



Full wwPDB EM Validation Report ⓘ

Nov 10, 2024 – 02:55 pm GMT

PDB ID : 8QMA
EMDB ID : EMD-18496
Title : Structure of the plastid-encoded RNA polymerase complex (PEP) from *Sinapis alba*
Authors : do Prado, P.F.V.; Ahrens, F.M.; Pfannschmidt, T.; Hillen, H.S.
Deposited on : 2023-09-21
Resolution : 3.50 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

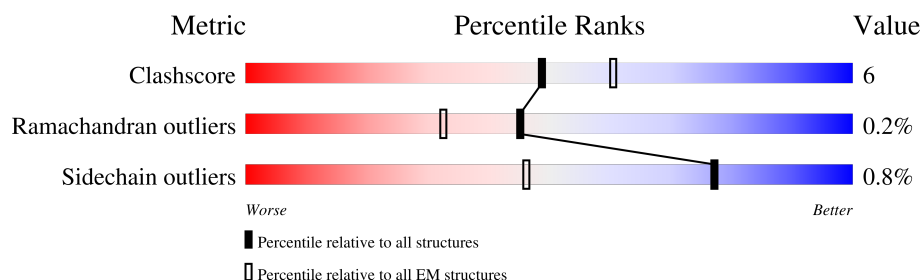
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.













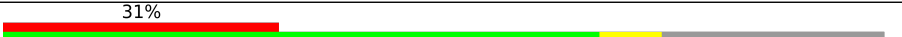
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	G	264	
2	H	529	
3	K	334	
4	L	297	
5	M	184	
5	N	184	
6	O	768	
7	P	162	

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Mol	Chain	Length	Quality of chain
8	R	140	
9	S	460	
10	A	1072	
11	B	1373	
12	C	327	
12	D	327	
13	E	911	
14	F	675	
15	I	611	
16	J	483	
17	T	680	

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 52064 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 PAP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	214	Total	C	N	O	S	0	0
			1766	1137	300	323	6		

- Molecule 2 is a protein called PAP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	224	Total	C	N	O	S	0	0
			1892	1193	341	348	10		

- Molecule 3 is a protein called PAP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	200	Total	C	N	O	S	0	0
			1681	1062	295	317	7		

- Molecule 4 is a protein called PAP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	222	Total	C	N	O	S	0	0
			1801	1158	306	333	4		

- Molecule 5 is a protein called PAP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	114	Total	C	N	O	S	0	0
			925	590	147	179	9		
5	N	108	Total	C	N	O	S	0	0
			867	552	138	168	9		

- Molecule 6 is a protein called PAP11.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	O	194	Total	C	N	O	S	0	0
			1538	950	272	306	10		

- Molecule 7 is a protein called PAP12 (DNA-directed RNA polymerase subunit omega).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	65	Total	C	N	O	S	0	0
			530	332	91	105	2		

- Molecule 8 is a protein called PTAC18.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	100	Total	C	N	O	S	0	0
			852	555	144	150	3		

- Molecule 9 is a protein called PAP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	384	Total	C	N	O	S	0	0
			3104	1985	520	584	15		

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	789	Total	C	N	O	S	0	0
			6310	4042	1093	1154	21		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit beta”.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	931	Total	C	N	O	S	0	0
			7445	4765	1316	1339	25		

- Molecule 12 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	210	Total	C	N	O	S	0	0
			1666	1054	294	310	8		
12	D	278	Total	C	N	O	S	0	0
			2249	1440	393	407	9		

- Molecule 13 is a protein called PAP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	632	Total	C	N	O	S	0	0
			5075	3214	882	946	33		

- Molecule 14 is a protein called PAP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	483	Total	C	N	O	S	0	0
			4060	2593	706	746	15		

- Molecule 15 is a protein called FLN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	338	Total	C	N	O	S	0	0
			2645	1684	439	502	20		

- Molecule 16 is a protein called PAP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	426	Total	C	N	O	S	0	0
			3477	2227	591	639	20		

- Molecule 17 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	509	Total	C	N	O	S	0	0
			4151	2674	726	732	19		

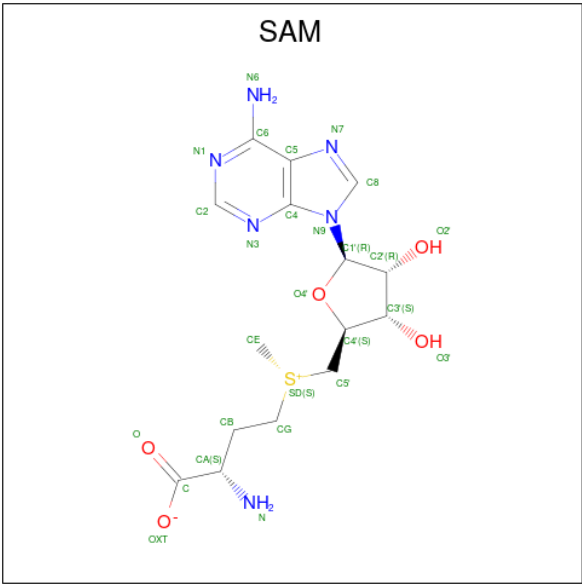
- Molecule 18 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	G	1	Total	Fe	0
			1	1	
18	L	1	Total	Fe	0
			1	1	

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
19	B	1	Total	Zn	0
			1	1	

- Molecule 20 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S) (labeled as "Ligand of Interest" by depositor).

