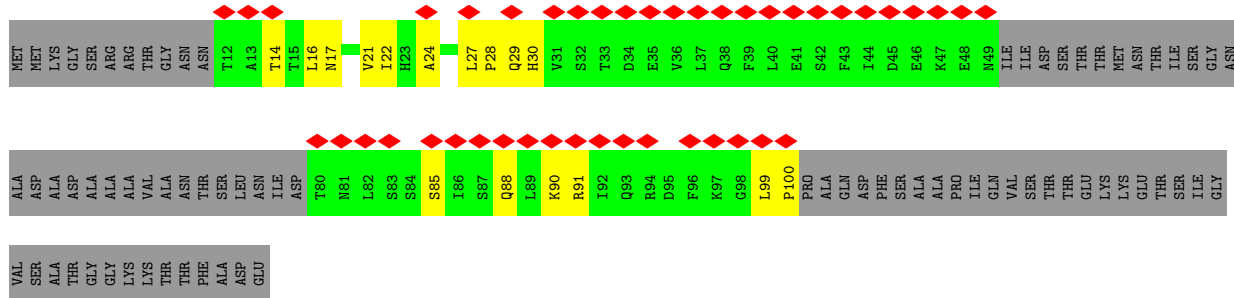
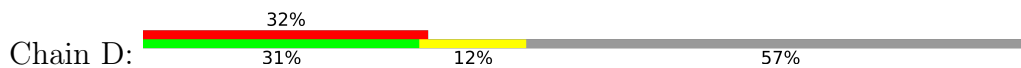




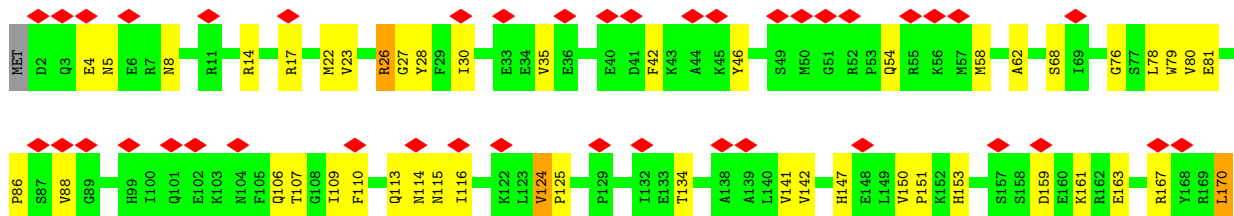
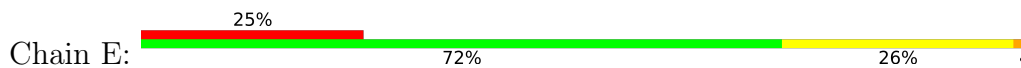
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

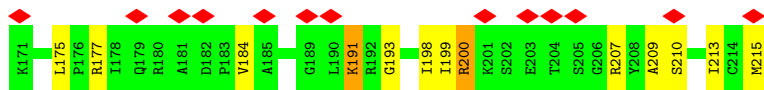


• Molecule 4: DNA-directed RNA polymerase I subunit RPA14

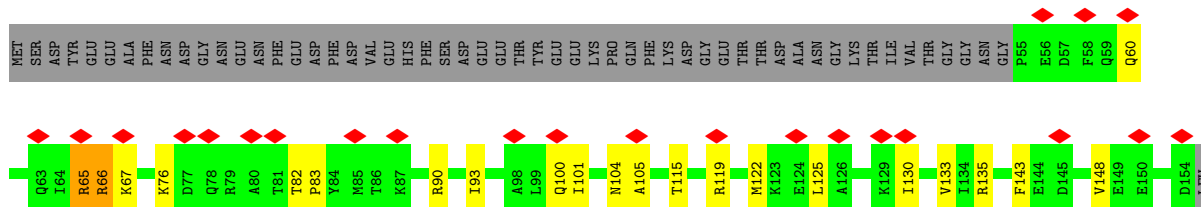


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

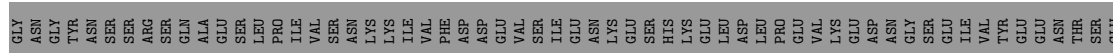
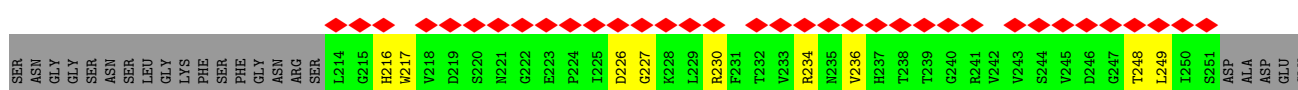
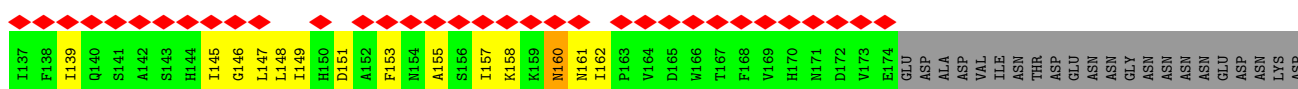
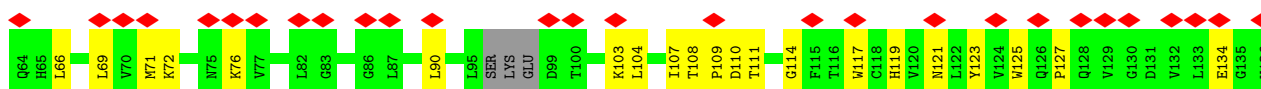
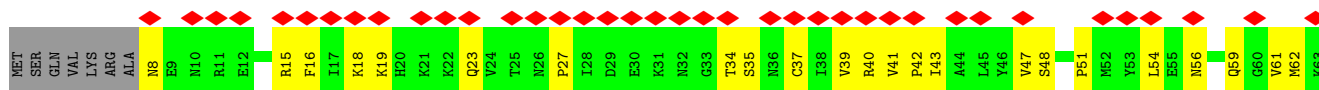




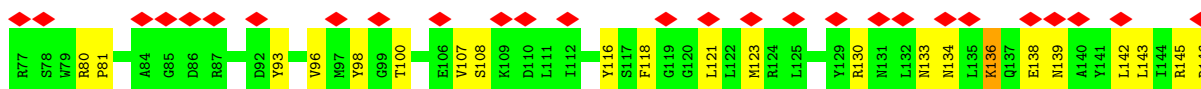
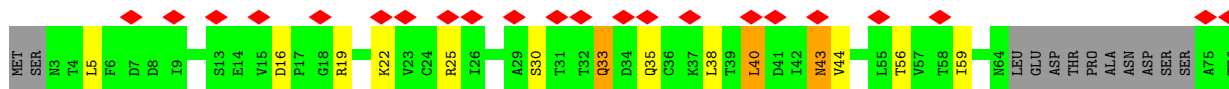
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



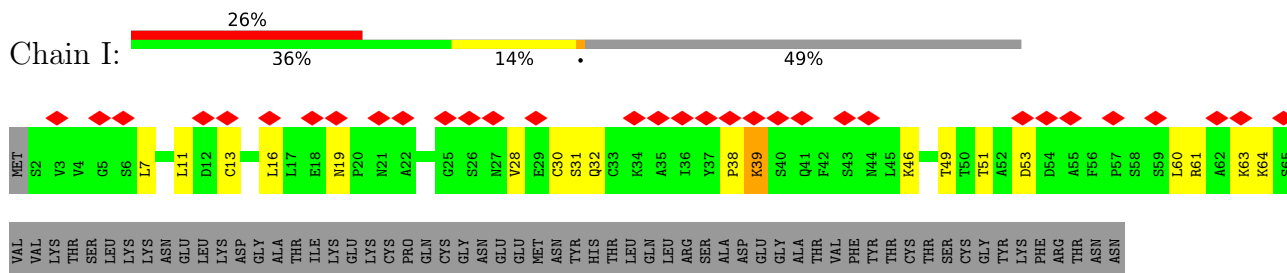
- Molecule 7: DNA-directed RNA polymerase I subunit RPA43



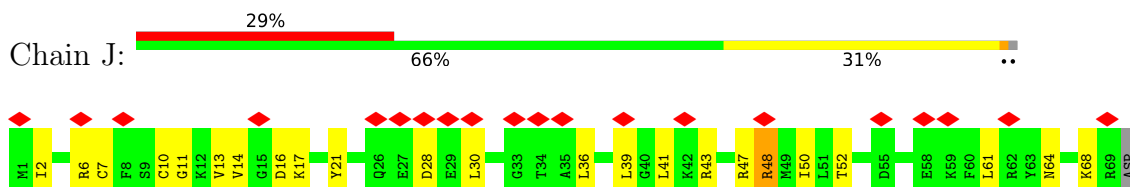
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



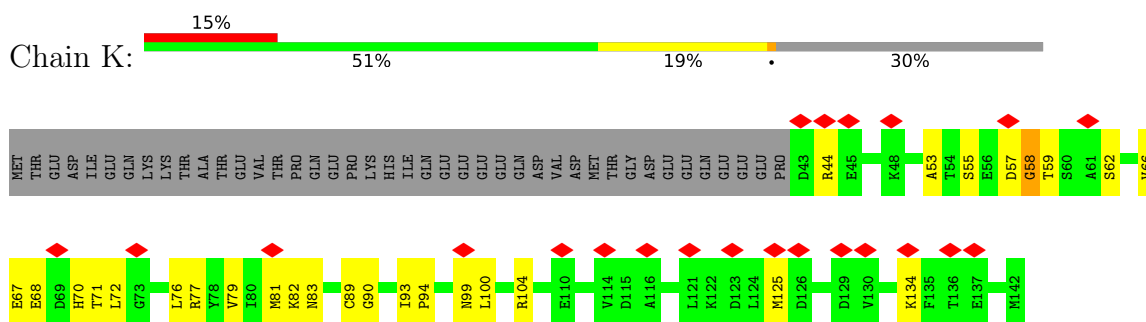
- Molecule 9: DNA-directed RNA polymerase I subunit RPA12



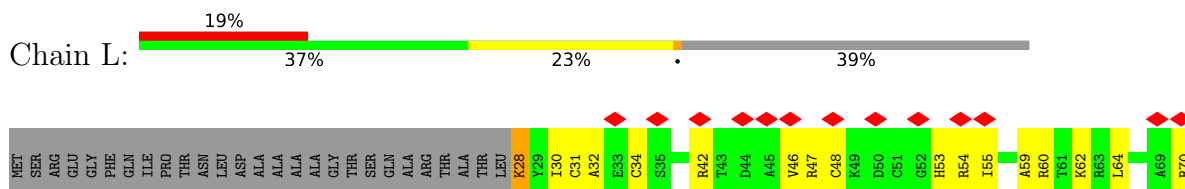
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



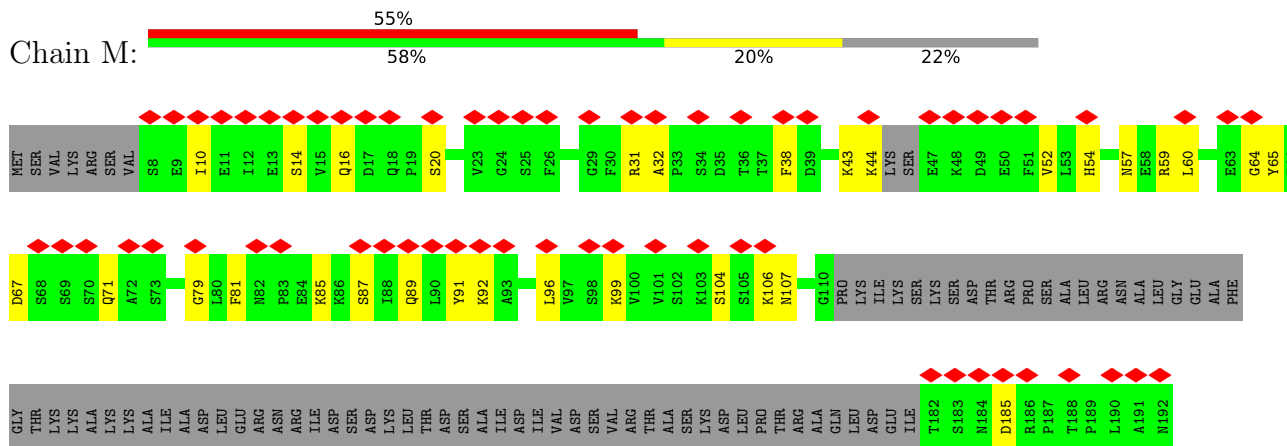
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