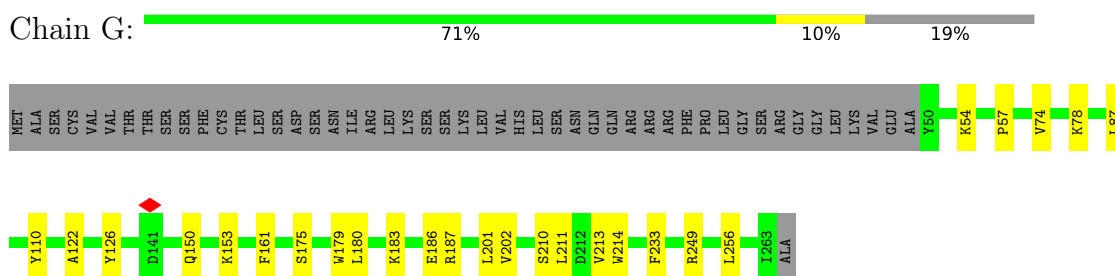


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
20	J	1	27	15	6	5	1	0

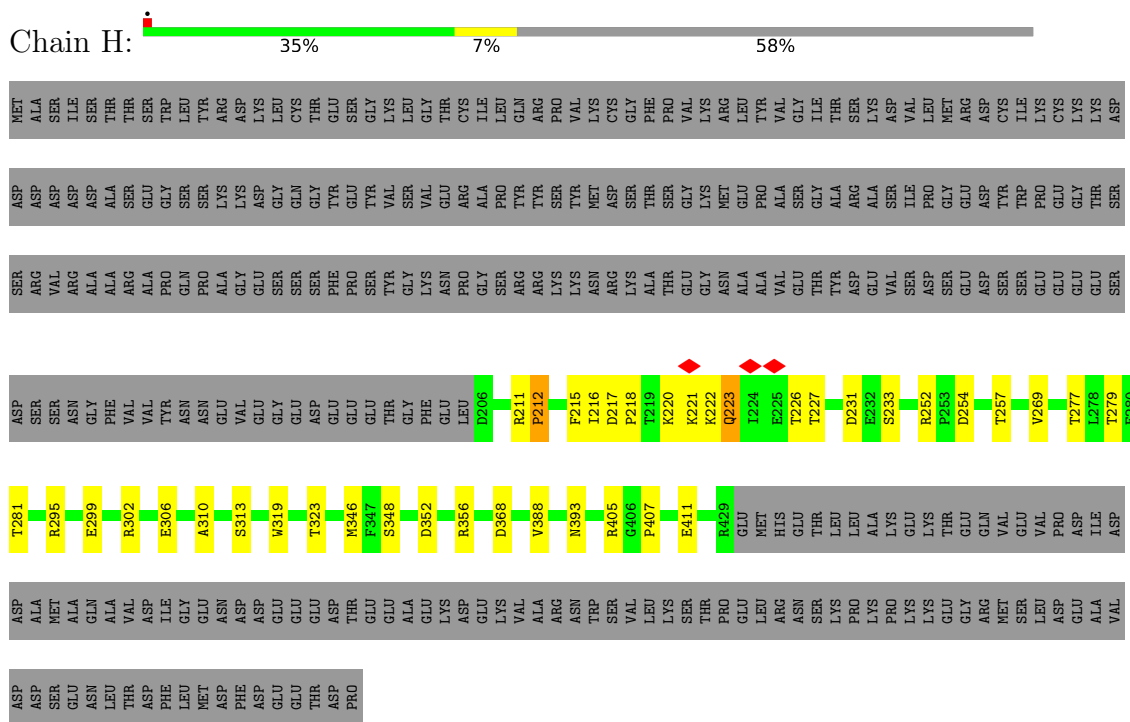
3 Residue-property plots

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: PAP4

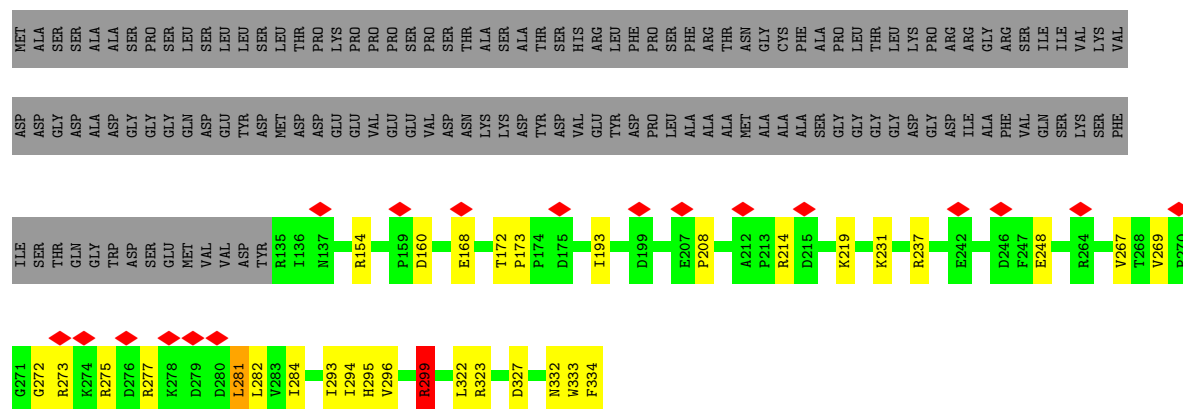


- Molecule 2: PAP5



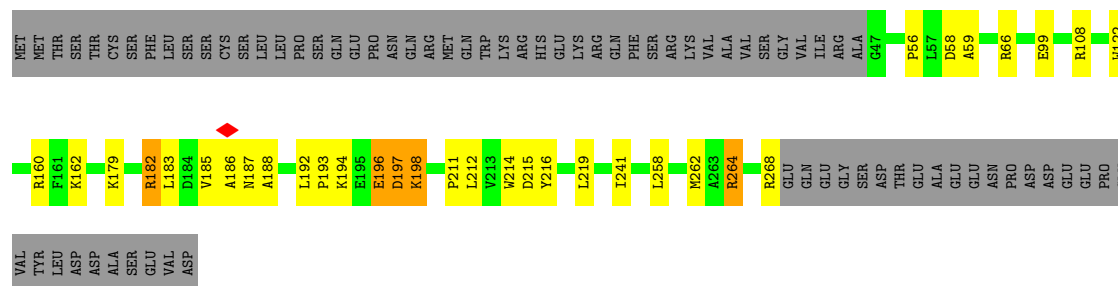
- Molecule 3: PAP8