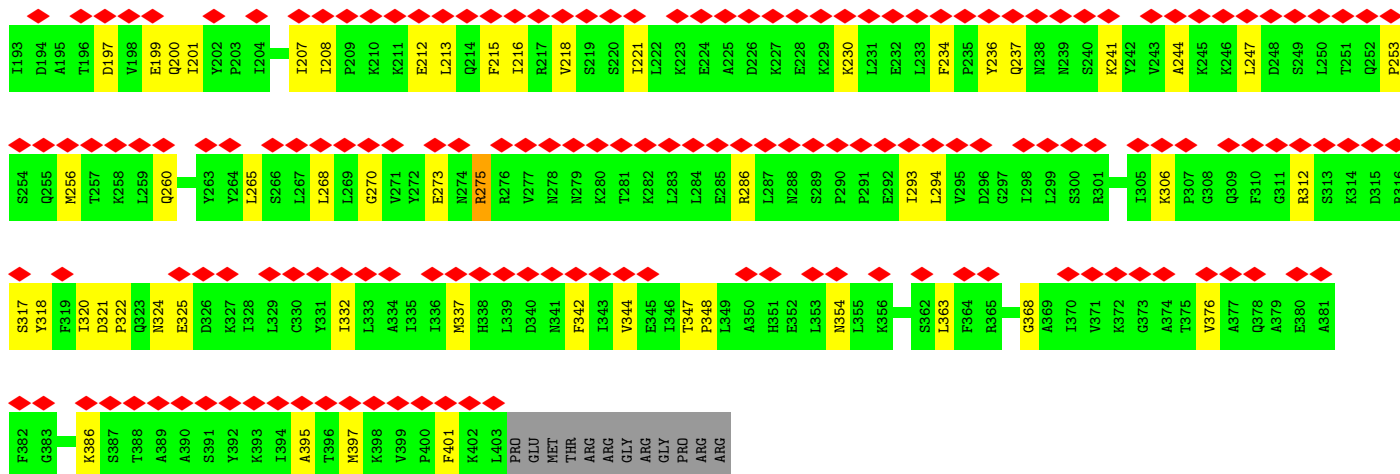


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

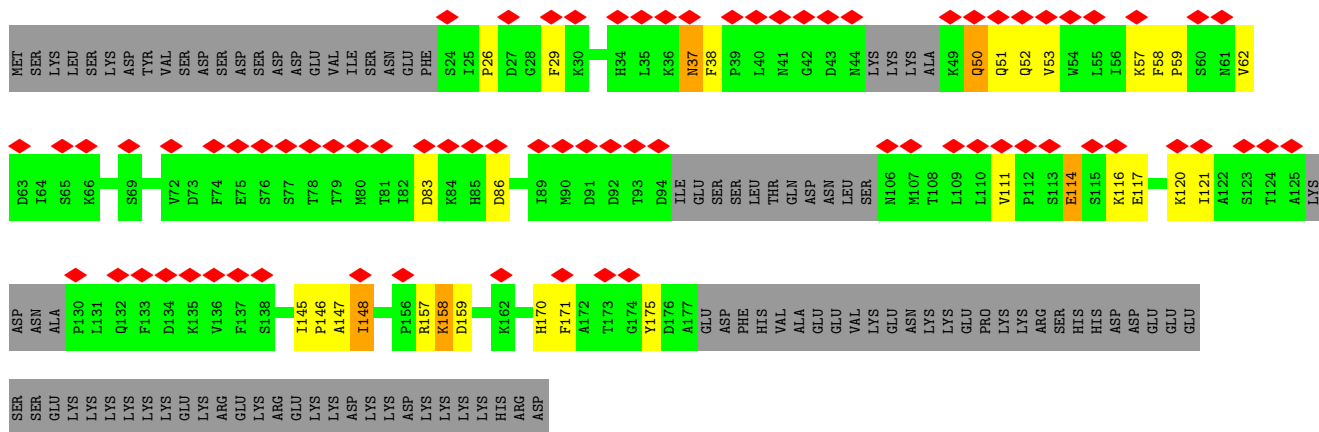


- Molecule 13: DNA-directed RNA polymerase I subunit RPA49

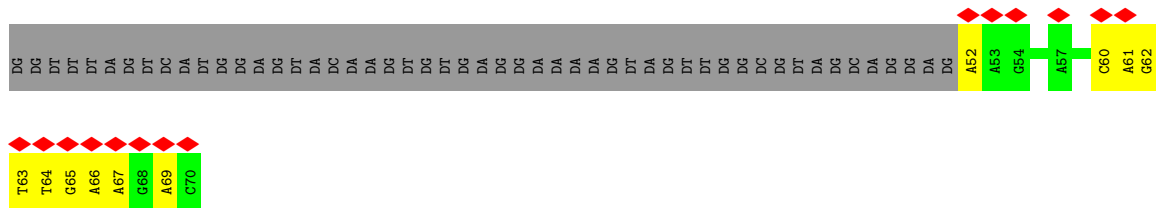




● Molecule 14: DNA-directed RNA polymerase I subunit RPA34



● Molecule 15: Non-template DNA




● Molecule 16: Template DNA



DT
DG
DA
DC
DT
DA
DA
DA
DC
DC

• Molecule 17: RNA




G
A
G
G4
U5
A6
C7
U8
U9
C10

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	13412	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.198	Depositor
Minimum map value	-0.125	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	237.6, 237.6, 237.6	wwPDB
Map dimensions	176, 176, 176	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.28	3/11782 (0.0%)	0.48	7/15913 (0.0%)
2	B	0.25	1/9506 (0.0%)	0.46	3/12847 (0.0%)
3	C	0.24	0/2469	0.42	0/3347
4	D	0.23	0/473	0.46	0/641
5	E	0.24	0/1787	0.41	0/2406
6	F	0.23	0/838	0.40	0/1129
7	G	0.24	0/1637	0.43	0/2226
8	H	0.24	0/1093	0.46	0/1480
9	I	0.25	0/478	0.47	0/647
10	J	0.23	0/578	0.44	0/775
11	K	0.48	2/795 (0.3%)	0.81	4/1072 (0.4%)
12	L	0.22	0/346	0.43	0/457
13	M	0.24	0/2620	0.44	0/3536
14	N	0.24	0/1090	0.49	0/1466
15	S	0.49	0/448	0.82	0/690
16	T	0.49	0/568	0.96	1/874 (0.1%)
17	R	0.11	0/160	0.69	0/246
All	All	0.27	6/36668 (0.0%)	0.49	15/49752 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
11	K	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	445	GLY	CA-C	-10.24	1.35	1.51
11	K	57	ASP	N-CA	9.99	1.66	1.46
1	A	449	GLY	N-CA	9.55	1.60	1.46
1	A	763	GLY	N-CA	6.76	1.56	1.46
2	B	1064	LYS	N-CA	5.39	1.57	1.46
11	K	57	ASP	CA-CB	5.27	1.65	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	57	ASP	N-CA-C	-14.07	73.00	111.00
1	A	449	GLY	N-CA-C	-13.59	79.14	113.10
2	B	1064	LYS	N-CA-C	-11.77	79.22	111.00
11	K	57	ASP	CB-CA-C	-11.66	87.07	110.40
11	K	58	GLY	N-CA-C	-10.02	88.05	113.10
1	A	763	GLY	N-CA-C	-9.60	89.11	113.10
11	K	57	ASP	N-CA-CB	-8.16	95.91	110.60
1	A	445	GLY	N-CA-C	-8.11	92.83	113.10
1	A	764	SER	N-CA-C	-7.18	91.62	111.00
16	T	20	DT	O4'-C4'-C3'	-6.67	101.83	104.50
1	A	445	GLY	CA-C-O	-6.25	109.35	120.60
1	A	450	LYS	N-CA-C	-6.23	94.17	111.00
2	B	1064	LYS	CB-CA-C	-5.87	98.67	110.40
1	A	448	SER	C-N-CA	-5.47	110.81	122.30
2	B	1154	ASP	CB-CG-OD2	5.22	123.00	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	247	GLY	Mainchain
1	A	445	GLY	Mainchain
11	K	58	GLY	Mainchain

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	11571	0	11650	379	0
2	B	9301	0	9194	260	0
3	C	2418	0	2401	72	0
4	D	467	0	468	11	0
5	E	1751	0	1776	37	0
6	F	823	0	841	17	0
7	G	1600	0	1600	45	0
8	H	1075	0	1046	30	0
9	I	472	0	473	16	0
10	J	569	0	585	21	0
11	K	785	0	782	19	0
12	L	344	0	363	13	0
13	M	2573	0	2653	58	0
14	N	1070	0	1085	27	0
15	S	397	0	213	9	0
16	T	509	0	285	10	0
17	R	145	0	75	0	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	I	1	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
All	All	35876	0	35490	901	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 13.

All (901) 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)
2:B:811:LEU:HD22	2:B:825:PHE:CZ	1.47	1.47
13:M:197:ASP:OD2	13:M:199:GLU:OE1	1.53	1.26
2:B:811:LEU:CD2	2:B:825:PHE:CZ	2.18	1.25
2:B:1104:CYS:HB3	2:B:1107:CYS:SG	1.90	1.11
13:M:368:GLY:O	13:M:397:MET:HE1	1.52	1.09
10:J:7:CYS:HB3	10:J:10:CYS:SG	2.00	1.01
1:A:449:GLY:O	1:A:450:LYS:HG2	1.59	1.00
1:A:248:PHE:O	1:A:249:THR:HG23	1.63	0.97
1:A:248:PHE:HZ	16:T:16:DC:OP1	1.48	0.96
1:A:449:GLY:O	1:A:450:LYS:CG	2.13	0.96
2:B:811:LEU:HD22	2:B:825:PHE:CE2	2.00	0.95
1:A:757:ASN:CG	1:A:764:SER:O	2.06	0.93

Continued on next page...

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:PHE:HB3	1:A:442:LYS:HG3	1.51	0.92
1:A:449:GLY:O	1:A:450:LYS:CB	2.18	0.90
2:B:1063:ARG:HA	2:B:1067:GLY:H	1.36	0.89
2:B:811:LEU:CD2	2:B:825:PHE:CE2	2.55	0.88
13:M:368:GLY:O	13:M:397:MET:CE	2.23	0.87
1:A:757:ASN:ND2	1:A:764:SER:O	2.06	0.87
2:B:811:LEU:HD22	2:B:825:PHE:HZ	1.40	0.83
1:A:760:TRP:HB2	1:A:764:SER:HB3	1.62	0.82
1:A:247:GLY:O	1:A:248:PHE:HB2	1.83	0.79
2:B:811:LEU:HD21	2:B:825:PHE:CZ	2.17	0.78
2:B:811:LEU:HD21	2:B:825:PHE:CE1	2.17	0.78
1:A:757:ASN:CB	1:A:764:SER:O	2.32	0.78
2:B:962:MET:HG3	2:B:1031:VAL:HG21	1.67	0.77
1:A:248:PHE:O	1:A:249:THR:CG2	2.32	0.77
1:A:985:ARG:HG3	1:A:987:TYR:H	1.50	0.76
1:A:681:THR:HG21	1:A:781:LEU:H	1.50	0.76
1:A:449:GLY:O	1:A:450:LYS:HB2	1.86	0.75
1:A:757:ASN:HB3	1:A:764:SER:HB2	1.68	0.74
2:B:651:ARG:HH21	2:B:669:GLN:HE22	1.35	0.74
2:B:811:LEU:CD2	2:B:825:PHE:CE1	2.69	0.74
2:B:239:VAL:H	2:B:361:HIS:HB3	1.53	0.74
1:A:249:THR:HG21	1:A:435:ASN:ND2	2.03	0.73
5:E:17:ARG:HH22	5:E:35:VAL:HG13	1.53	0.73
1:A:757:ASN:HB3	1:A:764:SER:O	1.88	0.73
1:A:866:LYS:HD3	1:A:866:LYS:H	1.54	0.73
1:A:250:LYS:CG	1:A:314:TYR:CD1	2.72	0.72
2:B:359:LEU:HD11	2:B:370:LYS:HG3	1.70	0.72
2:B:705:PRO:HD2	2:B:920:ARG:HG3	1.71	0.71
2:B:58:GLY:HA3	2:B:62:ASN:HD22	1.55	0.71
2:B:104:ILE:HG23	2:B:137:LEU:HD23	1.69	0.71
1:A:248:PHE:CZ	16:T:16:DC:OP1	2.39	0.70
1:A:462:LYS:H	1:A:466:LEU:HB2	1.56	0.70
3:C:80:ALA:HB3	3:C:102:GLY:HA2	1.74	0.70
1:A:709:ARG:HG2	1:A:710:SER:H	1.57	0.69
1:A:250:LYS:O	1:A:251:ILE:C	2.27	0.69
1:A:1272:VAL:HG12	1:A:1292:ILE:HA	1.72	0.69
2:B:1189:LEU:HD11	2:B:1196:LEU:HB2	1.75	0.69
6:F:119:ARG:NH2	6:F:122:MET:SD	2.65	0.69
1:A:757:ASN:HB3	1:A:764:SER:CB	2.23	0.69
7:G:145:ILE:HG22	7:G:157:ILE:HG12	1.75	0.68
5:E:124:VAL:HG23	5:E:125:PRO:HD3	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:CYS:CB	1:A:65:CYS:SG	2.82	0.67
1:A:249:THR:CG2	1:A:435:ASN:ND2	2.57	0.67
5:E:46:TYR:O	5:E:54:GLN:NE2	2.27	0.67
1:A:249:THR:HG21	1:A:435:ASN:HD21	1.58	0.66
4:D:28:PRO:HB3	7:G:41:VAL:HG22	1.77	0.66
13:M:337:MET:SD	13:M:344:VAL:CG2	2.83	0.66
3:C:165:ARG:HB3	3:C:189:PRO:HB3	1.78	0.66
13:M:368:GLY:C	13:M:397:MET:CE	2.64	0.66
6:F:93:ILE:HD11	6:F:125:LEU:HD12	1.77	0.66
2:B:675:ALA:HB3	2:B:689:VAL:HG12	1.78	0.66
2:B:558:VAL:HG12	2:B:560:ARG:H	1.61	0.65
15:S:63:DT:H2''	15:S:64:DT:H3'	1.78	0.65
1:A:647:ALA:HA	1:A:651:ALA:HB3	1.78	0.65
1:A:85:CYS:SG	1:A:86:TYR:N	2.70	0.65
3:C:132:ILE:HB	3:C:208:CYS:HB3	1.77	0.65
3:C:54:PHE:HB3	3:C:300:PHE:HB2	1.78	0.64
2:B:656:LEU:HD11	2:B:689:VAL:HG13	1.78	0.64
7:G:134:GLU:OE1	7:G:230:ARG:NH2	2.30	0.64
9:I:11:LEU:HD22	13:M:31:ARG:HD3	1.77	0.64
2:B:17:ARG:NH1	2:B:758:ASP:OD2	2.30	0.64
1:A:65:CYS:HB3	1:A:75:HIS:NE2	2.12	0.64
1:A:490:ILE:HG23	1:A:494:GLU:HB2	1.78	0.64
7:G:37:CYS:SG	7:G:125:TRP:NE1	2.70	0.64
1:A:102:CYS:HB3	1:A:105:CYS:SG	2.37	0.64
3:C:58:ASN:OD1	3:C:296:ASN:ND2	2.29	0.64
1:A:247:GLY:O	1:A:248:PHE:CB	2.44	0.64
1:A:250:LYS:HG2	1:A:314:TYR:CE1	2.32	0.64
8:H:98:TYR:OH	8:H:139:ASN:OD1	2.07	0.64
1:A:250:LYS:HG2	1:A:314:TYR:CD1	2.32	0.64
1:A:991:LYS:HE3	1:A:993:GLN:HB2	1.79	0.64
1:A:600:MET:O	2:B:1082:HIS:NE2	2.31	0.64
1:A:943:ILE:O	1:A:985:ARG:NH1	2.31	0.64
2:B:752:VAL:HB	2:B:979:GLN:HE21	1.63	0.64
1:A:246:ASP:HB3	1:A:249:THR:O	1.98	0.63
2:B:636:GLN:NE2	2:B:671:TYR:OH	2.31	0.63
4:D:99:LEU:HD22	4:D:100:PRO:HD2	1.80	0.63
2:B:898:LEU:HD11	12:L:46:VAL:HG11	1.80	0.63
1:A:1634:LEU:HD22	1:A:1643:VAL:HG21	1.79	0.63
2:B:931:TRP:HE1	2:B:935:ASP:HB2	1.63	0.63
13:M:207:ILE:HG22	13:M:208:ILE:HG13	1.81	0.63
1:A:438:ILE:HD12	1:A:456:VAL:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:7:DA:H2''	16:T:8:DA:H5''	1.81	0.62
1:A:652:ASN:O	1:A:656:GLN:NE2	2.32	0.62
7:G:148:LEU:HB3	7:G:151:ASP:HA	1.80	0.62
2:B:216:ALA:HA	2:B:234:ILE:HG22	1.80	0.62
1:A:481:ARG:NH2	1:A:634:ASN:OD1	2.33	0.62
2:B:748:GLN:HB2	2:B:769:PHE:HA	1.79	0.62
1:A:1635:ASP:HA	1:A:1640:ARG:HH11	1.64	0.62
2:B:262:PHE:HB2	2:B:269:TYR:HB2	1.81	0.62
4:D:85:SER:HA	4:D:88:GLN:HE21	1.64	0.62
1:A:449:GLY:C	1:A:450:LYS:HG2	2.19	0.62
2:B:1006:ASN:ND2	2:B:1010:ASN:OD1	2.32	0.62
13:M:265:LEU:HD13	13:M:268:LEU:HD22	1.81	0.62
14:N:58:PHE:HB2	14:N:62:VAL:HG11	1.82	0.62
1:A:54:LEU:HA	1:A:75:HIS:HB2	1.82	0.61
1:A:1556:GLU:OE2	5:E:153:HIS:NE2	2.32	0.61
2:B:733:LEU:HD21	2:B:743:ARG:HD3	1.82	0.61
13:M:337:MET:SD	13:M:344:VAL:HG21	2.40	0.61
8:H:43:ASN:HD22	8:H:44:VAL:H	1.48	0.61
16:T:20:DT:H2''	16:T:21:DG:H5'	1.83	0.61
1:A:613:THR:O	1:A:615:ARG:NH2	2.33	0.61
1:A:489:ASN:ND2	11:K:94:PRO:O	2.33	0.61
1:A:510:PRO:HB3	1:A:576:LYS:HE3	1.81	0.61
2:B:848:ILE:HA	2:B:882:ILE:HD11	1.82	0.61
2:B:137:LEU:HD12	2:B:158:CYS:HB2	1.83	0.61
6:F:135:ARG:HD2	6:F:143:PHE:HB2	1.82	0.61
1:A:1264:SER:HB2	1:A:1493:CYS:HB3	1.82	0.61
2:B:310:LEU:HG	9:I:16:LEU:HD21	1.82	0.61
2:B:1016:GLY:O	3:C:69:ARG:NH2	2.33	0.61
10:J:10:CYS:SG	10:J:11:GLY:N	2.73	0.61
1:A:369:LEU:HD22	1:A:370:PRO:HD2	1.82	0.61
2:B:982:THR:HG23	2:B:985:ILE:HD13	1.82	0.60
1:A:1660:VAL:HG22	7:G:103:LYS:HG2	1.81	0.60
2:B:252:TYR:OH	2:B:305:ARG:NH1	2.33	0.60
3:C:80:ALA:HA	3:C:208:CYS:HA	1.82	0.60
1:A:248:PHE:C	1:A:249:THR:HG23	2.21	0.60
14:N:148:ILE:O	14:N:148:ILE:HG22	2.02	0.60
1:A:23:GLU:OE1	2:B:1130:ARG:NH1	2.34	0.60
1:A:920:PHE:O	8:H:19:ARG:NH1	2.35	0.60
1:A:1311:GLU:O	1:A:1315:ASN:ND2	2.34	0.60
2:B:280:LEU:HG	2:B:370:LYS:HD2	1.83	0.60
7:G:51:PRO:HA	7:G:54:LEU:HG	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:59:ILE:HG12	8:H:142:LEU:HG	1.83	0.60
1:A:628:PHE:HB2	2:B:785:ASP:HB3	1.83	0.60
1:A:940:VAL:HA	1:A:943:ILE:HG22	1.83	0.60
2:B:129:ARG:HH21	2:B:890:ASP:HA	1.67	0.60
2:B:586:VAL:HB	2:B:593:ILE:HD11	1.84	0.60
2:B:795:GLU:HG2	3:C:217:ALA:H	1.66	0.60
1:A:447:THR:HG22	1:A:448:SER:H	1.67	0.60
1:A:658:LEU:HD11	1:A:663:GLY:HA2	1.84	0.60
1:A:1027:LEU:HD23	1:A:1588:MET:HG2	1.82	0.60
2:B:158:CYS:HB3	2:B:457:ILE:HD13	1.84	0.60
5:E:28:TYR:OH	5:E:76:GLY:O	2.19	0.60
13:M:337:MET:SD	13:M:344:VAL:HG23	2.42	0.60
2:B:101:GLN:HB3	2:B:140:LYS:HB3	1.82	0.60
2:B:421:LEU:HD22	2:B:424:ILE:HD11	1.83	0.60
2:B:690:GLU:OE2	2:B:695:ASN:ND2	2.34	0.60
2:B:15:ASP:HA	2:B:978:ALA:HB3	1.84	0.60
2:B:1202:PRO:HD2	4:D:21:VAL:HG21	1.82	0.60
4:D:22:ILE:HG23	7:G:76:LYS:HG3	1.84	0.60
13:M:234:PHE:O	13:M:237:GLN:NE2	2.35	0.59
1:A:649:ASN:OD1	6:F:90:ARG:NH1	2.34	0.59
1:A:699:CYS:O	1:A:815:ARG:NH2	2.36	0.59
7:G:42:PRO:HA	7:G:121:ASN:HA	1.84	0.59
2:B:745:GLN:HE21	2:B:800:TYR:HB3	1.68	0.59
2:B:803:MET:SD	2:B:909:ARG:NH1	2.72	0.59
1:A:721:LYS:NZ	8:H:93:TYR:O	2.35	0.59
2:B:655:TYR:O	2:B:659:ASP:HA	2.03	0.59
13:M:44:LYS:H	14:N:29:PHE:HD2	1.50	0.59
1:A:1657:LEU:HB2	6:F:133:VAL:HB	1.84	0.59
2:B:292:ILE:HD13	2:B:375:LEU:HD11	1.84	0.59
2:B:795:GLU:OE2	3:C:218:LYS:NZ	2.36	0.59
3:C:164:ALA:HB3	3:C:189:PRO:HA	1.84	0.59
3:C:240:LYS:HD3	3:C:265:ALA:H	1.67	0.59
1:A:243:PHE:HB3	1:A:251:ILE:HD11	1.85	0.59
2:B:654:ARG:NH1	2:B:661:GLU:OE1	2.36	0.59
1:A:866:LYS:HD3	1:A:866:LYS:N	2.18	0.59
1:A:937:ASN:HA	1:A:940:VAL:HG22	1.85	0.59
2:B:240:ARG:HD2	2:B:244:THR:HG23	1.85	0.59
11:K:62:SER:OG	11:K:104:ARG:NH1	2.35	0.59
1:A:14:VAL:HG13	1:A:1632:GLU:HB2	1.85	0.58
1:A:654:ASP:HB2	1:A:803:PRO:HB2	1.84	0.58
1:A:1274:GLU:OE2	1:A:1288:ARG:NH2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:676:VAL:HG23	2:B:677:THR:HG22	1.84	0.58
12:L:30:ILE:HD11	12:L:59:ALA:HB2	1.84	0.58
14:N:117:GLU:OE2	14:N:120:LYS:NZ	2.30	0.58
1:A:248:PHE:O	1:A:249:THR:CB	2.51	0.58
1:A:687:PHE:HB3	1:A:691:GLN:HB2	1.85	0.58
6:F:65:ARG:HD3	6:F:66:ARG:HD2	1.86	0.58
6:F:100:GLN:HE21	7:G:54:LEU:HD12	1.67	0.58
1:A:462:LYS:HG3	1:A:463:LYS:H	1.68	0.58
3:C:75:VAL:HG21	3:C:313:ILE:HD11	1.85	0.58
1:A:569:SER:OG	4:D:17:ASN:ND2	2.36	0.58
1:A:117:ARG:NH1	1:A:136:LEU:O	2.34	0.58
2:B:863:ASP:OD2	2:B:870:LYS:NZ	2.29	0.58
1:A:366:ARG:HH22	2:B:1183:LYS:HE2	1.68	0.58
2:B:812:ALA:O	2:B:813:LEU:HB2	2.03	0.58
1:A:1502:PRO:O	1:A:1525:ASN:ND2	2.37	0.58
3:C:271:ARG:NH1	14:N:175:TYR:OH	2.36	0.58
1:A:99:ARG:HD2	1:A:228:LEU:HD23	1.86	0.58
2:B:40:GLU:HB3	2:B:550:ARG:HH22	1.68	0.58
2:B:476:LEU:HD13	2:B:477:ASP:H	1.68	0.58
1:A:884:ARG:NH1	1:A:961:VAL:O	2.37	0.57
14:N:50:GLN:HE22	14:N:52:GLN:HB3	1.69	0.57
1:A:247:GLY:O	1:A:248:PHE:HD2	1.85	0.57
2:B:163:VAL:HG11	2:B:169:ARG:HB2	1.85	0.57
5:E:62:ALA:HB3	5:E:78:LEU:HB3	1.85	0.57
8:H:56:THR:HB	8:H:145:ARG:HB2	1.85	0.57
1:A:1038:ILE:HD11	1:A:1047:GLN:HB2	1.84	0.57
1:A:1047:GLN:NE2	1:A:1587:ASP:OD2	2.37	0.57
1:A:24:ILE:HA	1:A:27:LEU:HD22	1.86	0.57
1:A:843:ARG:NH1	1:A:945:CYS:O	2.37	0.57
3:C:41:GLU:HB3	3:C:57:ILE:HB	1.85	0.57
2:B:1097:ASP:OD1	2:B:1180:PHE:N	2.31	0.57
1:A:444:GLN:NE2	1:A:446:ARG:HD3	2.19	0.57
1:A:708:THR:HG21	1:A:741:PRO:HA	1.84	0.57
1:A:977:MET:HG3	1:A:983:LYS:HG3	1.85	0.57
2:B:292:ILE:HD12	2:B:379:ARG:HH11	1.68	0.57
13:M:368:GLY:C	13:M:397:MET:HE2	2.24	0.57
1:A:247:GLY:O	1:A:248:PHE:CD2	2.58	0.57
1:A:463:LYS:HZ1	1:A:468:ARG:HH22	1.51	0.57
1:A:1130:ALA:HB1	6:F:82:THR:HB	1.87	0.57
3:C:93:GLN:HE21	3:C:96:VAL:HG13	1.69	0.57
1:A:525:ASN:O	1:A:554:ARG:NH1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:105:PRO:HD3	10:J:6:ARG:HD2	1.87	0.57
7:G:108:THR:HG22	7:G:110:ASP:H	1.69	0.57
1:A:250:LYS:O	1:A:250:LYS:HG3	2.04	0.56
3:C:114:THR:OG1	3:C:130:ASN:ND2	2.36	0.56
9:I:30:CYS:SG	9:I:31:SER:N	2.78	0.56
2:B:207:ILE:HD12	2:B:505:ARG:HA	1.87	0.56
2:B:572:PRO:O	2:B:576:THR:OG1	2.23	0.56
1:A:248:PHE:O	1:A:249:THR:OG1	2.21	0.56
1:A:336:GLN:NE2	1:A:348:LYS:O	2.38	0.56
1:A:670:ILE:HD12	1:A:671:GLN:H	1.69	0.56
1:A:700:ILE:HG23	1:A:706:HIS:HB2	1.87	0.56
1:A:709:ARG:H	1:A:709:ARG:HD2	1.71	0.56
1:A:760:TRP:HB2	1:A:764:SER:CB	2.33	0.56
1:A:795:HIS:HE1	1:A:1061:SER:HB2	1.70	0.56
1:A:1298:ASP:OD1	1:A:1298:ASP:N	2.34	0.56
1:A:836:THR:HG23	1:A:917:MET:HA	1.86	0.56
1:A:964:LYS:NZ	2:B:671:TYR:O	2.38	0.56
1:A:1655:ASP:OD1	1:A:1655:ASP:N	2.38	0.56
2:B:310:LEU:HD12	9:I:16:LEU:HD11	1.87	0.56
2:B:70:GLU:HG2	2:B:98:SER:HB2	1.88	0.56
2:B:966:SER:HB3	2:B:1029:GLY:HA3	1.87	0.56
2:B:219:ARG:HG2	2:B:221:SER:H	1.71	0.56
8:H:22:LYS:O	8:H:43:ASN:ND2	2.38	0.56
1:A:1226:VAL:HG12	1:A:1227:MET:HG3	1.88	0.56
2:B:265:ARG:HG3	2:B:474:SER:HA	1.88	0.56
2:B:741:LEU:HB2	2:B:804:TYR:HB2	1.87	0.56
2:B:784:ASP:H	2:B:950:ASN:HD22	1.52	0.56
1:A:1012:LYS:NZ	1:A:1201:THR:O	2.39	0.56
1:A:701:ARG:HG2	1:A:703:GLU:HG3	1.86	0.55
2:B:773:VAL:N	2:B:1029:GLY:O	2.36	0.55
2:B:935:ASP:OD1	3:C:69:ARG:NH1	2.39	0.55
3:C:269:ASP:OD2	3:C:271:ARG:NH1	2.39	0.55
10:J:17:LYS:HD3	10:J:39:LEU:HB3	1.87	0.55
3:C:96:VAL:HA	3:C:99:HIS:CD2	2.41	0.55
1:A:9:SER:HB2	2:B:1176:VAL:HG22	1.89	0.55
1:A:245:LYS:NZ	15:S:60:DC:OP1	2.38	0.55
1:A:248:PHE:HB3	1:A:442:LYS:CG	2.33	0.55
1:A:1236:PRO:HG2	1:A:1523:GLY:HA2	1.87	0.55
2:B:1074:MET:SD	2:B:1074:MET:N	2.79	0.55
1:A:593:PRO:HB3	16:T:21:DG:H1'	1.87	0.55
1:A:1657:LEU:HD13	7:G:104:LEU:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:40:LEU:HD13	8:H:123:MET:HE1	1.88	0.55
2:B:476:LEU:HD12	2:B:478:LEU:HD22	1.88	0.55
12:L:31:CYS:CB	12:L:34:CYS:SG	2.95	0.55
13:M:81:PHE:HE1	14:N:52:GLN:HE21	1.54	0.55
1:A:96:ILE:HG23	1:A:228:LEU:HD21	1.88	0.55
1:A:911:CYS:SG	1:A:912:VAL:N	2.79	0.55
2:B:1157:GLN:NE2	2:B:1171:ASN:OD1	2.39	0.55
2:B:810:ASP:OD1	2:B:811:LEU:N	2.39	0.55
13:M:85:LYS:HE3	13:M:87:SER:HB3	1.87	0.55
1:A:1275:THR:HG22	9:I:46:LYS:HG3	1.89	0.55
1:A:753:ASN:HD22	1:A:754:LYS:H	1.55	0.54
2:B:811:LEU:O	2:B:812:ALA:HB3	2.06	0.54
5:E:151:PRO:HB3	5:E:200:ARG:HB3	1.89	0.54
2:B:210:ARG:HB2	2:B:399:HIS:HB3	1.88	0.54
2:B:550:ARG:HB2	2:B:650:LEU:HB2	1.89	0.54
2:B:772:VAL:HA	2:B:1030:VAL:HG12	1.89	0.54
1:A:472:MET:SD	1:A:1614:SER:OG	2.61	0.54
1:A:1077:LEU:HD13	1:A:1169:LEU:HD12	1.88	0.54
2:B:531:VAL:HG23	2:B:715:ASN:HB3	1.88	0.54
1:A:250:LYS:CG	1:A:314:TYR:HD1	1.94	0.54
1:A:425:ASN:O	1:A:428:VAL:HG12	2.07	0.54
2:B:251:HIS:HE1	2:B:261:ARG:HD3	1.72	0.54
11:K:67:GLU:HA	11:K:99:ASN:HB3	1.89	0.54
3:C:117:ASP:HB3	3:C:120:LEU:HD23	1.90	0.54
14:N:37:ASN:HD22	14:N:38:PHE:N	2.06	0.54
1:A:62:CYS:HB3	1:A:65:CYS:SG	2.44	0.54
1:A:828:CYS:SG	1:A:829:GLY:N	2.80	0.54
1:A:1187:ILE:HG13	2:B:1080:ILE:HG23	1.88	0.54
9:I:28:VAL:H	9:I:38:PRO:HD3	1.73	0.54
2:B:1043:LYS:O	2:B:1063:ARG:NH2	2.40	0.54
8:H:38:LEU:HD21	8:H:40:LEU:HD23	1.90	0.54
1:A:249:THR:CG2	1:A:435:ASN:HD22	2.20	0.54
1:A:325:ASP:OD2	1:A:329:ARG:NH1	2.40	0.54
1:A:827:THR:HA	2:B:951:PRO:HG2	1.90	0.54
3:C:39:ASP:O	3:C:58:ASN:ND2	2.41	0.54
13:M:201:ILE:HD11	13:M:401:PHE:HB2	1.89	0.54
2:B:249:VAL:HG22	2:B:261:ARG:HG2	1.90	0.53
13:M:16:GLN:HE21	13:M:92:LYS:H	1.56	0.53
1:A:1643:VAL:HG23	1:A:1644:GLY:H	1.73	0.53
2:B:623:ASP:HA	2:B:663:ILE:HD11	1.89	0.53
8:H:98:TYR:CE1	8:H:139:ASN:OD1	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:253:PRO:O	13:M:256:MET:HG2	2.07	0.53
1:A:196:ALA:HA	1:A:201:ARG:HH21	1.74	0.53
2:B:720:GLN:O	2:B:724:GLN:HB2	2.08	0.53
1:A:59:ARG:HH11	13:M:322:PRO:HD3	1.72	0.53
1:A:759:TYR:O	8:H:19:ARG:NH2	2.34	0.53
1:A:1097:TYR:HD2	1:A:1123:VAL:HG12	1.73	0.53
2:B:161:LEU:HD22	2:B:162:PRO:HD2	1.91	0.53
2:B:277:LEU:HD23	2:B:374:LEU:HD12	1.91	0.53
10:J:14:VAL:HB	10:J:50:ILE:HD11	1.90	0.53
1:A:58:LEU:O	1:A:59:ARG:HG3	2.09	0.53
1:A:640:ASN:HD21	2:B:1094:ASN:HD22	1.56	0.53
1:A:1111:GLU:HG2	1:A:1112:PRO:HD2	1.91	0.53
2:B:585:CYS:HA	2:B:595:TRP:HB3	1.90	0.53
3:C:65:ASN:HD22	3:C:68:ARG:HH21	1.55	0.53
1:A:585:ASP:HA	1:A:644:ARG:HH21	1.73	0.53