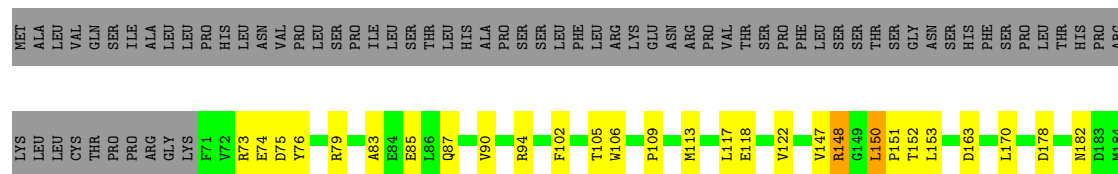
• Molecule 4: PAP9

Chain L: 64% 9% 25%



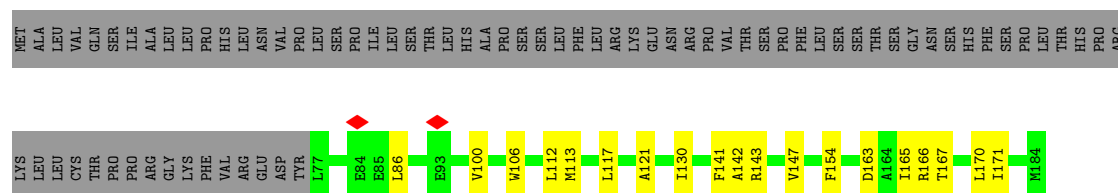
• Molecule 5: PAP10

Chain M: 47% 14% 38%



• Molecule 5: PAP10

Chain N: 48% 10% 41%

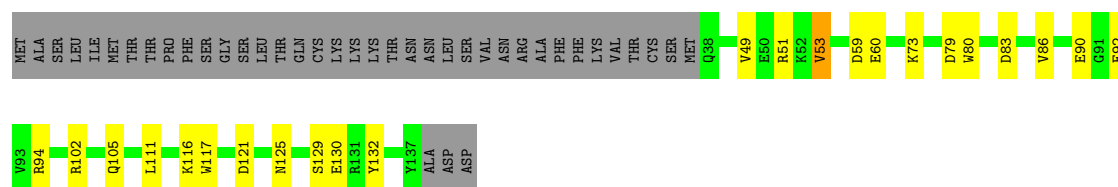


• Molecule 6: PAP11

Chain O: 16% 20% 5% 75%

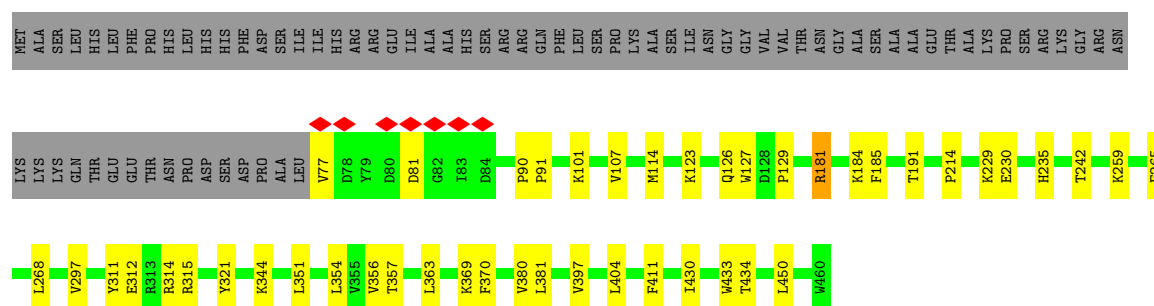


Chain R:  55% 16% 29%