2:B:492:ASN:HB3	2:B:495:ARG:HG3	1.89	0.53
7:G:139:ILE:O	7:G:146:GLY:N	2.42	0.53
1:A:435:ASN:HA	1:A:438:ILE:HG22	1.91	0.53
1:A:998:HIS:CE1	2:B:712:SER:H	2.27	0.53
1:A:1024:THR:O	1:A:1028:GLU:HB2	2.08	0.53
7:G:107:ILE:HA	7:G:114:GLY:HA2	1.89	0.53
9:I:13:CYS:HB2	9:I:32:GLN:HE21	1.74	0.53
1:A:671:GLN:HG2	1:A:934:LYS:HB2	1.90	0.53
1:A:720:PHE:HB2	8:H:96:VAL:HB	1.91	0.53
1:A:1237:GLN:HE22	1:A:1520:VAL:HB	1.74	0.53
1:A:1531:ASP:OD1	1:A:1532:GLN:NE2	2.42	0.53
13:M:215:PHE:HD2	13:M:293:ILE:HG21	1.74	0.53
2:B:44:PRO:HG3	2:B:551:ILE:HB	1.91	0.52
5:E:198:ILE:HD11	5:E:210:SER:HB3	1.91	0.52
7:G:158:LYS:H	7:G:161:ASN:HD21	1.57	0.52
8:H:118:PHE:HD2	8:H:121:LEU:HB3	1.73	0.52
2:B:555:GLN:HG3	2:B:645:GLY:HA2	1.90	0.52
3:C:240:LYS:HA	3:C:244:ALA:HB2	1.91	0.52
2:B:300:SER:HB2	9:I:49:THR:HG22	1.92	0.52
2:B:1006:ASN:HB3	3:C:276:SER:HB2	1.90	0.52
1:A:748:ASN:HD21	1:A:773:ASP:H	1.57	0.52
2:B:480:GLN:O	2:B:484:TYR:OH	2.27	0.52
7:G:147:LEU:HB2	7:G:155:ALA:HB3	1.90	0.52
2:B:791:LYS:HE3	2:B:932:PRO:HB3	1.92	0.52
3:C:324:LYS:HG2	11:K:72:LEU:HD21	1.92	0.52
1:A:763:GLY:HA2	1:A:765:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:52:VAL:HG11	14:N:26:PRO:HD2	1.91	0.52
2:B:597:SER:HB3	2:B:600:GLN:HG2	1.92	0.52
2:B:1195:ARG:HH22	2:B:1197:ARG:HE	1.58	0.52
1:A:344:ASN:HD21	1:A:348:LYS:H	1.58	0.52
1:A:590:ASN:ND2	2:B:1075:GLU:OE1	2.43	0.52
1:A:1510:PRO:HG3	1:A:1520:VAL:HG13	1.92	0.52
2:B:501:ARG:HG3	2:B:544:HIS:HB2	1.92	0.52
2:B:677:THR:OG1	2:B:679:GLN:OE1	2.20	0.52
3:C:87:ASN:OD1	3:C:203:SER:OG	2.21	0.52
3:C:294:VAL:HG12	3:C:296:ASN:H	1.75	0.52
8:H:33:GLN:HE22	8:H:35:GLN:HB3	1.75	0.52
1:A:461:GLU:HB3	1:A:464:GLU:HA	1.91	0.52
1:A:1563:VAL:O	1:A:1567:ASN:HB2	2.09	0.52
1:A:1616:GLU:HG2	16:T:18:DC:H5''	1.92	0.52
2:B:16:PHE:HD1	2:B:978:ALA:HB2	1.75	0.52
1:A:87:ASN:O	1:A:91:PHE:N	2.39	0.51
1:A:123:ARG:NH2	1:A:333:CYS:O	2.43	0.51
1:A:753:ASN:ND2	1:A:754:LYS:H	2.08	0.51
5:E:42:PHE:O	5:E:46:TYR:HB3	2.09	0.51
1:A:139:ILE:HG21	1:A:184:LYS:HD3	1.91	0.51
1:A:332:GLN:HE21	1:A:336:GLN:HG2	1.75	0.51
2:B:1114:GLN:HE21	2:B:1129:ARG:CZ	2.23	0.51
7:G:27:PRO:O	7:G:35:SER:OG	2.25	0.51
1:A:370:PRO:HB3	1:A:379:GLU:HA	1.92	0.51
3:C:246:ARG:HA	3:C:249:LYS:HE2	1.92	0.51
1:A:943:ILE:HD11	2:B:960:ILE:HG21	1.93	0.51
3:C:68:ARG:HB2	3:C:227:TYR:CE2	2.45	0.51
3:C:78:VAL:HG22	3:C:210:LEU:HG	1.92	0.51
13:M:218:VAL:HA	13:M:221:ILE:HD13	1.92	0.51
1:A:1260:LYS:HB3	1:A:1505:ASP:HA	1.93	0.51
2:B:586:VAL:HG13	2:B:640:LEU:HD12	1.92	0.51
15:S:65:DG:H2''	15:S:66:DA:C8	2.46	0.51
2:B:219:ARG:NH1	15:S:52:DA:OP1	2.39	0.51
3:C:77:SER:HB2	3:C:221:PRO:HD3	1.93	0.51
5:E:17:ARG:NH1	5:E:35:VAL:O	2.44	0.51
10:J:41:LEU:O	10:J:47:ARG:NE	2.43	0.51
13:M:14:SER:HB3	13:M:89:GLN:HB2	1.92	0.51
1:A:470:HIS:HB3	2:B:1181:VAL:HG11	1.92	0.51
1:A:582:LYS:HD2	1:A:584:ARG:HH21	1.76	0.51
3:C:73:SER:OG	3:C:74:GLU:OE1	2.29	0.51
7:G:15:ARG:HH21	7:G:18:LYS:HD2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:31:CYS:SG	12:L:32:ALA:N	2.83	0.51
2:B:495:ARG:HG2	2:B:723:LYS:HG2	1.93	0.51
2:B:679:GLN:HE21	14:N:157:ARG:HB2	1.76	0.51
2:B:790:ASN:HD22	2:B:791:LYS:N	2.08	0.51
2:B:810:ASP:C	2:B:811:LEU:HD12	2.31	0.51
1:A:550:SER:OG	1:A:553:GLN:OE1	2.24	0.50
1:A:1498:ILE:HG23	1:A:1499:ARG:HD3	1.94	0.50
14:N:158:LYS:H	14:N:158:LYS:HD3	1.75	0.50
3:C:322:LYS:HE2	11:K:125:MET:HG3	1.93	0.50
1:A:1197:SER:HA	1:A:1200:MET:HG2	1.92	0.50
3:C:94:ASP:OD1	3:C:95:GLU:N	2.44	0.50
10:J:48:ARG:O	10:J:52:THR:OG1	2.19	0.50
1:A:700:ILE:O	1:A:706:HIS:ND1	2.45	0.50
1:A:964:LYS:HE2	1:A:971:PRO:HB3	1.92	0.50
1:A:1088:HIS:HB3	1:A:1089:LEU:HD22	1.93	0.50
1:A:1121:ASP:OD1	1:A:1121:ASP:N	2.45	0.50
2:B:711:GLN:HB3	2:B:713:PRO:HD2	1.92	0.50
8:H:118:PHE:HZ	8:H:142:LEU:HD22	1.77	0.50
1:A:719:ILE:HD12	1:A:725:LEU:HD23	1.93	0.50
5:E:4:GLU:O	5:E:8:ASN:ND2	2.45	0.50
1:A:729:LYS:NZ	1:A:779:GLY:O	2.31	0.50
1:A:1646:LEU:HD11	7:G:109:PRO:HB2	1.93	0.50
13:M:376:VAL:O	13:M:386:LYS:NZ	2.44	0.50
3:C:188:ASP:OD1	3:C:188:ASP:N	2.45	0.50
1:A:512:THR:HG22	1:A:513:ALA:H	1.77	0.49
1:A:611:GLU:HB2	1:A:615:ARG:HH12	1.77	0.49
2:B:372:ARG:HH12	2:B:594:GLY:HA2	1.78	0.49
2:B:491:ILE:HG23	2:B:495:ARG:HD3	1.95	0.49
9:I:60:LEU:HD23	9:I:60:LEU:H	1.77	0.49
1:A:73:PRO:O	1:A:366:ARG:NH2	2.45	0.49
2:B:811:LEU:N	2:B:811:LEU:CD1	2.74	0.49
1:A:988:SER:HB2	2:B:988:GLU:HA	1.95	0.49
5:E:86:PRO:HA	5:E:113:GLN:HE21	1.77	0.49
13:M:306:LYS:O	13:M:317:SER:OG	2.31	0.49
1:A:953:GLU:OE1	1:A:1203:ASN:ND2	2.44	0.49
2:B:963:PHE:O	2:B:1027:TYR:OH	2.30	0.49
11:K:89:CYS:SG	11:K:90:GLY:N	2.86	0.49
1:A:581:ILE:HD11	1:A:605:VAL:HG21	1.95	0.49
1:A:1626:VAL:HG11	2:B:1194:ILE:HG13	1.94	0.49
2:B:750:PRO:HA	2:B:770:ASN:HD21	1.76	0.49
5:E:110:PHE:HB2	5:E:134:THR:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:67:ASP:HB2	13:M:71:GLN:HB2	1.94	0.49
1:A:513:ALA:HA	1:A:516:ILE:HG23	1.95	0.49
1:A:763:GLY:HA3	8:H:25:ARG:NH1	2.28	0.49
1:A:947:LEU:HD21	1:A:982:VAL:HG11	1.94	0.49
1:A:1072:ASN:HB3	1:A:1075:ALA:HB3	1.94	0.49
2:B:246:GLN:NE2	2:B:356:ARG:O	2.45	0.49
2:B:939:SER:O	3:C:226:SER:OG	2.19	0.49
2:B:1006:ASN:ND2	2:B:1010:ASN:O	2.38	0.49
5:E:80:VAL:HA	5:E:109:ILE:HB	1.95	0.49
1:A:111:LYS:H	1:A:111:LYS:HD2	1.78	0.49
1:A:336:GLN:O	1:A:340:HIS:ND1	2.45	0.49
2:B:404:LEU:HD11	2:B:551:ILE:HG21	1.95	0.49
2:B:939:SER:OG	2:B:1011:GLU:OE2	2.29	0.49
7:G:162:ILE:HG22	7:G:249:LEU:HD12	1.95	0.49
13:M:322:PRO:HA	13:M:325:GLU:HB2	1.95	0.49
1:A:1510:PRO:HD3	1:A:1520:VAL:HG22	1.94	0.49
2:B:565:LEU:HD21	2:B:586:VAL:HG11	1.93	0.49
2:B:567:SER:HB2	14:N:59:PRO:HB3	1.95	0.49
12:L:31:CYS:HB3	12:L:34:CYS:SG	2.53	0.49
13:M:241:LYS:HG3	13:M:244:ALA:HB3	1.95	0.49
1:A:57:PHE:O	1:A:60:ASN:ND2	2.46	0.48
1:A:911:CYS:O	1:A:915:GLY:N	2.27	0.48
2:B:282:HIS:HA	2:B:323:ARG:NE	2.28	0.48
2:B:476:LEU:HD13	2:B:477:ASP:N	2.28	0.48
2:B:713:PRO:O	2:B:717:TYR:HB2	2.13	0.48
7:G:234:ARG:HB2	7:G:248:THR:HG23	1.95	0.48
1:A:440:SER:H	1:A:457:LYS:HZ1	1.61	0.48
1:A:770:LEU:HD23	1:A:777:LEU:HD12	1.95	0.48
1:A:827:THR:HG21	2:B:1026:ILE:HA	1.94	0.48
1:A:495:ILE:HB	1:A:605:VAL:HG12	1.95	0.48
2:B:52:LEU:HA	2:B:60:LEU:H	1.77	0.48
5:E:22:MET:O	5:E:26:ARG:HB2	2.12	0.48
2:B:1064:LYS:C	2:B:1066:HIS:H	2.16	0.48
3:C:124:GLU:N	3:C:124:GLU:OE1	2.46	0.48
1:A:866:LYS:N	1:A:866:LYS:CD	2.76	0.48
1:A:1549:VAL:O	1:A:1553:TYR:HB2	2.13	0.48
2:B:499:HIS:HA	2:B:502:MET:HG2	1.94	0.48
1:A:51:ASP:OD1	1:A:52:LEU:N	2.46	0.48
1:A:226:LYS:HG3	1:A:227:LEU:H	1.79	0.48
1:A:947:LEU:HD23	1:A:947:LEU:H	1.77	0.48
2:B:195:ILE:HG22	2:B:200:GLU:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:321:GLN:NE2	13:M:104:SER:OG	2.42	0.48
2:B:545:PHE:HB3	2:B:549:CYS:SG	2.54	0.48
2:B:609:ARG:HH12	2:B:668:GLU:HG3	1.78	0.48
3:C:240:LYS:HD3	3:C:264:GLU:HA	1.95	0.48
1:A:316:LEU:H	1:A:316:LEU:HD23	1.79	0.48
1:A:462:LYS:HG2	1:A:466:LEU:HD23	1.96	0.48
2:B:748:GLN:HB3	10:J:52:THR:HG22	1.96	0.48
2:B:1064:LYS:HB2	2:B:1065:ARG:NH1	2.28	0.48
2:B:1099:THR:HG22	2:B:1178:ILE:O	2.13	0.48
1:A:959:VAL:HG12	1:A:965:THR:HG22	1.95	0.48
1:A:1501:ILE:HG23	1:A:1504:ILE:HG23	1.96	0.48
2:B:570:VAL:HA	2:B:596:VAL:HG11	1.96	0.48
1:A:435:ASN:HB2	1:A:442:LYS:HE2	1.96	0.48
1:A:1049:MET:HG2	1:A:1054:ALA:HB2	1.95	0.48
2:B:1039:MET:HG3	2:B:1043:LYS:HG2	1.96	0.48
1:A:483:VAL:HA	1:A:632:GLU:HB3	1.96	0.48
2:B:320:LEU:HG	2:B:326:VAL:HG22	1.95	0.48
13:M:213:LEU:HD12	13:M:216:ILE:HD12	1.96	0.48
4:D:91:ARG:HB3	7:G:151:ASP:OD1	2.14	0.47
9:I:61:ARG:HH21	9:I:64:LYS:HD3	1.79	0.47
1:A:484:ILE:HB	1:A:616:LEU:HD23	1.96	0.47
2:B:810:ASP:O	2:B:811:LEU:HD12	2.13	0.47
13:M:347:THR:OG1	13:M:348:PRO:HD3	2.14	0.47
1:A:691:GLN:O	1:A:695:TYR:HB2	2.15	0.47
9:I:13:CYS:SG	13:M:59:ARG:NH2	2.83	0.47
2:B:253:LEU:HD12	2:B:257:GLN:HB2	1.96	0.47
5:E:159:ASP:OD1	5:E:159:ASP:N	2.43	0.47
7:G:69:LEU:HD22	7:G:72:LYS:HE3	1.95	0.47
1:A:720:PHE:HE1	8:H:98:TYR:HB2	1.79	0.47
1:A:1056:ASP:OD1	1:A:1057:ILE:N	2.47	0.47
1:A:1619:CYS:O	1:A:1623:THR:HG23	2.15	0.47
5:E:27:GLY:O	5:E:68:SER:OG	2.23	0.47
13:M:32:ALA:HB1	14:N:121:ILE:HG21	1.97	0.47
1:A:256:LEU:HD22	1:A:260:GLN:HG2	1.95	0.47
1:A:621:THR:OG1	1:A:626:ALA:O	2.31	0.47
2:B:288:ILE:O	2:B:292:ILE:HG12	2.15	0.47
3:C:190:ASP:HB2	10:J:16:ASP:HB2	1.96	0.47
7:G:56:ASN:ND2	7:G:59:GLN:OE1	2.47	0.47
1:A:361:VAL:HG23	2:B:1191:ALA:HA	1.96	0.47
1:A:527:PRO:HA	1:A:580:HIS:CE1	2.50	0.47
1:A:709:ARG:HG2	1:A:710:SER:N	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1326:GLU:HA	1:A:1329:ILE:HG22	1.95	0.47
2:B:251:HIS:CE1	2:B:261:ARG:HD3	2.49	0.47
4:D:24:ALA:HA	7:G:43:ILE:HG22	1.97	0.47
5:E:46:TYR:CE1	5:E:58:MET:HG3	2.49	0.47
13:M:67:ASP:HB2	13:M:71:GLN:HE21	1.79	0.47
13:M:321:ASP:OD1	13:M:324:ASN:ND2	2.47	0.47
1:A:184:LYS:NZ	1:A:185:ARG:HE	2.13	0.47
1:A:1025:LYS:HD2	1:A:1615:TYR:CG	2.50	0.47
8:H:107:VAL:HG12	8:H:108:SER:H	1.80	0.47
13:M:312:ARG:NH1	13:M:317:SER:OG	2.40	0.47
1:A:6:PRO:HB3	7:G:111:THR:HG21	1.96	0.47
1:A:843:ARG:O	1:A:847:LEU:HB2	2.15	0.47
5:E:163:GLU:O	5:E:167:ARG:HB2	2.15	0.47
8:H:136:LYS:H	8:H:136:LYS:HD2	1.79	0.47
1:A:248:PHE:CD1	1:A:442:LYS:HB2	2.50	0.47
1:A:1162:ASN:OD1	1:A:1165:LYS:NZ	2.40	0.47
3:C:145:ASP:OD1	3:C:146:ALA:N	2.46	0.47
1:A:450:LYS:O	1:A:451:VAL:HB	2.15	0.46
1:A:466:LEU:HD22	1:A:469:LYS:HB3	1.97	0.46
1:A:797:LEU:HA	1:A:800:VAL:HG22	1.97	0.46
2:B:91:LEU:HD23	2:B:91:LEU:H	1.79	0.46
2:B:201:LYS:HE3	2:B:465:LEU:HB3	1.97	0.46
2:B:718:GLN:HA	2:B:721:MET:HG2	1.97	0.46
1:A:669:LEU:HD22	1:A:673:HIS:CG	2.51	0.46
2:B:72:VAL:HG12	2:B:96:SER:HA	1.96	0.46
6:F:65:ARG:HH22	7:G:117:TRP:HZ3	1.64	0.46
9:I:39:LYS:H	9:I:39:LYS:HD3	1.81	0.46
1:A:827:THR:HG21	2:B:1026:ILE:HG22	1.98	0.46
1:A:1443:GLN:HE22	1:A:1462:PHE:H	1.63	0.46
1:A:1490:GLU:OE2	1:A:1494:ARG:NH2	2.49	0.46
2:B:321:GLN:HG3	9:I:32:GLN:HB3	1.96	0.46
7:G:139:ILE:H	7:G:146:GLY:HA3	1.81	0.46
1:A:835:LEU:HD11	1:A:840:ASN:HB3	1.97	0.46
2:B:65:VAL:HA	2:B:68:ILE:HB	1.96	0.46
8:H:93:TYR:HD2	8:H:143:LEU:HB3	1.81	0.46
1:A:54:LEU:H	1:A:54:LEU:HD23	1.80	0.46
1:A:1006:LEU:HA	1:A:1009:THR:HB	1.98	0.46
2:B:787:MET:N	2:B:926:VAL:O	2.46	0.46
3:C:162:VAL:HG22	3:C:193:LEU:HD12	1.98	0.46
15:S:60:DC:H2''	15:S:61:DA:C8	2.51	0.46
1:A:603:HIS:CE1	1:A:653:THR:HB	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:ILE:HD12	2:B:518:ARG:HB3	1.97	0.46
1:A:1657:LEU:HD11	6:F:135:ARG:HE	1.80	0.46
2:B:209:GLN:HE22	2:B:237:ARG:HB2	1.80	0.46
1:A:1112:PRO:HG2	1:A:1114:TYR:CE2	2.51	0.46
2:B:866:LEU:HD12	13:M:354:ASN:HB3	1.98	0.46
2:B:934:ILE:HG13	3:C:69:ARG:HD3	1.97	0.46
3:C:40:PHE:HD2	11:K:134:LYS:HD2	1.81	0.46
3:C:247:PHE:HB2	3:C:285:PHE:HE2	1.81	0.46
13:M:268:LEU:HD21	13:M:332:ILE:HD13	1.98	0.46
1:A:534:THR:HG23	1:A:580:HIS:CD2	2.50	0.46
1:A:866:LYS:O	1:A:867:ASP:HB2	2.16	0.46
2:B:47:GLY:HA3	2:B:553:THR:HG21	1.98	0.46
1:A:57:PHE:HB2	1:A:365:THR:HG21	1.98	0.45
1:A:1326:GLU:HG3	1:A:1454:HIS:HD2	1.81	0.45
10:J:43:ARG:O	10:J:47:ARG:HG2	2.15	0.45
11:K:66:VAL:HG12	11:K:100:LEU:HD13	1.98	0.45
1:A:480:ALA:HB3	1:A:635:MET:HB3	1.98	0.45
1:A:596:HIS:HB2	1:A:1191:GLN:HE21	1.81	0.45
1:A:1568:ASN:O	1:A:1572:ARG:HG2	2.16	0.45
2:B:571:ALA:HA	14:N:57:LYS:HE2	1.99	0.45
2:B:718:GLN:HB2	2:B:922:GLY:HA2	1.99	0.45
10:J:2:ILE:H	10:J:2:ILE:HG13	1.65	0.45
14:N:86:ASP:OD1	14:N:86:ASP:N	2.49	0.45
14:N:147:ALA:C	14:N:148:ILE:HG13	2.36	0.45
1:A:363:PRO:O	1:A:368:ARG:NE	2.48	0.45
1:A:688:THR:HG22	1:A:691:GLN:HG2	1.97	0.45
1:A:1224:GLU:O	1:A:1228:THR:OG1	2.29	0.45
1:A:1659:LYS:HA	7:G:103:LYS:O	2.17	0.45
2:B:71:LYS:HD3	2:B:421:LEU:HD12	1.98	0.45
2:B:372:ARG:HH22	2:B:594:GLY:HA2	1.81	0.45
2:B:598:HIS:CE1	2:B:631:PRO:HD3	2.51	0.45
2:B:1112:THR:O	2:B:1129:ARG:HG2	2.17	0.45
8:H:5:LEU:O	8:H:133:ASN:ND2	2.49	0.45
12:L:53:HIS:HE1	12:L:55:ILE:HB	1.82	0.45
13:M:212:GLU:HB3	13:M:294:LEU:HD23	1.99	0.45
1:A:1459:LYS:HB2	1:A:1473:LYS:HB3	1.99	0.45
1:A:30:LYS:HB2	1:A:30:LYS:HZ2	1.81	0.45
1:A:1167:ARG:HA	1:A:1170:MET:HE2	1.98	0.45
1:A:1238:MET:HA	1:A:1543:SER:HA	1.98	0.45
2:B:426:ALA:HA	2:B:429:ARG:HG2	1.99	0.45
3:C:123:ASP:OD1	3:C:123:ASP:N	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PHE:N	1:A:331:GLU:OE2	2.50	0.45
1:A:817:PHE:HA	1:A:820:TYR:HB3	1.98	0.45
1:A:335:LEU:HA	1:A:338:VAL:HG12	1.98	0.45
1:A:588:LEU:HD22	1:A:589:MET:H	1.81	0.45
1:A:1248:ASP:OD1	1:A:1517:ARG:NH2	2.50	0.45
1:A:1437:ASN:ND2	1:A:1438:ASN:H	2.15	0.45
5:E:199:ILE:HG22	5:E:209:ALA:HB2	1.99	0.45
11:K:55:SER:OG	11:K:59:THR:N	2.49	0.45
1:A:749:LEU:H	1:A:771:PHE:HB2	1.81	0.45
1:A:827:THR:HB	2:B:776:ILE:HD12	1.99	0.45
1:A:1046:VAL:HG22	1:A:1591:ARG:HH21	1.82	0.45
2:B:770:ASN:HD22	10:J:52:THR:HG21	1.81	0.45
2:B:790:ASN:HB2	2:B:946:ASP:HA	1.99	0.45
2:B:810:ASP:C	2:B:811:LEU:CD1	2.85	0.45
5:E:14:ARG:HB3	5:E:141:VAL:O	2.17	0.45
5:E:106:GLN:OE1	5:E:107:THR:OG1	2.30	0.45
1:A:263:ASN:HA	1:A:266:VAL:HG12	1.99	0.45
1:A:1006:LEU:HD23	1:A:1006:LEU:H	1.82	0.45
1:A:1090:ASP:OD1	1:A:1091:VAL:N	2.50	0.45
2:B:874:TYR:CE2	2:B:876:SER:HB3	2.52	0.45
6:F:101:ILE:HA	6:F:105:ALA:HB3	1.99	0.45
1:A:175:SER:HA	1:A:178:LEU:HD23	1.99	0.45
1:A:226:LYS:HD2	1:A:226:LYS:HA	1.75	0.45
1:A:749:LEU:HB2	1:A:771:PHE:CD2	2.52	0.45
2:B:800:TYR:OH	3:C:95:GLU:OE1	2.22	0.45
2:B:889:GLY:HA3	2:B:898:LEU:HD22	1.99	0.45
5:E:5:ASN:HA	5:E:8:ASN:HD21	1.82	0.45
13:M:81:PHE:O	14:N:51:GLN:HA	2.17	0.45
1:A:485:SER:O	1:A:616:LEU:N	2.48	0.44
1:A:670:ILE:HD12	1:A:671:GLN:N	2.33	0.44
1:A:1538:VAL:HG11	5:E:142:VAL:HG11	1.99	0.44
1:A:1657:LEU:HD11	6:F:135:ARG:NE	2.32	0.44
1:A:712:ILE:HG22	1:A:738:ASN:HB3	1.99	0.44
1:A:753:ASN:HB3	1:A:755:ILE:HG13	1.98	0.44
1:A:1457:ILE:HA	1:A:1474:LEU:HG	1.98	0.44
3:C:69:ARG:NH1	11:K:70:HIS:HB2	2.31	0.44
1:A:79:ILE:HD12	1:A:390:LEU:HD22	1.99	0.44
1:A:673:HIS:CD2	1:A:817:PHE:HB2	2.52	0.44
4:D:14:THR:HG23	4:D:16:LEU:H	1.81	0.44
5:E:79:TRP:NE1	5:E:81:GLU:HB2	2.33	0.44
7:G:47:VAL:HG11	7:G:61:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:56:THR:HG21	8:H:145:ARG:HD2	2.00	0.44
1:A:184:LYS:HA	1:A:187:GLU:HG2	1.99	0.44
1:A:500:VAL:HG21	1:A:612:LYS:HD2	2.00	0.44
1:A:986:PHE:HE1	1:A:990:ILE:HD13	1.83	0.44
1:A:1004:GLU:HA	1:A:1007:ILE:HB	1.99	0.44
1:A:1076:LEU:HD11	1:A:1169:LEU:HD21	1.99	0.44
2:B:234:ILE:HG12	2:B:381:LEU:HB2	2.00	0.44
2:B:566:TYR:HA	2:B:570:VAL:HB	1.99	0.44
11:K:76:LEU:HA	11:K:79:VAL:HG12	1.99	0.44
14:N:170:HIS:CG	14:N:171:PHE:H	2.35	0.44
3:C:54:PHE:HE2	3:C:56:LEU:HD12	1.82	0.44
15:S:62:DG:H2"	15:S:63:DT:C6	2.52	0.44
1:A:699:CYS:SG	1:A:816:LEU:HA	2.57	0.44
1:A:1034:TYR:HA	1:A:1181:PRO:HB2	2.00	0.44
1:A:1088:HIS:NE2	6:F:83:PRO:HB2	2.32	0.44
1:A:1250:GLN:O	1:A:1253:THR:OG1	2.31	0.44
3:C:198:PRO:O	10:J:64:ASN:ND2	2.50	0.44
12:L:31:CYS:HB2	12:L:48:CYS:SG	2.57	0.44
13:M:65:TYR:OH	13:M:99:LYS:NZ	2.47	0.44
13:M:236:TYR:OH	13:M:273:GLU:OE1	2.35	0.44
14:N:37:ASN:HD22	14:N:38:PHE:H	1.65	0.44
1:A:579:ARG:CZ	1:A:582:LYS:HD3	2.47	0.44
2:B:211:ARG:HH12	2:B:646:HIS:HB2	1.82	0.44
3:C:127:THR:OG1	3:C:130:ASN:OD1	2.35	0.44
7:G:226:ASP:OD1	7:G:227:GLY:N	2.45	0.44
13:M:57:ASN:HD22	13:M:60:LEU:HD22	1.81	0.44
1:A:12:THR:HA	1:A:1634:LEU:HD11	1.98	0.44
1:A:123:ARG:O	1:A:126:GLN:NE2	2.45	0.44
1:A:748:ASN:ND2	1:A:773:ASP:H	2.15	0.44
2:B:614:GLU:HG3	2:B:616:LYS:HG2	1.99	0.44
8:H:98:TYR:CZ	8:H:139:ASN:OD1	2.70	0.44
8:H:100:THR:HG22	8:H:138:GLU:HA	2.00	0.44
13:M:20:SER:OG	13:M:91:TYR:OH	2.24	0.44
1:A:991:LYS:HE2	1:A:994:GLU:HG2	1.99	0.44
4:D:30:HIS:HA	7:G:39:VAL:HG23	2.00	0.44
1:A:217:LYS:HA	1:A:220:VAL:HG12	2.00	0.43
1:A:460:LEU:O	1:A:466:LEU:HB3	2.18	0.43
1:A:608:LEU:HB2	1:A:610:ASN:HD22	1.82	0.43
1:A:1292:ILE:O	1:A:1471:GLU:HA	2.16	0.43
5:E:161:LYS:NZ	5:E:193:GLY:O	2.41	0.43
8:H:133:ASN:OD1	8:H:134:ASN:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:SER:OG	1:A:29:ALA:N	2.51	0.43
1:A:118:TYR:HE2	1:A:226:LYS:HE2	1.83	0.43
1:A:138:GLU:H	1:A:138:GLU:HG3	1.59	0.43
1:A:942:GLN:HG2	1:A:947:LEU:HA	2.00	0.43
1:A:1045:LEU:H	1:A:1045:LEU:HD23	1.83	0.43
2:B:1065:ARG:O	2:B:1066:HIS:HB3	2.18	0.43
3:C:69:ARG:HD2	11:K:71:THR:HG23	1.99	0.43
8:H:80:ARG:HD2	8:H:81:PRO:HD2	1.99	0.43
16:T:21:DG:OP2	16:T:21:DG:H3'	2.17	0.43
1:A:34:ASN:HA	1:A:35:PRO:HD3	1.92	0.43
1:A:701:ARG:NH1	11:K:93:ILE:O	2.50	0.43
1:A:885:ASP:N	1:A:885:ASP:OD1	2.51	0.43
1:A:887:ASN:OD1	1:A:888:LYS:N	2.52	0.43
2:B:133:TYR:HB2	2:B:195:ILE:HD11	2.00	0.43
2:B:260:PHE:CE1	2:B:273:VAL:HG12	2.54	0.43
2:B:402:VAL:N	2:B:647:SER:OG	2.51	0.43
5:E:114:ASN:OD1	5:E:115:ASN:N	2.49	0.43
5:E:147:HIS:HB3	5:E:150:VAL:HG22	1.99	0.43
13:M:79:GLY:O	14:N:53:VAL:HA	2.18	0.43
2:B:625:GLU:HB2	2:B:648:ARG:HH11	1.83	0.43
5:E:88:VAL:HB	5:E:116:ILE:HG23	2.00	0.43
5:E:175:LEU:HB2	5:E:213:ILE:HD13	2.00	0.43
5:E:191:LYS:H	5:E:191:LYS:HD2	1.82	0.43
1:A:747:ILE:H	1:A:747:ILE:HG13	1.66	0.43
2:B:204:ARG:HH22	2:B:504:HIS:CG	2.36	0.43
3:C:216:HIS:CE1	12:L:70:ARG:HE	2.37	0.43
7:G:62:MET:HA	7:G:66:LEU:HB3	2.01	0.43
8:H:16:ASP:OD1	8:H:16:ASP:N	2.51	0.43
1:A:442:LYS:HE3	1:A:442:LYS:HB3	1.78	0.43
2:B:76:GLY:H	2:B:432:ILE:HD11	1.84	0.43
2:B:656:LEU:HB2	2:B:657:PRO:HD3	2.00	0.43
2:B:1064:LYS:C	2:B:1066:HIS:N	2.71	0.43
13:M:230:LYS:HD2	13:M:247:LEU:HD21	1.99	0.43
1:A:446:ARG:HG3	1:A:447:THR:H	1.83	0.43
1:A:527:PRO:HA	1:A:580:HIS:HE1	1.82	0.43
1:A:568:VAL:HA	1:A:571:HIS:HB2	2.00	0.43
1:A:947:LEU:HD11	1:A:982:VAL:HG21	2.01	0.43
2:B:317:TYR:HD1	2:B:320:LEU:HB2	1.83	0.43
2:B:711:GLN:HB2	2:B:714:ARG:HG2	2.00	0.43
5:E:23:VAL:HG13	5:E:30:ILE:HG13	2.01	0.43
7:G:34:THR:HG21	7:G:134:GLU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:270:GLY:O	13:M:286:ARG:NH2	2.49	0.43
14:N:111:VAL:O	14:N:120:LYS:HB2	2.18	0.43
1:A:324:LEU:HA	1:A:327:VAL:HG22	2.01	0.43
2:B:325:GLN:HG2	13:M:107:ASN:HD21	1.84	0.43
2:B:560:ARG:HH22	2:B:618:PRO:HG2	1.83	0.43
2:B:1099:THR:HB	2:B:1180:PHE:CZ	2.54	0.43
1:A:757:ASN:CB	1:A:764:SER:HB2	2.45	0.43
1:A:935:GLY:HA2	1:A:939:ASN:HD22	1.83	0.43
2:B:218:ILE:HG23	2:B:231:HIS:HD2	1.83	0.43
2:B:555:GLN:OE1	2:B:646:HIS:N	2.51	0.43
2:B:990:ASP:HB3	14:N:159:ASP:HB3	2.01	0.43
1:A:1600:ARG:HB2	1:A:1621:PHE:HZ	1.83	0.43
1:A:1659:LYS:HG3	6:F:133:VAL:HG21	2.01	0.43
5:E:46:TYR:CE1	5:E:54:GLN:HG2	2.54	0.43
15:S:69:DA:H5'	15:S:69:DA:C8	2.54	0.43
2:B:1047:ARG:HD2	2:B:1066:HIS:O	2.19	0.42
3:C:195:LYS:HB2	10:J:61:LEU:HD11	2.01	0.42
13:M:318:TYR:HE2	13:M:320:ILE:HD11	1.84	0.42
14:N:50:GLN:NE2	14:N:52:GLN:HB3	2.34	0.42
1:A:14:VAL:HG11	1:A:1610:PHE:HE2	1.84	0.42
1:A:181:LEU:O	1:A:185:ARG:HG2	2.18	0.42
1:A:658:LEU:HD12	1:A:1058:THR:HA	2.00	0.42
1:A:985:ARG:NH2	1:A:986:PHE:HB2	2.34	0.42
1:A:1108:HIS:NE2	1:A:1111:GLU:O	2.50	0.42
1:A:481:ARG:HD3	2:B:1045:GLN:NE2	2.34	0.42
1:A:1559:ARG:HG2	1:A:1586:ALA:HB1	2.02	0.42
1:A:1612:LYS:HG2	1:A:1621:PHE:CD2	2.55	0.42
2:B:551:ILE:HD13	2:B:649:MET:HA	2.00	0.42
3:C:279:VAL:HG23	3:C:280:LEU:HD12	2.01	0.42
7:G:16:PHE:HA	7:G:19:LYS:HE2	2.01	0.42
7:G:90:LEU:HD21	7:G:119:HIS:ND1	2.34	0.42
9:I:51:THR:HG22	9:I:53:ASP:H	1.85	0.42
1:A:481:ARG:NH1	1:A:632:GLU:OE2	2.52	0.42
2:B:585:CYS:SG	2:B:587:GLN:NE2	2.70	0.42
2:B:775:VAL:HG12	2:B:951:PRO:HG3	2.01	0.42
3:C:139:LYS:HG2	3:C:201:GLU:HB2	2.00	0.42
3:C:243:SER:HB2	3:C:285:PHE:CZ	2.55	0.42
15:S:66:DA:H2''	15:S:67:DA:C8	2.54	0.42
1:A:1008:ASP:O	1:A:1012:LYS:HG3	2.19	0.42
1:A:1108:HIS:CE1	1:A:1111:GLU:HB3	2.54	0.42
1:A:1114:TYR:CD1	1:A:1115:LYS:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1562:ILE:O	1:A:1566:ILE:HG13	2.19	0.42
2:B:673:ASN:ND2	2:B:685:VAL:O	2.49	0.42
2:B:778:TYR:CD1	2:B:937:PRO:HD3	2.54	0.42
2:B:856:ASP:O	2:B:858:ILE:HD12	2.19	0.42
3:C:200:GLN:NE2	10:J:64:ASN:OD1	2.33	0.42
1:A:245:LYS:H	1:A:245:LYS:HD2	1.85	0.42
1:A:1002:GLY:HA3	2:B:712:SER:HB3	2.01	0.42
2:B:1192:MET:H	2:B:1192:MET:HG3	1.75	0.42
1:A:584:ARG:NH1	6:F:115:THR:OG1	2.41	0.42
2:B:843:ASP:OD2	12:L:28:LYS:NZ	2.51	0.42
2:B:1011:GLU:O	2:B:1026:ILE:HG13	2.20	0.42
7:G:40:ARG:HD3	7:G:123:TYR:CE1	2.54	0.42
1:A:701:ARG:NH2	11:K:94:PRO:HA	2.35	0.42
1:A:781:LEU:HD11	1:A:786:TYR:HE1	1.84	0.42
1:A:1314:GLN:HA	1:A:1317:ILE:HG22	2.01	0.42
2:B:372:ARG:NE	2:B:573:ALA:O	2.53	0.42
3:C:31:TRP:CG	11:K:82:LYS:HD3	2.54	0.42
7:G:160:ASN:O	7:G:160:ASN:ND2	2.48	0.42
14:N:83:ASP:N	14:N:83:ASP:OD1	2.53	0.42
16:T:20:DT:C2'	16:T:21:DG:H5'	2.49	0.42
1:A:518:GLU:HG3	1:A:579:ARG:HH22	1.85	0.42
1:A:537:GLN:HE21	1:A:576:LYS:N	2.18	0.42
1:A:1309:SER:N	1:A:1312:GLU:OE2	2.53	0.42
2:B:445:TYR:HA	2:B:448:ARG:HG2	2.01	0.42
2:B:543:ASN:OD1	2:B:543:ASN:N	2.53	0.42
3:C:40:PHE:CD2	11:K:134:LYS:HD2	2.55	0.42
13:M:43:LYS:HD2	14:N:29:PHE:H	1.85	0.42
15:S:61:DA:H2''	15:S:62:DG:N7	2.35	0.42
1:A:119:ALA:O	1:A:123:ARG:HB2	2.20	0.42
1:A:184:LYS:HE3	1:A:184:LYS:HB3	1.84	0.42
1:A:1221:ARG:NH2	1:A:1544:ASN:OD1	2.53	0.42
13:M:199:GLU:HG3	13:M:342:PHE:HE1	1.84	0.42
1:A:239:PHE:CG	1:A:260:GLN:HG3	2.55	0.41
1:A:1104:TYR:OH	1:A:1119:LYS:NZ	2.45	0.41
2:B:375:LEU:HA	2:B:378:ILE:HG22	2.02	0.41
2:B:644:GLY:HA2	2:B:648:ARG:CZ	2.50	0.41
2:B:773:VAL:HG21	2:B:1031:VAL:HB	2.02	0.41
2:B:1039:MET:HG2	2:B:1042:ASP:HB3	2.01	0.41
3:C:31:TRP:HA	3:C:35:LYS:NZ	2.35	0.41
7:G:47:VAL:HG22	7:G:48:SER:H	1.85	0.41
9:I:7:LEU:HD11	9:I:16:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:21:DG:OP2	16:T:22:DA:OP2	2.38	0.41
2:B:526:GLY:HA3	2:B:651:ARG:HH22	1.84	0.41
2:B:724:GLN:NE2	2:B:1037:ARG:HB3	2.35	0.41
2:B:784:ASP:H	2:B:950:ASN:ND2	2.16	0.41
2:B:848:ILE:HG22	12:L:60:ARG:HD2	2.02	0.41
2:B:936:MET:HB2	2:B:936:MET:HE3	1.94	0.41
3:C:88:ASN:HB2	12:L:60:ARG:NH1	2.35	0.41
7:G:127:PRO:HG2	7:G:236:VAL:HG11	2.02	0.41
10:J:36:LEU:HD22	10:J:39:LEU:HD12	2.02	0.41
1:A:1105:ARG:HH21	5:E:207:ARG:NH1	2.18	0.41
1:A:1314:GLN:NE2	1:A:1460:TYR:OH	2.38	0.41
2:B:73:ILE:HG22	2:B:95:LEU:HD11	2.02	0.41
2:B:238:SER:HB2	2:B:361:HIS:H	1.84	0.41
2:B:1195:ARG:HH12	2:B:1197:ARG:HB2	1.86	0.41
3:C:84:TYR:HB3	12:L:64:LEU:HD11	2.01	0.41
8:H:30:SER:OG	8:H:33:GLN:O	2.26	0.41
10:J:68:LYS:HE2	10:J:68:LYS:HB3	1.93	0.41
13:M:64:GLY:HA3	13:M:96:LEU:HD21	2.01	0.41
1:A:85:CYS:SG	1:A:431:GLN:NE2	2.92	0.41
1:A:1086:ILE:H	1:A:1086:ILE:HG13	1.75	0.41
2:B:256:GLY:HA3	2:B:308:LEU:HD22	2.02	0.41
2:B:317:TYR:CD1	2:B:320:LEU:HB2	2.55	0.41
2:B:589:ASP:N	2:B:589:ASP:OD1	2.53	0.41
8:H:98:TYR:HE1	8:H:139:ASN:OD1	2.01	0.41
11:K:53:ALA:O	11:K:104:ARG:NH2	2.48	0.41
13:M:10:ILE:HD12	13:M:10:ILE:HA	1.94	0.41
1:A:122:LEU:HB3	1:A:337:TYR:CD2	2.55	0.41
1:A:344:ASN:ND2	1:A:348:LYS:H	2.19	0.41
1:A:486:PRO:HB2	1:A:618:TYR:HE1	1.85	0.41
1:A:1122:PRO:HG3	5:E:207:ARG:NH1	2.35	0.41
1:A:1479:ASP:OD1	1:A:1479:ASP:N	2.54	0.41
2:B:292:ILE:HD12	2:B:379:ARG:NH1	2.33	0.41
2:B:812:ALA:O	2:B:813:LEU:CB	2.68	0.41
1:A:996:TYR:OH	2:B:524:SER:OG	2.38	0.41
1:A:1025:LYS:HG3	1:A:1026:GLN:HG3	2.02	0.41
1:A:1599:ASN:OD1	1:A:1602:GLY:N	2.48	0.41
2:B:746:THR:O	2:B:748:GLN:HG2	2.21	0.41
2:B:791:LYS:HE3	2:B:791:LYS:HB3	1.90	0.41
10:J:21:TYR:HB2	10:J:39:LEU:HD11	2.03	0.41
10:J:28:ASP:HB3	10:J:30:LEU:HD23	2.01	0.41
13:M:38:PHE:HB2	13:M:54:HIS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LYS:HE2	1:A:314:TYR:CA	2.35	0.41
1:A:842:TRP:CE2	1:A:910:LYS:HE3	2.55	0.41
1:A:1592:GLN:HB2	1:A:1596:LEU:HD21	2.03	0.41
2:B:492:ASN:ND2	2:B:722:GLY:O	2.54	0.41
3:C:163:TYR:HE1	3:C:192:LEU:HD23	1.85	0.41
3:C:258:ILE:HG22	3:C:265:ALA:HB2	2.02	0.41
13:M:256:MET:O	13:M:260:GLN:N	2.41	0.41
1:A:753:ASN:HD21	1:A:782:ASP:HB3	1.85	0.41
2:B:258:VAL:HG11	2:B:378:ILE:HD11	2.03	0.41
5:E:153:HIS:CE1	5:E:184:VAL:HG11	2.56	0.41
14:N:145:ILE:HD12	14:N:146:PRO:HD2	2.03	0.41
1:A:462:LYS:HG2	1:A:466:LEU:HB2	2.02	0.41
1:A:604:LYS:H	1:A:604:LYS:HD2	1.86	0.41
1:A:732:ILE:HA	1:A:735:VAL:HG12	2.02	0.41
1:A:794:VAL:HB	1:A:810:LEU:HD21	2.02	0.41
1:A:946:LEU:HD13	1:A:948:GLY:N	2.36	0.41
1:A:1039:ARG:HH12	5:E:170:LEU:HD23	1.85	0.41
1:A:1597:ALA:H	1:A:1602:GLY:HA3	1.86	0.41
2:B:280:LEU:HB2	2:B:371:PHE:CE1	2.56	0.41
2:B:537:SER:OG	2:B:538:PRO:HD3	2.21	0.41
2:B:558:VAL:HG11	2:B:561:ILE:HG12	2.02	0.41
2:B:627:GLY:HA3	2:B:667:PHE:HD2	1.86	0.41
2:B:767:ASN:OD1	2:B:767:ASN:N	2.54	0.41
3:C:78:VAL:HG12	3:C:208:CYS:SG	2.61	0.41
9:I:11:LEU:HD13	13:M:31:ARG:H	1.86	0.41
1:A:943:ILE:HD12	1:A:943:ILE:HA	1.91	0.41
11:K:77:ARG:NH2	11:K:89:CYS:HB3	2.36	0.41
1:A:535:GLN:HB2	1:A:578:TYR:CD2	2.56	0.40
2:B:345:SER:OG	2:B:348:GLU:OE1	2.24	0.40
6:F:130:ILE:HG23	6:F:148:VAL:HG11	2.03	0.40
8:H:116:TYR:HB3	8:H:123:MET:HB2	2.03	0.40
12:L:47:ARG:NH2	12:L:54:ARG:HH22	2.19	0.40
13:M:344:VAL:HB	13:M:395:ALA:HB3	2.02	0.40
14:N:114:GLU:OE1	14:N:116:LYS:N	2.54	0.40
1:A:99:ARG:HH21	1:A:228:LEU:HD23	1.86	0.40
1:A:468:ARG:O	2:B:1070:ARG:NH1	2.51	0.40
1:A:535:GLN:HB2	1:A:578:TYR:HD2	1.86	0.40
1:A:671:GLN:HA	1:A:933:ALA:HB1	2.02	0.40
2:B:230:SER:HB2	2:B:252:TYR:HD2	1.87	0.40
2:B:1063:ARG:HH11	16:T:24:DG:H4'	1.84	0.40
3:C:90:SER:HA	3:C:200:GLN:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:103:LEU:HD11	10:J:6:ARG:HB2	2.03	0.40
3:C:136:LEU:O	3:C:203:SER:HA	2.21	0.40
3:C:232:GLN:HB2	3:C:294:VAL:HG23	2.02	0.40
7:G:216:HIS:CD2	7:G:217:TRP:H	2.39	0.40
1:A:463:LYS:HZ1	1:A:468:ARG:NH2	2.19	0.40
1:A:841:LYS:HE3	1:A:841:LYS:HB3	1.90	0.40
1:A:879:LEU:HA	1:A:882:ILE:HG12	2.03	0.40
3:C:100:ARG:HD2	10:J:2:ILE:HD13	2.04	0.40
1:A:477:ASN:ND2	2:B:1048:SER:O	2.54	0.40
1:A:904:THR:HA	1:A:907:VAL:HG22	2.04	0.40
1:A:1128:ASN:O	1:A:1131:LYS:HG2	2.22	0.40
2:B:37:LEU:HB3	2:B:760:TYR:HE1	1.87	0.40
2:B:324:THR:O	2:B:328:GLN:HG2	2.21	0.40
2:B:967:LEU:HD11	2:B:1009:GLY:HA3	2.03	0.40
2:B:1132:SER:HA	2:B:1169:GLY:HA3	2.04	0.40
3:C:165:ARG:HD3	3:C:165:ARG:H	1.86	0.40
7:G:161:ASN:HB2	7:G:248:THR:HA	2.03	0.40
1:A:468:ARG:HA	1:A:472:MET:HB2	2.03	0.40
1:A:753:ASN:ND2	1:A:784:SER:HB3	2.37	0.40
1:A:797:LEU:HD22	1:A:801:TYR:CE2	2.56	0.40
2:B:526:GLY:HA3	2:B:651:ARG:NH2	2.37	0.40
2:B:791:LYS:HB3	2:B:932:PRO:HB3	2.02	0.40
4:D:27:LEU:HD23	7:G:23:GLN:HE21	1.86	0.40
6:F:82:THR:HA	6:F:83:PRO:HD3	1.92	0.40
7:G:62:MET:HG3	7:G:66:LEU:HD23	2.02	0.40
7:G:149:ILE:HG23	7:G:153:PHE:HB2	2.03	0.40
11:K:66:VAL:O	11:K:68:GLU:HG2	2.21	0.40
13:M:275:ARG:H	13:M:275:ARG:HD3	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	1450/1664 (87%)	1375 (95%)	71 (5%)	4 (0%)	41	76
2	B	1160/1203 (96%)	1097 (95%)	63 (5%)	0	100	100
3	C	300/335 (90%)	289 (96%)	11 (4%)	0	100	100
4	D	55/137 (40%)	54 (98%)	1 (2%)	0	100	100
5	E	212/215 (99%)	208 (98%)	4 (2%)	0	100	100
6	F	98/155 (63%)	95 (97%)	3 (3%)	0	100	100
7	G	196/326 (60%)	191 (97%)	5 (3%)	0	100	100
8	H	130/146 (89%)	126 (97%)	4 (3%)	0	100	100
9	I	62/125 (50%)	56 (90%)	6 (10%)	0	100	100
10	J	67/70 (96%)	60 (90%)	7 (10%)	0	100	100
11	K	98/142 (69%)	96 (98%)	2 (2%)	0	100	100
12	L	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
13	M	317/415 (76%)	304 (96%)	13 (4%)	0	100	100
14	N	127/233 (54%)	106 (84%)	20 (16%)	1 (1%)	19	60
All	All	4313/5236 (82%)	4097 (95%)	211 (5%)	5 (0%)	54	85