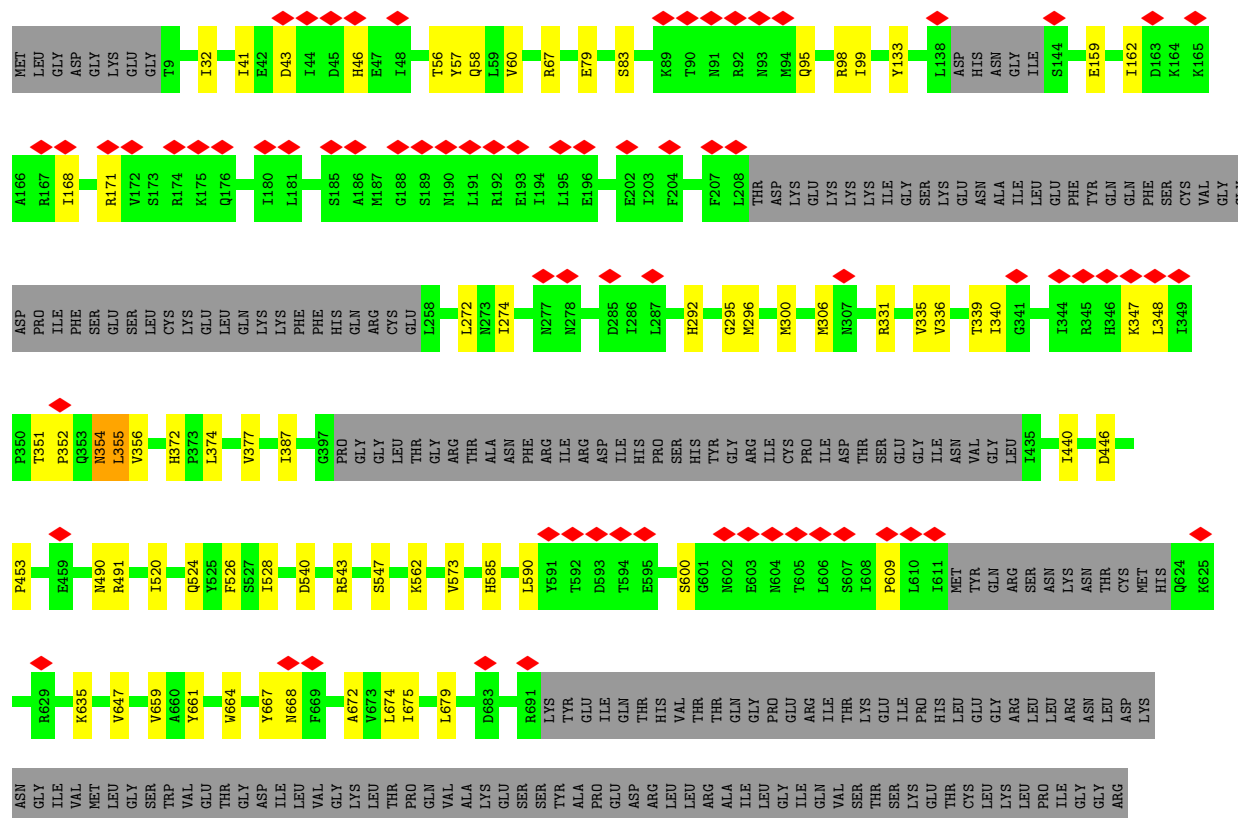
• Molecule 9: PAP6

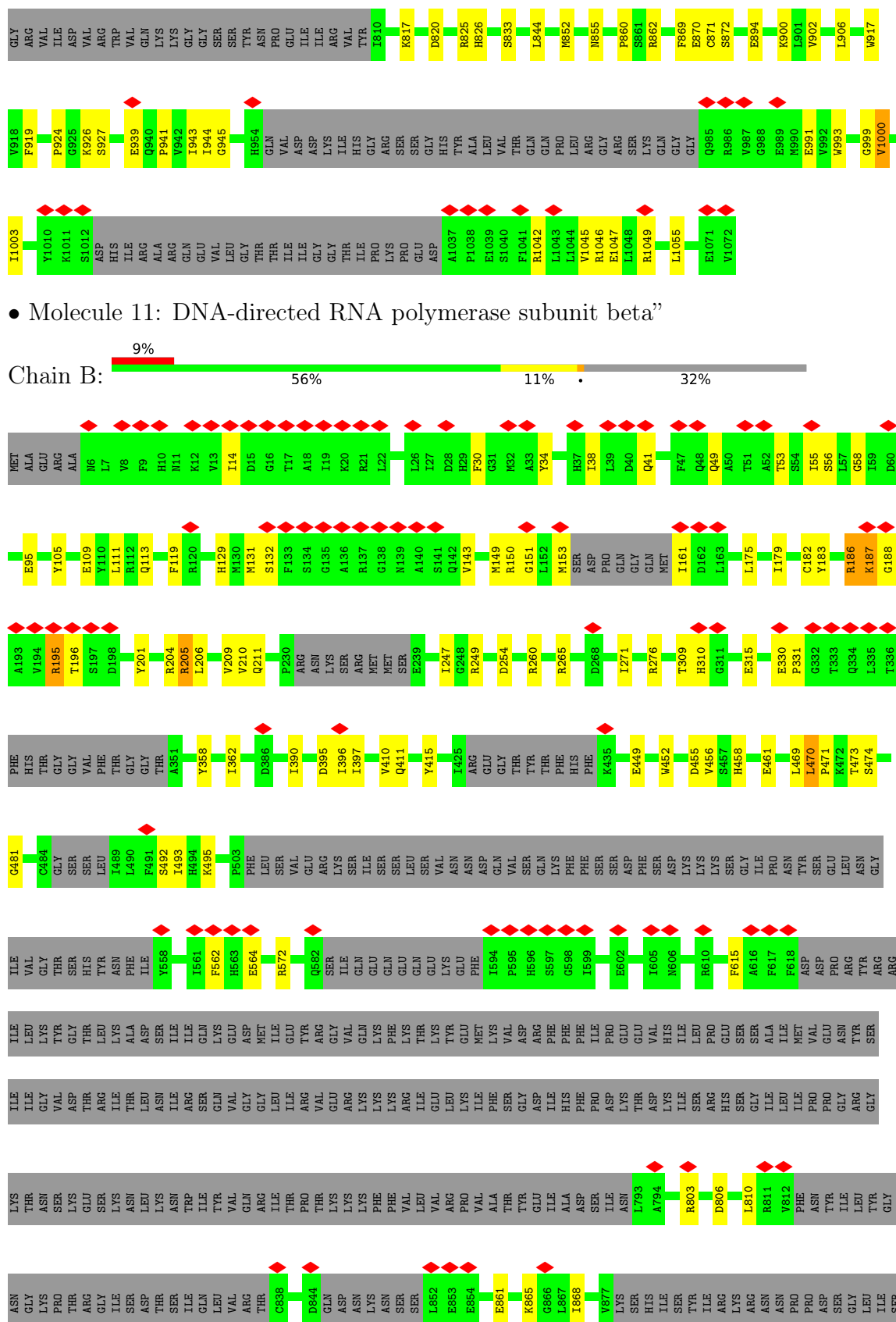
Chain S:  73% 10% 17%

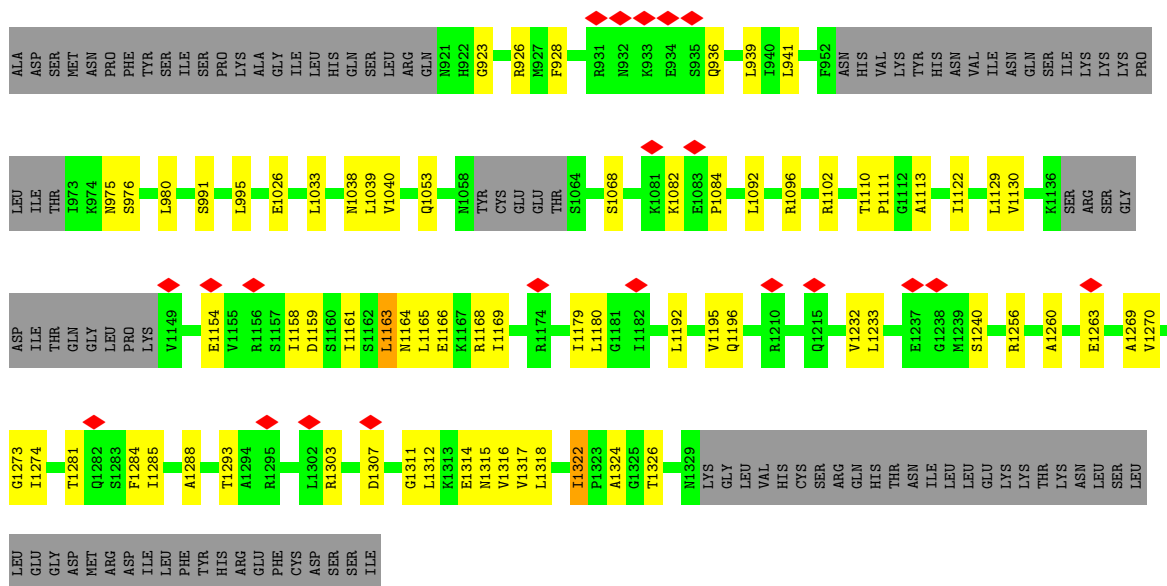


• Molecule 10: DNA-directed RNA polymerase subunit beta

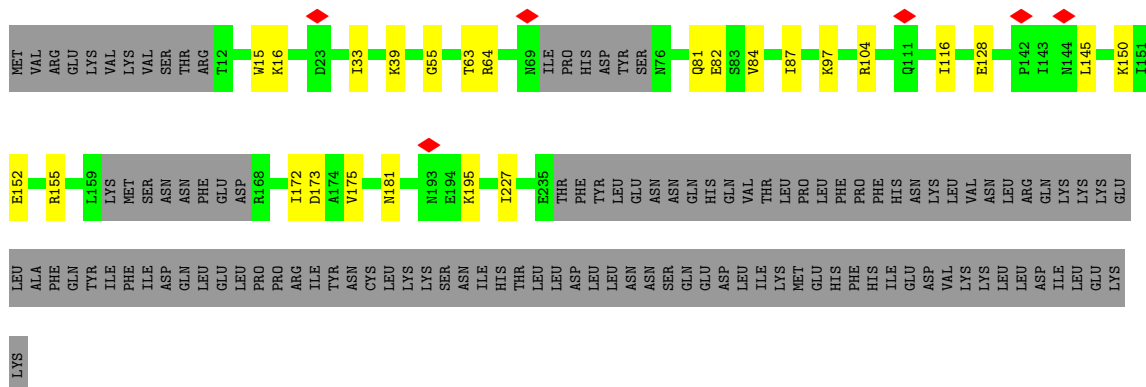
Chain A:  8% 63% 10% 26%



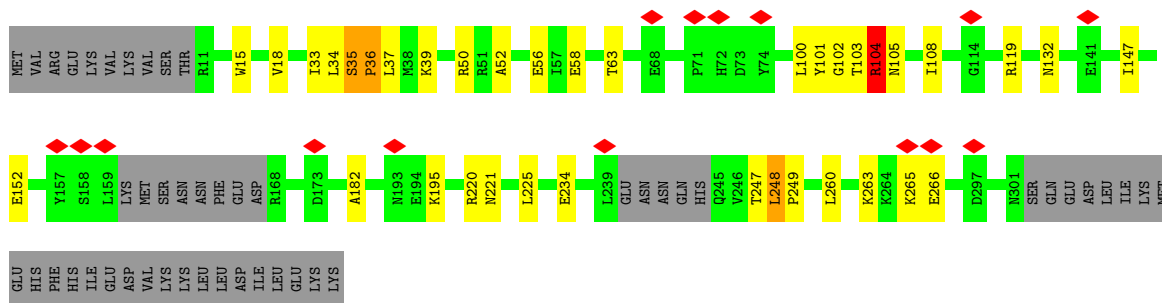
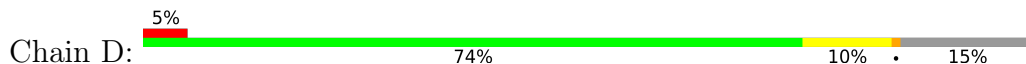