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	THR
1	A	248	PHE
1	A	450	LYS
1	A	227	LEU
14	N	148	ILE

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	1293/1465 (88%)	1254 (97%)	39 (3%)	41	63
2	B	1025/1053 (97%)	998 (97%)	27 (3%)	46	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	269/296 (91%)	261 (97%)	8 (3%)	41	63
4	D	56/116 (48%)	54 (96%)	2 (4%)	35	59
5	E	196/197 (100%)	189 (96%)	7 (4%)	35	59
6	F	90/137 (66%)	84 (93%)	6 (7%)	16	43
7	G	180/291 (62%)	177 (98%)	3 (2%)	60	78
8	H	117/128 (91%)	111 (95%)	6 (5%)	24	50
9	I	56/110 (51%)	53 (95%)	3 (5%)	22	49
10	J	64/65 (98%)	62 (97%)	2 (3%)	40	62
11	K	90/130 (69%)	87 (97%)	3 (3%)	38	61
12	L	38/57 (67%)	35 (92%)	3 (8%)	12	38
13	M	292/371 (79%)	287 (98%)	5 (2%)	60	78
14	N	125/220 (57%)	121 (97%)	4 (3%)	39	62
All	All	3891/4636 (84%)	3773 (97%)	118 (3%)	44	63

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ARG
1	A	92	ASN
1	A	111	LYS
1	A	138	GLU
1	A	230	ARG
1	A	259	LYS
1	A	399	LEU
1	A	417	ARG
1	A	457	LYS
1	A	512	THR
1	A	604	LYS
1	A	606	ARG
1	A	649	ASN
1	A	667	ARG
1	A	670	ILE
1	A	709	ARG
1	A	711	LYS
1	A	753	ASN
1	A	764	SER
1	A	786	TYR
1	A	866	LYS

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Mol	Chain	Res	Type
1	A	888	LYS
1	A	947	LEU
1	A	953	GLU
1	A	964	LYS
1	A	1021	ARG
1	A	1027	LEU
1	A	1063	MET
1	A	1079	LYS
1	A	1110	LYS
1	A	1221	ARG
1	A	1437	ASN
1	A	1494	ARG
1	A	1499	ARG
1	A	1506	ARG
1	A	1567	ASN
1	A	1590	THR
1	A	1591	ARG
1	A	1643	VAL
2	B	87	ASN
2	B	104	ILE
2	B	119	ARG
2	B	127	ARG
2	B	136	LYS
2	B	164	MET
2	B	168	ASN
2	B	209	GLN
2	B	224	ASN
2	B	315	LYS
2	B	323	ARG
2	B	343	ASP
2	B	470	LEU
2	B	476	LEU
2	B	528	LEU
2	B	595	TRP
2	B	651	ARG
2	B	658	LEU
2	B	716	MET
2	B	784	ASP
2	B	790	ASN
2	B	811	LEU
2	B	920	ARG
2	B	967	LEU

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Mol	Chain	Res	Type
2	B	1063	ARG
2	B	1074	MET
2	B	1171	ASN
3	C	93	GLN
3	C	165	ARG
3	C	232	GLN
3	C	271	ARG
3	C	277	ARG
3	C	295	ARG
3	C	316	LYS
3	C	329	LYS
4	D	29	GLN
4	D	90	LYS
5	E	26	ARG
5	E	124	VAL
5	E	170	LEU
5	E	177	ARG
5	E	191	LYS
5	E	200	ARG
5	E	215	MET
6	F	60	GLN
6	F	65	ARG
6	F	66	ARG
6	F	67	LYS
6	F	76	LYS
6	F	104	ASN
7	G	8	ASN
7	G	71	MET
7	G	160	ASN
8	H	33	GLN
8	H	40	LEU
8	H	43	ASN
8	H	130	ARG
8	H	136	LYS
8	H	146	ARG
9	I	19	ASN
9	I	39	LYS
9	I	63	LYS
10	J	13	VAL
10	J	48	ARG
11	K	44	ARG
11	K	81	MET

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Mol	Chain	Res	Type
11	K	83	ASN
12	L	28	LYS
12	L	42	ARG
12	L	62	LYS
13	M	106	LYS
13	M	185	ASP
13	M	200	GLN
13	M	275	ARG
13	M	363	LEU
14	N	37	ASN
14	N	50	GLN
14	N	114	GLU
14	N	158	LYS

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	332	GLN
1	A	344	ASN
1	A	444	GLN
1	A	489	ASN
1	A	521	GLN
1	A	537	GLN
1	A	580	HIS
1	A	603	HIS
1	A	610	ASN
1	A	640	ASN
1	A	642	ASN
1	A	691	GLN
1	A	748	ASN
1	A	753	ASN
1	A	795	HIS
1	A	939	ASN
1	A	998	HIS
1	A	1036	ASN
1	A	1237	GLN
1	A	1314	GLN
1	A	1437	ASN
1	A	1443	GLN
1	A	1454	HIS
1	A	1567	ASN
2	B	62	ASN

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Mol	Chain	Res	Type
2	B	128	GLN
2	B	224	ASN
2	B	231	HIS
2	B	251	HIS
2	B	532	HIS
2	B	598	HIS
2	B	669	GLN
2	B	715	ASN
2	B	745	GLN
2	B	748	GLN
2	B	770	ASN
2	B	790	ASN
2	B	950	ASN
2	B	979	GLN
2	B	1114	GLN
2	B	1115	GLN
3	C	65	ASN
3	C	93	GLN
3	C	130	ASN
3	C	216	HIS
3	C	301	ASN
4	D	17	ASN
4	D	29	GLN
4	D	88	GLN
5	E	8	ASN
5	E	113	GLN
6	F	60	GLN
6	F	104	ASN
7	G	23	GLN
7	G	67	ASN
7	G	216	HIS
8	H	33	GLN
8	H	43	ASN
9	I	19	ASN
9	I	21	ASN
10	J	53	HIS
11	K	52	GLN
11	K	64	GLN
11	K	83	ASN
13	M	71	GLN
13	M	107	ASN
13	M	323	GLN

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Mol	Chain	Res	Type
13	M	324	ASN
13	M	351	HIS
14	N	37	ASN
14	N	50	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
17	R	6/10 (60%)	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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

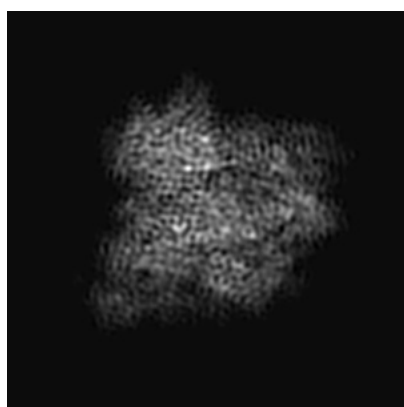
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3449. These allow visual inspection of the internal detail of the map and identification of artifacts.

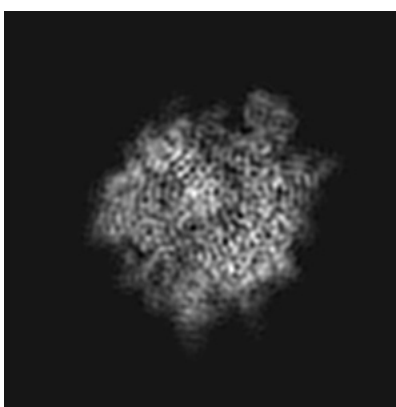
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

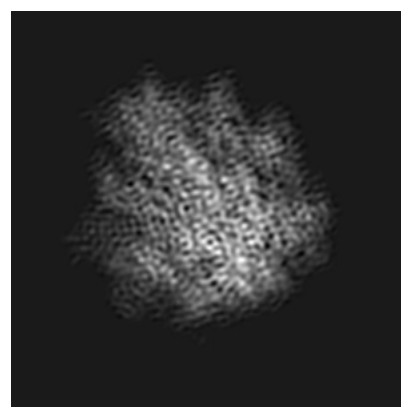
6.1.1 Primary map



X



Y

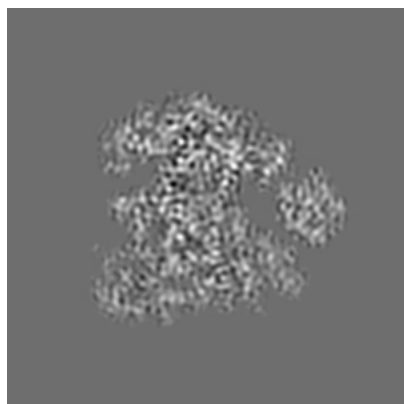


Z

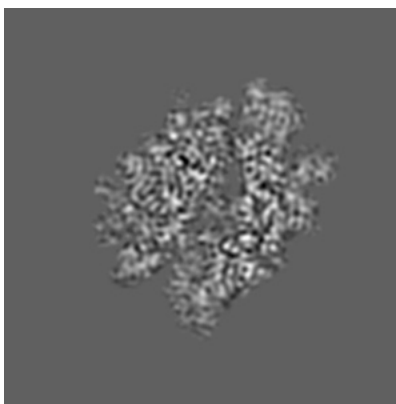
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

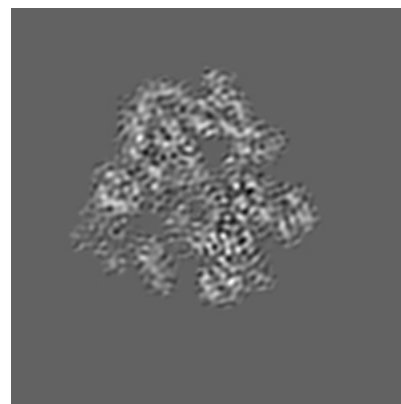
6.2.1 Primary map



X Index: 88



Y Index: 88

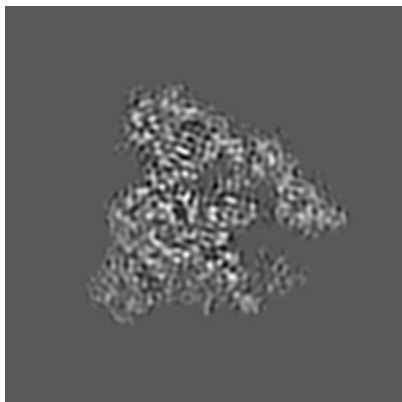


Z Index: 88

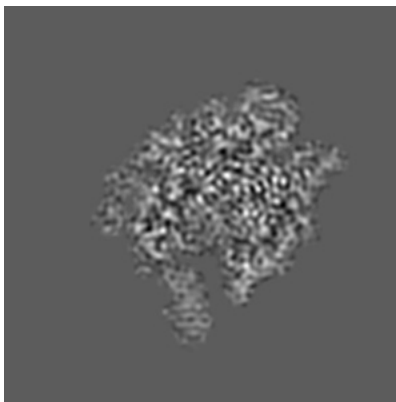
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

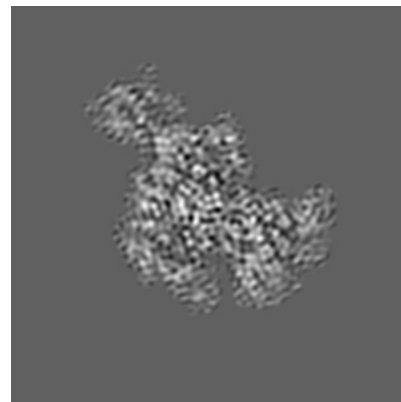
6.3.1 Primary map



X Index: 95



Y Index: 79



Z Index: 107

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

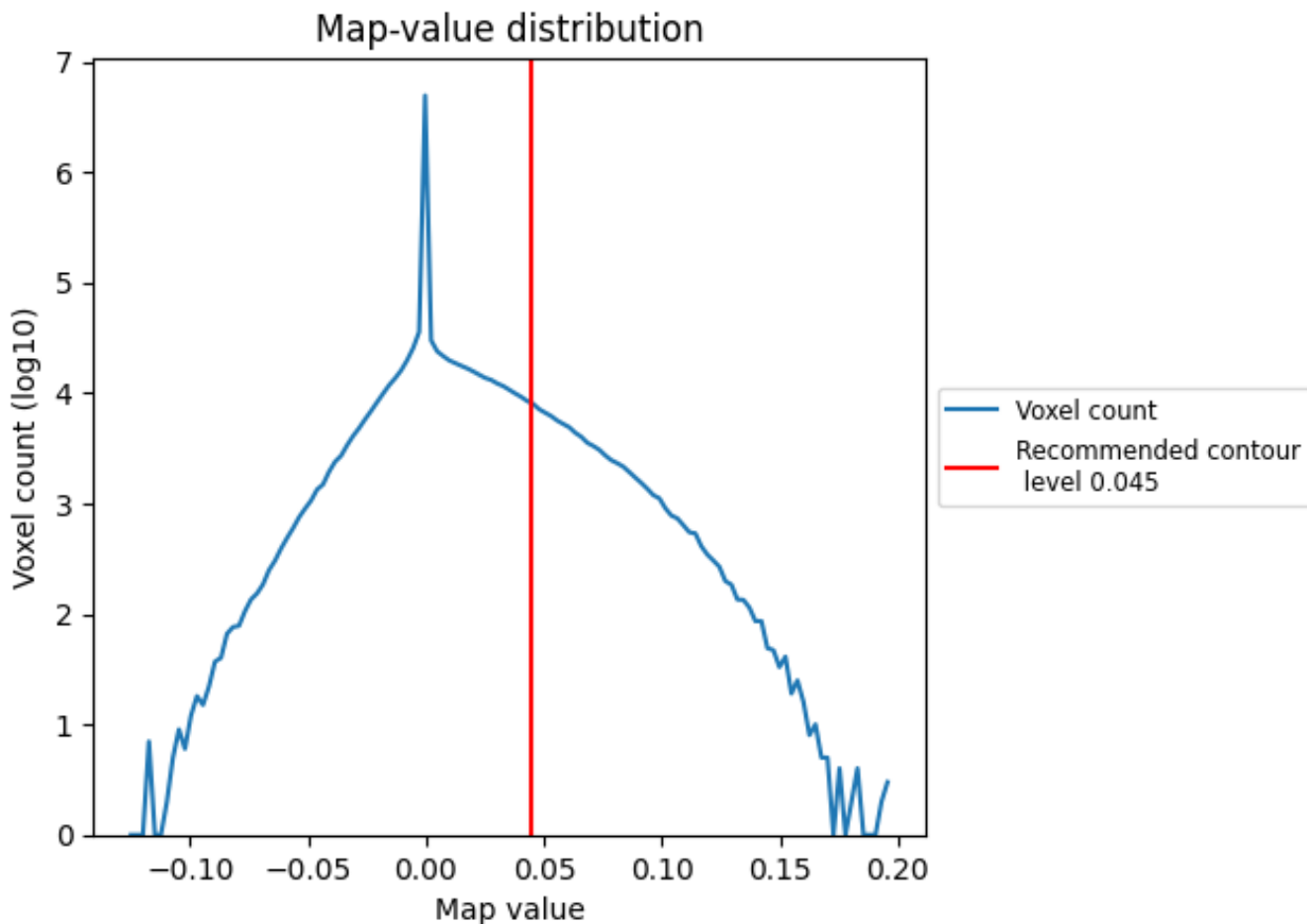
6.5 Mask visualisation

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

7 Map analysis [i](#)

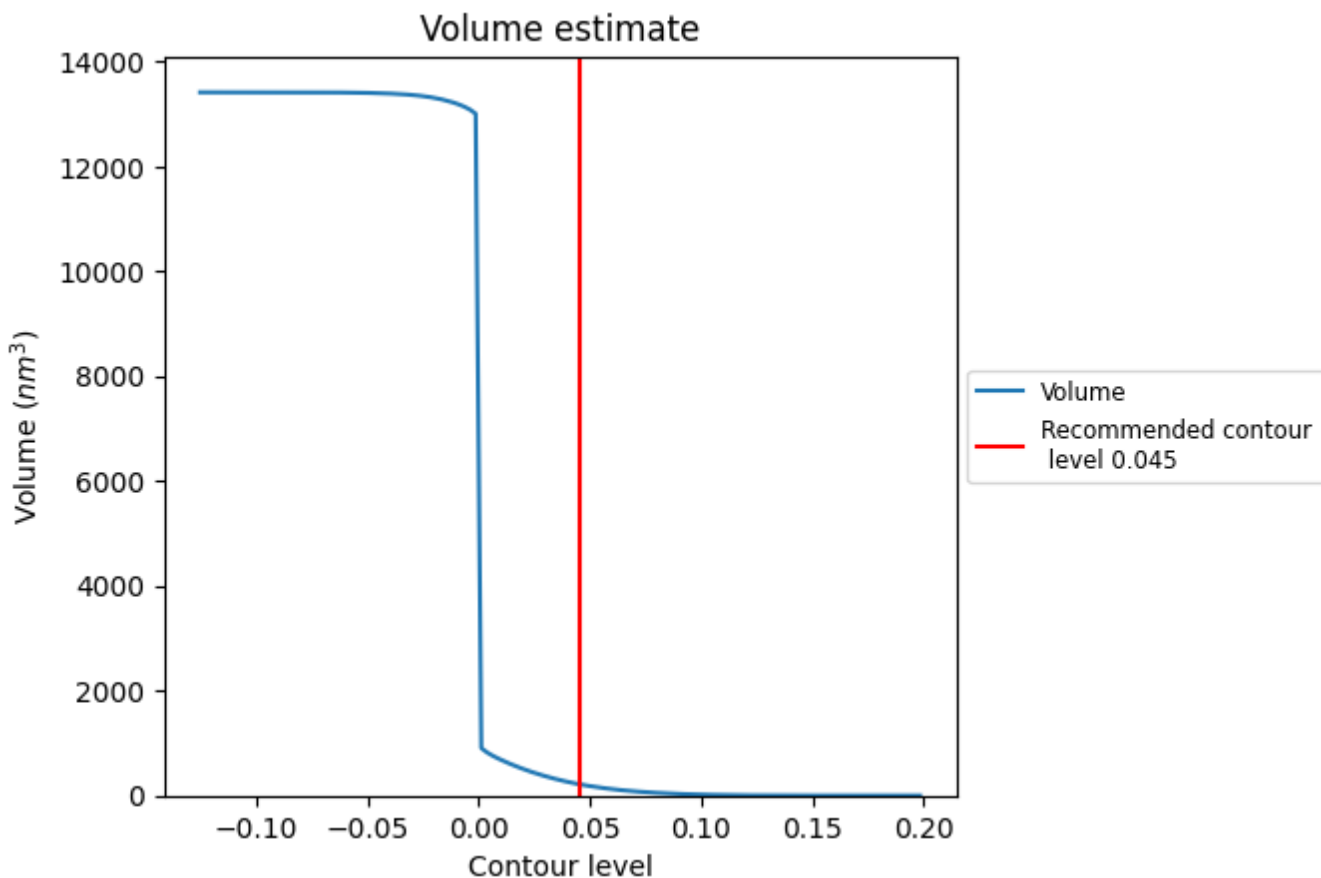
This section contains the results of statistical analysis of the map.