- Molecule 12: DNA-directed RNA polymerase subunit alpha

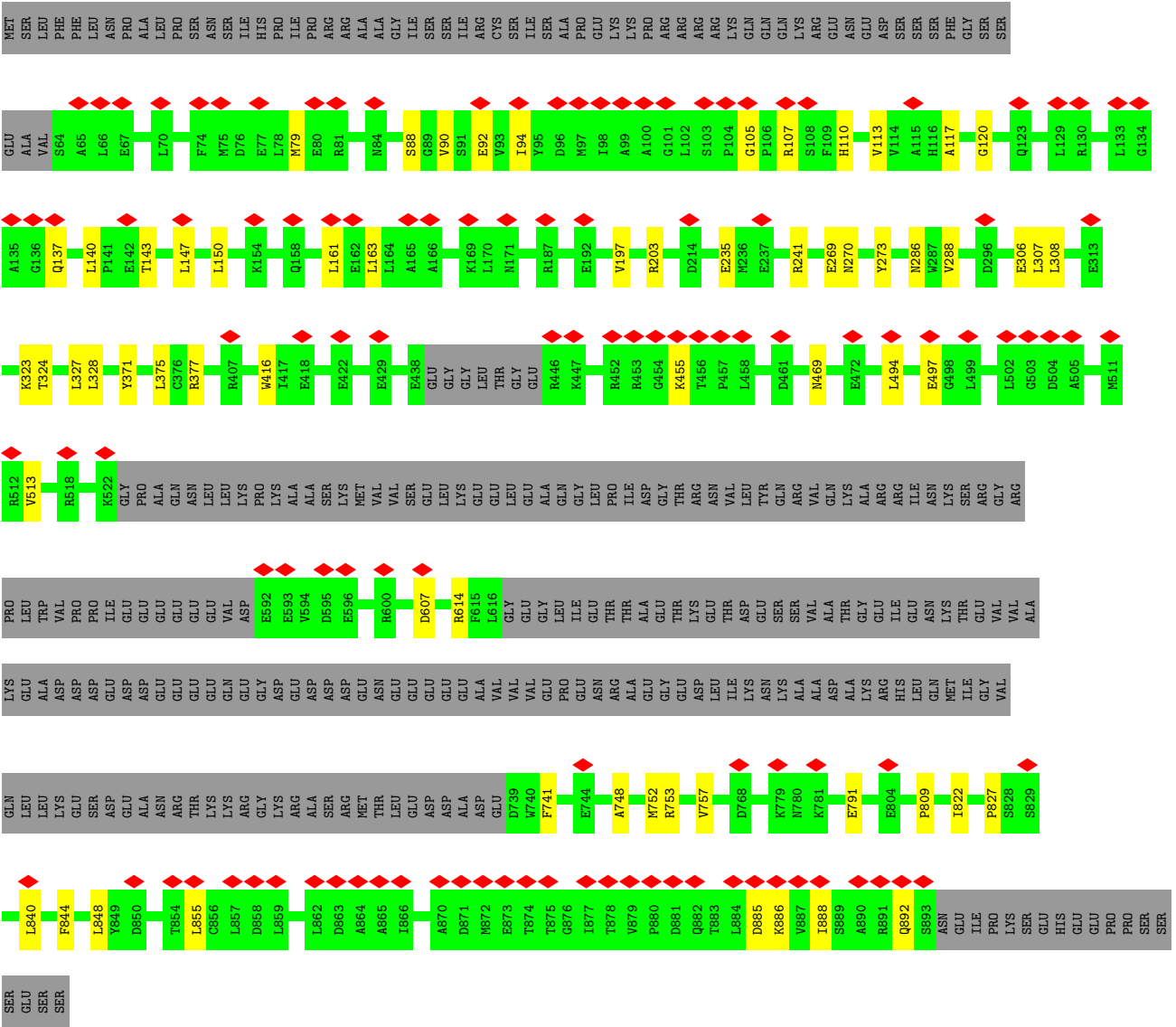


- Molecule 12: DNA-directed RNA polymerase subunit alpha

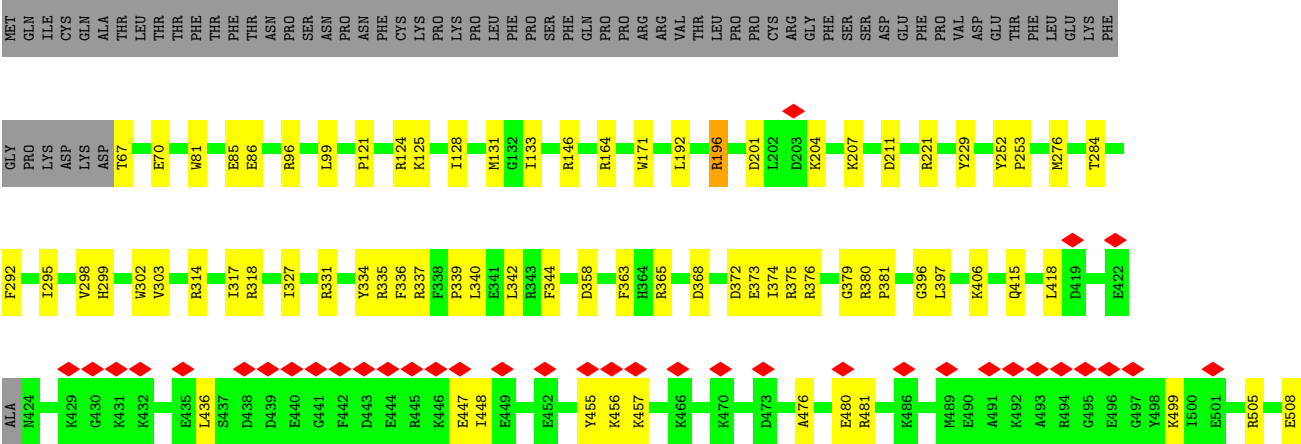


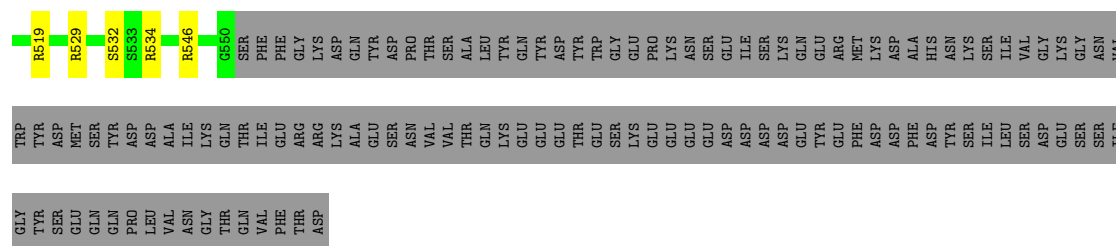
- Molecule 13: PAP1