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.

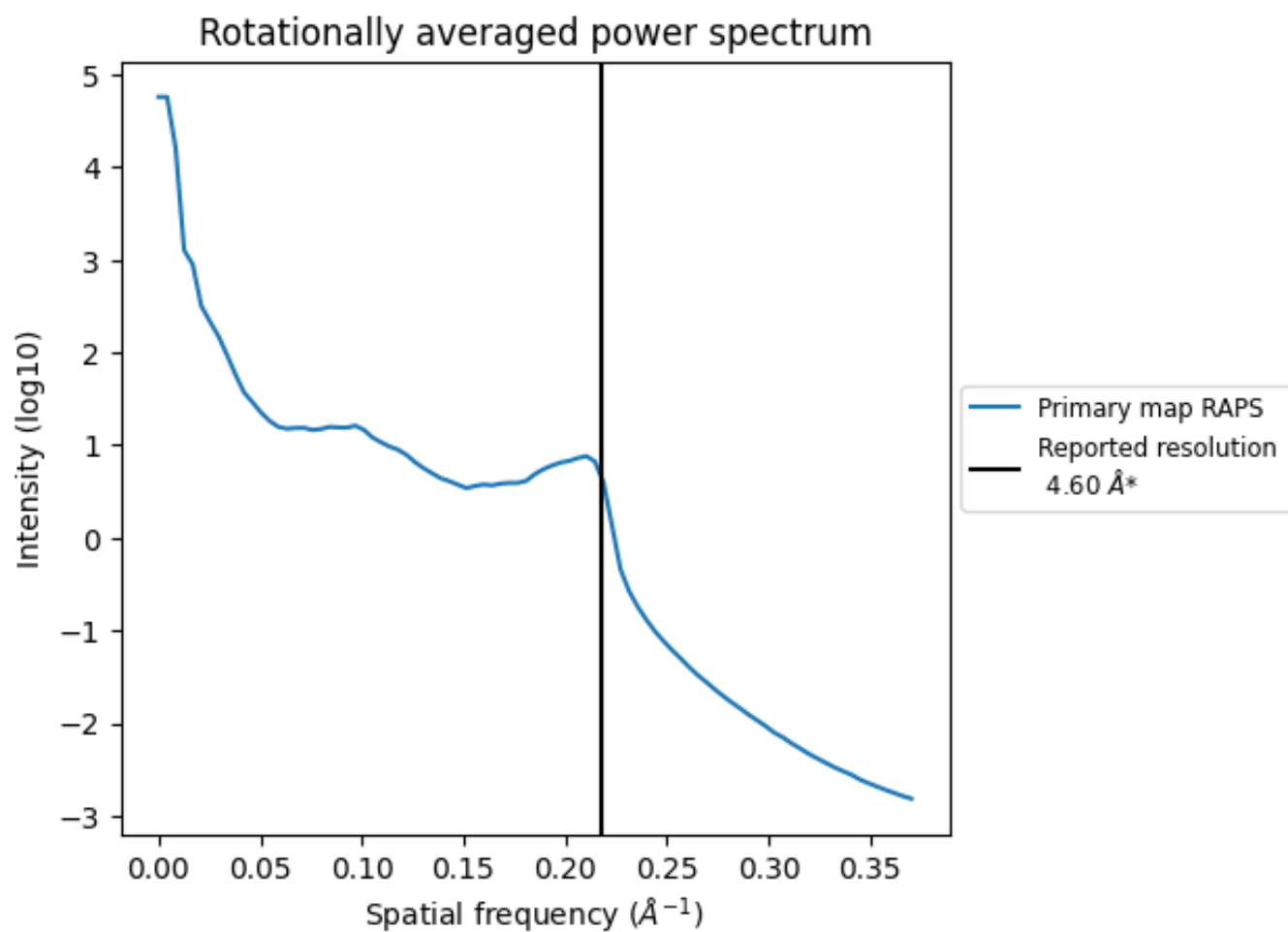
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 218 nm³; this corresponds to an approximate mass of 197 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](#)

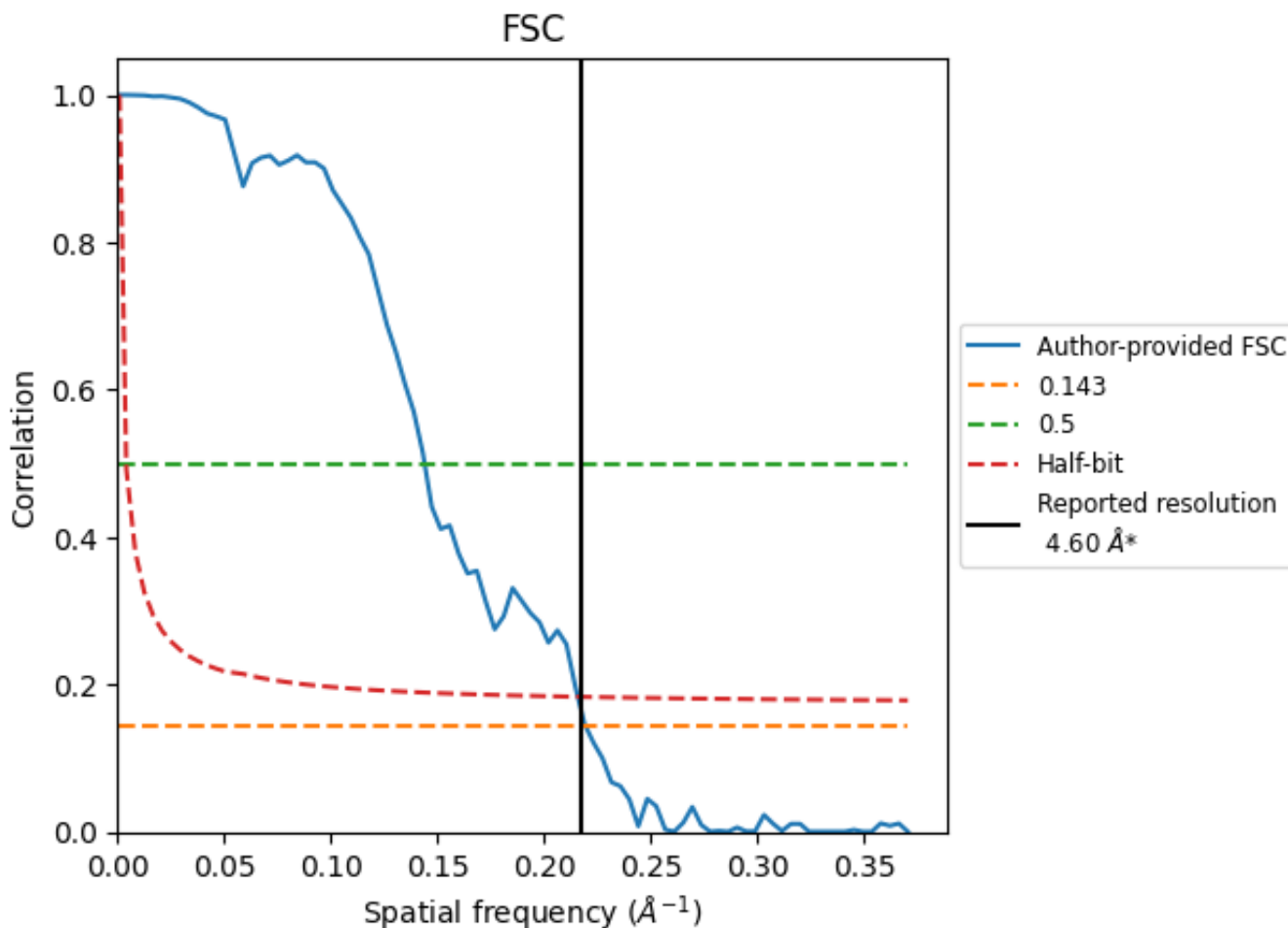


*Reported resolution corresponds to spatial frequency of 0.217\AA^{-1}

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

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

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



*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

8.2 Resolution estimates [i](#)

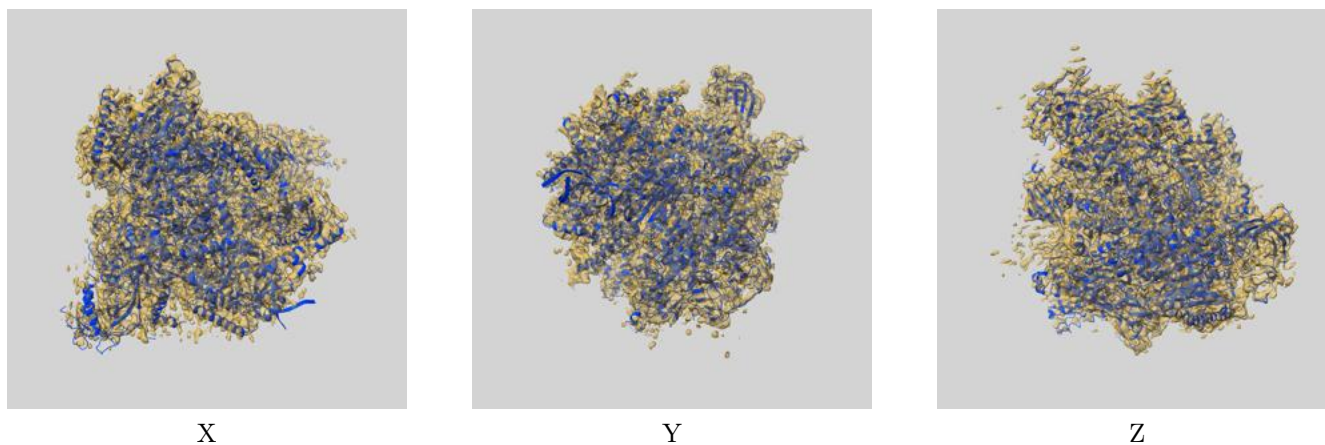
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.56	6.95	4.63
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3449 and PDB model 5M64. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



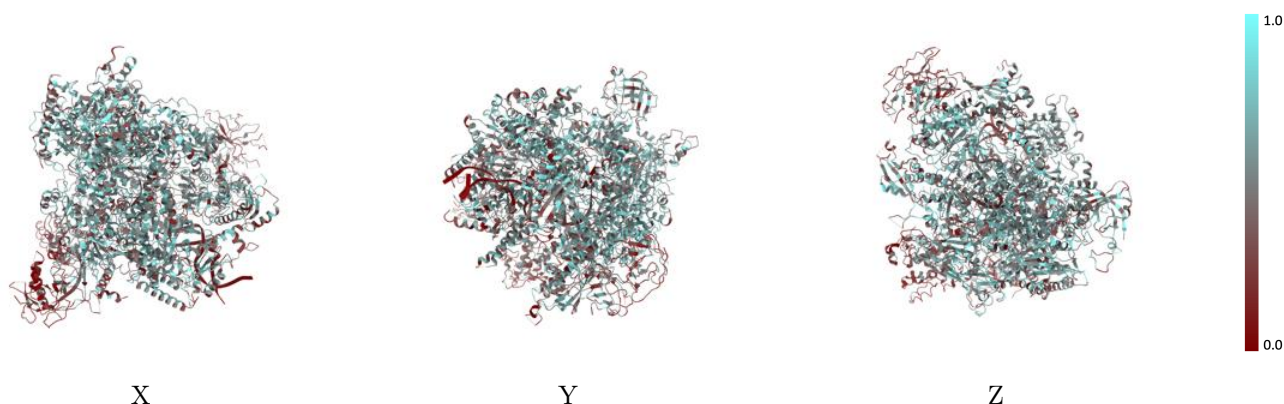
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



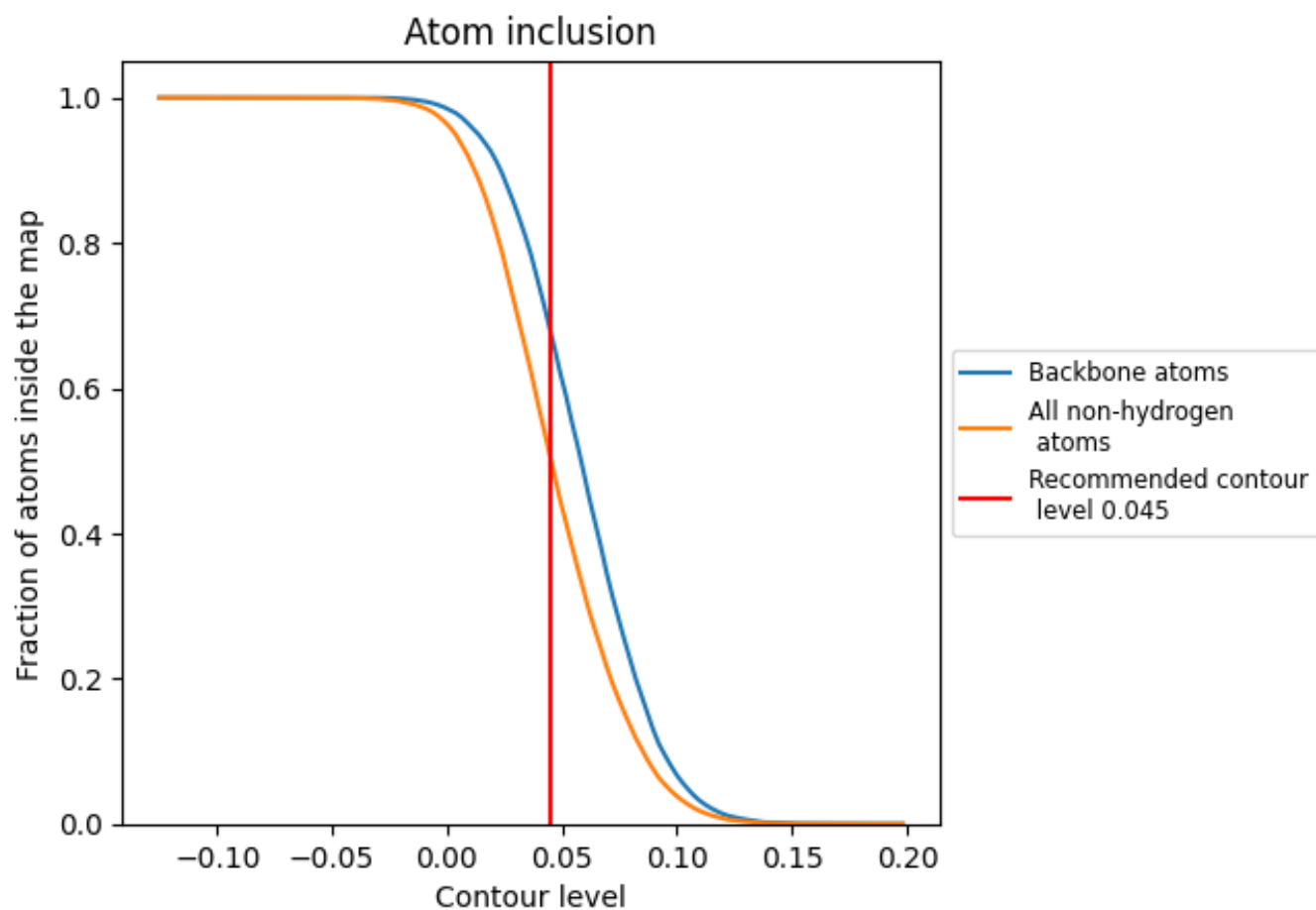
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 50% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5032	 0.2660
A	 0.5491	 0.2790
B	 0.5666	 0.2880
C	 0.5577	 0.3050
D	 0.2376	 0.2140
E	 0.5574	 0.2780
F	 0.5780	 0.3040
G	 0.3010	 0.2100
H	 0.5196	 0.2880
I	 0.4128	 0.1940
J	 0.5453	 0.2810
K	 0.5670	 0.3000
L	 0.5181	 0.2730
M	 0.2750	 0.1980
N	 0.3644	 0.2070
R	 0.2345	 0.1530
S	 0.2469	 0.0740
T	 0.2554	 0.1000