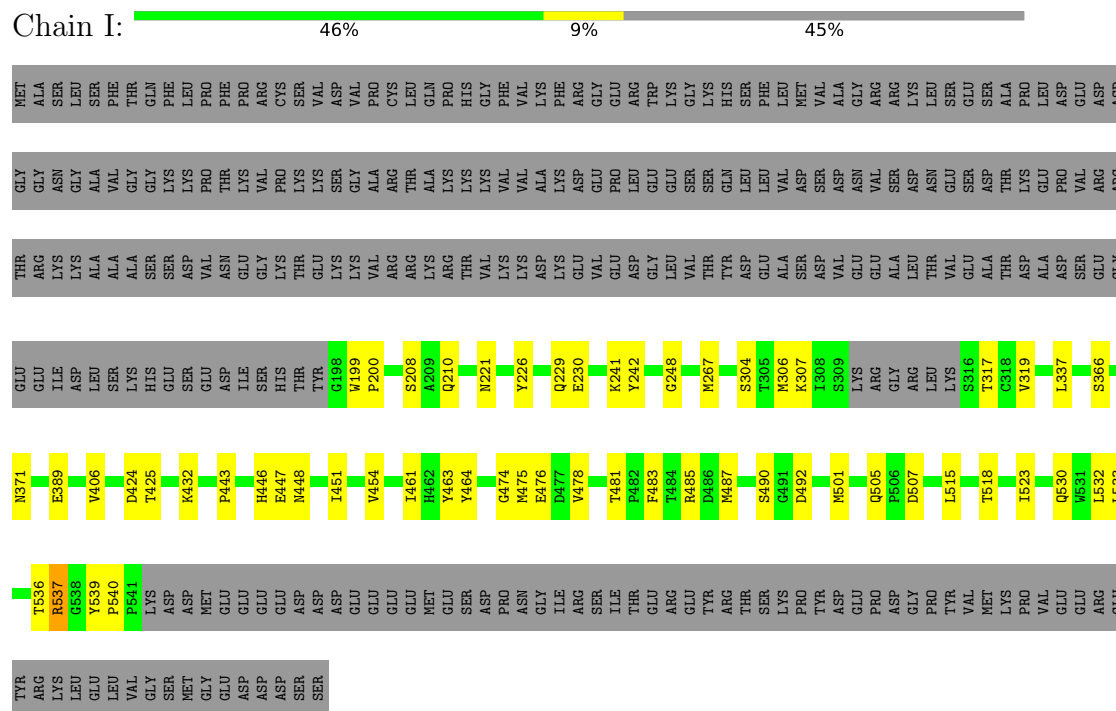


● Molecule 14: PAP3

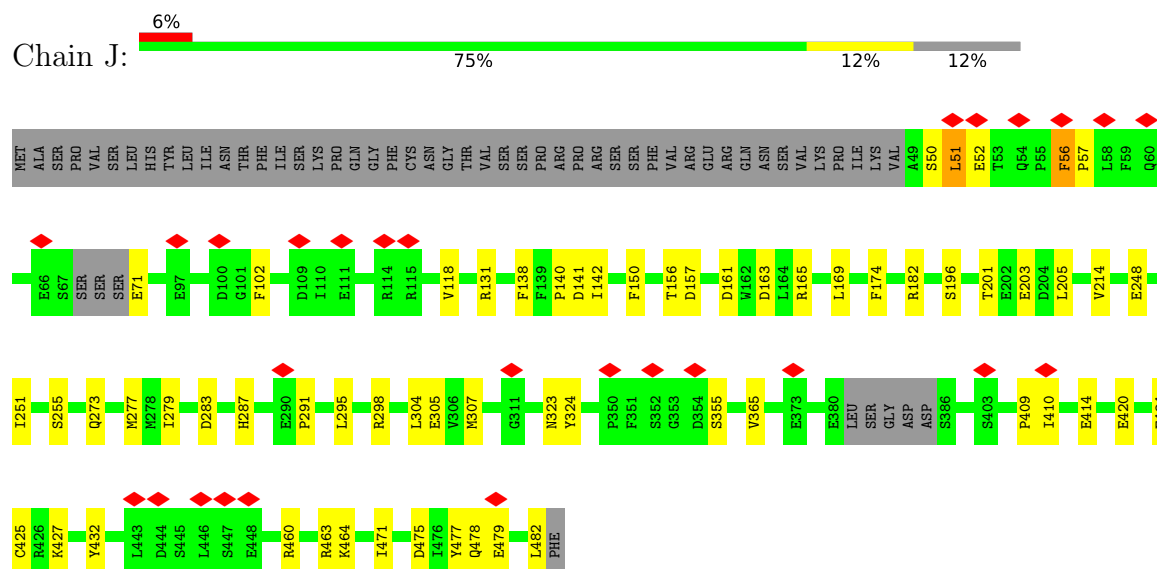




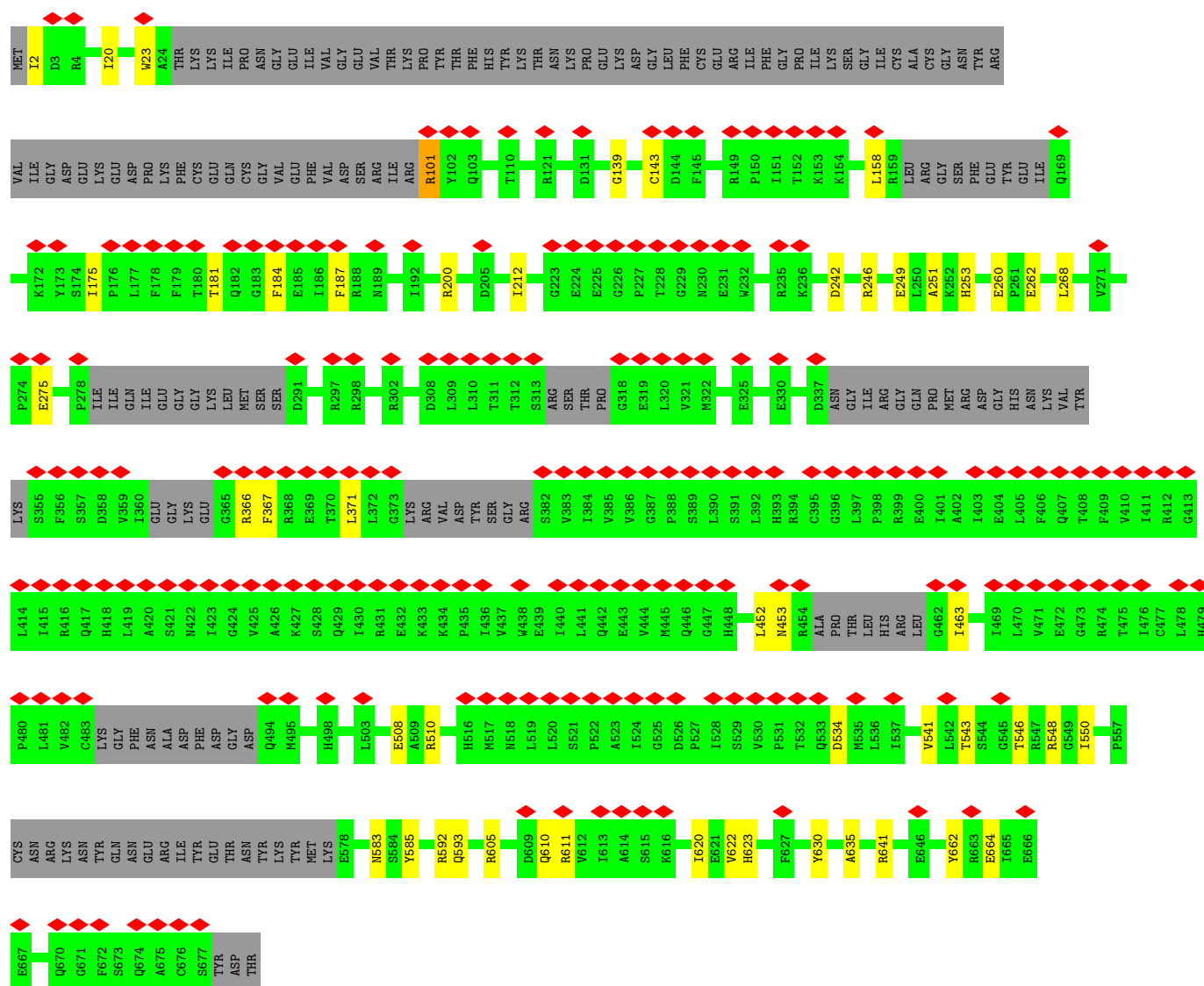
• Molecule 15: FLN2



• Molecule 16: PAP7



• Molecule 17: DNA-directed RNA polymerase subunit beta'



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123874	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)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.762	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.026	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	461.99997, 461.99997, 461.99997	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, SAM, 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	G	0.30	0/1820	0.49	0/2472
2	H	0.28	0/1941	0.56	0/2616
3	K	0.26	0/1722	0.55	0/2329
4	L	0.30	0/1855	0.54	0/2525
5	M	0.29	0/941	0.56	0/1271
5	N	0.28	0/881	0.59	0/1190
6	O	0.24	0/1568	0.54	0/2117
7	P	0.27	0/538	0.53	0/723
8	R	0.34	0/877	0.54	0/1187
9	S	0.31	0/3185	0.53	0/4320
10	A	0.28	0/6435	0.54	0/8690
11	B	0.28	0/7589	0.54	0/10256
12	C	0.26	0/1694	0.54	0/2292
12	D	0.27	0/2294	0.57	2/3107 (0.1%)
13	E	0.25	0/5178	0.53	1/6997 (0.0%)
14	F	0.29	0/4173	0.53	0/5628
15	I	0.27	0/2702	0.50	0/3661
16	J	0.26	0/3567	0.52	1/4829 (0.0%)
17	T	0.25	0/4238	0.51	0/5732
All	All	0.28	0/53198	0.53	4/71942 (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
3	K	0	1
4	L	0	4
6	O	0	1
11	B	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	C	0	1
12	D	0	2
14	F	0	2
15	I	0	1
17	T	0	1
All	All	0	17

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	35	SER	C-N-CD	-11.12	96.14	120.60
13	E	607	ASP	CB-CG-OD1	5.68	123.41	118.30
12	D	248	LEU	CA-CB-CG	-5.55	102.53	115.30
16	J	482	LEU	CA-CB-CG	5.36	127.62	115.30

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	B	186	ARG	Sidechain
11	B	195	ARG	Sidechain
11	B	205	ARG	Sidechain
11	B	249	ARG	Sidechain
12	C	155	ARG	Sidechain
12	D	104	ARG	Sidechain
12	D	35	SER	Peptide
14	F	196	ARG	Sidechain
14	F	534	ARG	Sidechain
15	I	537	ARG	Sidechain
3	K	214	ARG	Sidechain
4	L	108	ARG	Sidechain
4	L	160	ARG	Sidechain
4	L	182	ARG	Sidechain
4	L	264	ARG	Sidechain
6	O	690	ARG	Sidechain
17	T	605	ARG	Sidechain

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	G	1766	0	1691	16	0
2	H	1892	0	1857	30	0
3	K	1681	0	1648	24	0
4	L	1801	0	1732	23	0
5	M	925	0	919	23	0
5	N	867	0	867	15	0
6	O	1538	0	1470	21	0
7	P	530	0	510	11	0
8	R	852	0	836	15	0
9	S	3104	0	3026	30	0
10	A	6310	0	6385	84	0
11	B	7445	0	7523	120	0
12	C	1666	0	1685	16	0
12	D	2249	0	2288	20	0
13	E	5075	0	5030	44	0
14	F	4060	0	3959	65	0
15	I	2645	0	2629	46	0
16	J	3477	0	3414	42	0
17	T	4151	0	4219	46	0
18	G	1	0	0	0	0
18	L	1	0	0	0	0
19	B	1	0	0	0	0
20	J	27	0	22	1	0
All	All	52064	0	51710	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 6.

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)
10:A:99:ILE:HG21	10:A:354:ASN:HB2	1.56	0.88
9:S:184:LYS:HD3	9:S:185:PHE:H	1.38	0.87
17:T:20:ILE:HD13	17:T:23:TRP:HE1	1.44	0.82
11:B:493:ILE:HD11	14:F:374:ILE:HB	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:1163:LEU:HD13	11:B:1165:LEU:HB3	1.61	0.81
2:H:407:PRO:O	9:S:123:LYS:NZ	2.16	0.79
12:D:247:THR:HG23	15:I:537:ARG:HA	1.67	0.77
17:T:630:TYR:OH	17:T:641:ARG:NH1	2.18	0.76
11:B:1166:GLU:HA	11:B:1169:ILE:HG22	1.67	0.75
11:B:209:VAL:HG12	11:B:210:VAL:HG13	1.68	0.75
17:T:20:ILE:HA	17:T:23:TRP:CD1	2.22	0.75
3:K:272:GLY:O	3:K:275:ARG:NH1	2.21	0.74
10:A:1045:VAL:HG23	10:A:1055:LEU:HB3	1.70	0.74
5:N:143:ARG:NH2	15:I:389:GLU:OE1	2.21	0.73
10:A:1000:VAL:HG22	10:A:1003:ILE:HD13	1.69	0.72
2:H:211:ARG:HB3	2:H:212:PRO:HD2	1.70	0.72
13:E:113:VAL:HG11	13:E:143:THR:HG23	1.71	0.72
11:B:449:GLU:OE2	11:B:926:ARG:NH1	2.22	0.71
14:F:85:GLU:OE2	14:F:314:ARG:NH2	2.24	0.71
11:B:1196:GLN:HE22	13:E:741:PHE:H	1.38	0.71
11:B:410:VAL:HG12	11:B:411:GLN:H	1.57	0.69
2:H:299:GLU:OE2	2:H:302:ARG:NH2	2.24	0.69
13:E:844:PHE:HB3	13:E:848:LEU:HD12	1.73	0.69
13:E:147:LEU:HD22	13:E:163:LEU:HD22	1.74	0.68
10:A:543:ARG:HH21	10:A:862:ARG:HA	1.59	0.68
10:A:1049:ARG:HD2	17:T:23:TRP:CH2	2.29	0.68
14:F:406:LYS:NZ	14:F:447:GLU:OE2	2.26	0.68
12:C:39:LYS:HE2	12:C:195:LYS:HB2	1.75	0.67
3:K:248:GLU:OE2	3:K:275:ARG:NH2	2.27	0.67
5:M:79:ARG:NH2	5:M:85:GLU:OE2	2.25	0.66
11:B:1168:ARG:NH1	13:E:741:PHE:O	2.27	0.66
11:B:1240:SER:HB2	11:B:1263:GLU:HG3	1.78	0.66
6:O:576:ARG:NH1	6:O:591:ASP:OD2	2.28	0.66
15:I:461:ILE:HD12	15:I:523:ILE:HG12	1.78	0.65
5:M:106:TRP:HZ2	9:S:107:VAL:HG23	1.62	0.65
15:I:242:TYR:OH	15:I:476:GLU:OE2	2.15	0.65
5:N:167:THR:HG21	5:N:171:ILE:HD13	1.80	0.64
2:H:216:ILE:HD12	2:H:216:ILE:H	1.60	0.64
13:E:107:ARG:NH2	16:J:409:PRO:O	2.29	0.64
15:I:221:ASN:HD22	15:I:432:LYS:HB3	1.63	0.64
11:B:1161:ILE:HG22	11:B:1166:GLU:HB2	1.79	0.64
11:B:1285:ILE:HG21	11:B:1317:VAL:HG21	1.79	0.64
5:M:83:ALA:O	5:M:87:GLN:NE2	2.30	0.64
3:K:333:TRP:HZ2	17:T:550:ILE:HD11	1.63	0.64
16:J:50:SER:HB2	17:T:610:GLN:HE22	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:77:VAL:O	9:S:259:LYS:NZ	2.31	0.64
5:M:73:ARG:NH1	5:M:74:GLU:OE2	2.32	0.63
10:A:664:TRP:H	10:A:668:ASN:HD21	1.44	0.63
4:L:56:PRO:HG2	4:L:59:ALA:HB2	1.80	0.63
10:A:872:SER:HB3	10:A:906:LEU:HD11	1.80	0.63
4:L:211:PRO:HA	4:L:214:TRP:CE3	2.34	0.62
10:A:540:ASP:OD1	11:B:150:ARG:NH2	2.32	0.62
11:B:1316:VAL:HG13	11:B:1322:ILE:HD11	1.81	0.62
6:O:603:LEU:HA	6:O:606:VAL:HG12	1.81	0.62
16:J:355:SER:OG	16:J:420:GLU:OE1	2.13	0.62
10:A:1049:ARG:HD2	17:T:23:TRP:HH2	1.63	0.62
5:M:147:VAL:HG22	5:M:152:THR:HG21	1.81	0.61
14:F:455:TYR:CD2	14:F:456:LYS:HG2	2.34	0.61
2:H:348:SER:HA	12:D:18:VAL:HG13	1.82	0.61
12:C:64:ARG:HB3	12:C:150:LYS:HB2	1.83	0.61
15:I:446:HIS:CE1	15:I:448:ASN:HB2	2.35	0.61
7:P:133:VAL:HG22	7:P:138:PHE:HB2	1.83	0.61
5:M:73:ARG:HE	10:A:585:HIS:HE1	1.48	0.61
16:J:131:ARG:HG3	16:J:273:GLN:HE21	1.64	0.61
11:B:572:ARG:NH2	11:B:806:ASP:OD2	2.32	0.60
8:R:53:VAL:HG21	8:R:111:LEU:HB2	1.82	0.60
10:A:991:GLU:OE1	17:T:453:ASN:ND2	2.34	0.60
15:I:483:PHE:HB3	15:I:537:ARG:HD3	1.83	0.60
1:G:74:VAL:HG23	1:G:78:LYS:HE3	1.83	0.60
6:O:629:ARG:NH2	6:O:653:GLU:OE1	2.30	0.60
10:A:667:TYR:O	10:A:833:SER:OG	2.17	0.60
10:A:562:LYS:HG3	10:A:647:VAL:HB	1.84	0.60
12:C:97:LYS:NZ	12:C:128:GLU:OE1	2.35	0.60
10:A:659:VAL:HG22	10:A:852:MET:HB2	1.83	0.60
10:A:993:TRP:HH2	11:B:204:ARG:HG2	1.67	0.60
11:B:492:SER:O	11:B:495:LYS:NZ	2.34	0.60
11:B:1026:GLU:OE1	14:F:221:ARG:NH1	2.33	0.60
11:B:1260:ALA:HB1	13:E:308:LEU:HD22	1.82	0.60
17:T:158:LEU:HD21	17:T:175:ILE:HD13	1.84	0.59
6:O:725:GLN:O	6:O:731:LYS:HA	2.02	0.59
15:I:304:SER:OG	15:I:307:LYS:NZ	2.35	0.59
9:S:430:ILE:HG13	9:S:450:LEU:HD22	1.84	0.59
7:P:108:THR:HA	7:P:111:VAL:HG12	1.85	0.59
11:B:390:ILE:HG23	11:B:397:ILE:HG23	1.84	0.59
11:B:1033:LEU:HD23	11:B:1039:LEU:HD22	1.85	0.59
17:T:212:ILE:HD11	17:T:251:ALA:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:110:HIS:HB2	13:E:140:LEU:HD21	1.84	0.58
11:B:41:GLN:NE2	17:T:664:GLU:OE2	2.30	0.58
11:B:1129:LEU:HD23	11:B:1130:VAL:HG23	1.84	0.58
3:K:267:VAL:HG12	3:K:269:VAL:H	1.69	0.58
7:P:118:TYR:OH	7:P:127:HIS:HB2	2.03	0.58
10:A:347:LYS:NZ	10:A:348:LEU:O	2.37	0.58
10:A:490:ASN:OD1	10:A:491:ARG:N	2.37	0.58
10:A:926:LYS:HE2	10:A:941:PRO:HB2	1.85	0.58
11:B:68:LYS:HG3	11:B:111:LEU:HD11	1.86	0.58
12:C:81:GLN:NE2	12:C:82:GLU:OE2	2.34	0.58
10:A:1049:ARG:HB3	17:T:23:TRP:CH2	2.39	0.57
9:S:181:ARG:NH2	9:S:230:GLU:OE1	2.37	0.57
7:P:82:MET:HE3	17:T:510:ARG:HE	1.69	0.57
11:B:1288:ALA:HB1	11:B:1293:THR:HG23	1.86	0.57
11:B:470:LEU:HD13	11:B:1113:ALA:HB3	1.86	0.57
15:I:221:ASN:ND2	15:I:432:LYS:HB3	2.18	0.57
5:M:106:TRP:O	9:S:126:GLN:NE2	2.38	0.57
17:T:611:ARG:NH2	17:T:662:TYR:OH	2.38	0.57
16:J:57:PRO:HB3	16:J:102:PHE:HZ	1.69	0.57
11:B:564:GLU:O	14:F:499:LYS:NZ	2.26	0.56
11:B:1311:GLY:O	11:B:1315:ASN:ND2	2.37	0.56
14:F:380:ARG:HG3	14:F:380:ARG:HH11	1.70	0.56
12:C:104:ARG:HH12	15:I:505:GLN:HE22	1.52	0.56
14:F:335:ARG:NH2	14:F:368:ASP:OD2	2.32	0.56
4:L:197:ASP:O	4:L:198:LYS:HB2	2.06	0.56
14:F:124:ARG:O	14:F:128:ILE:HG12	2.05	0.56
17:T:242:ASP:OD2	17:T:246:ARG:NH1	2.39	0.56
12:D:15:TRP:HA	12:D:33:ILE:O	2.06	0.55
10:A:354:ASN:HB3	10:A:356:VAL:HG22	1.89	0.55
14:F:164:ARG:NH2	14:F:192:LEU:HD13	2.20	0.55
10:A:844:LEU:HD22	10:A:944:ILE:HD13	1.89	0.55
10:A:943:ILE:HG22	11:B:56:SER:HB3	1.88	0.55
11:B:1068:SER:HB2	14:F:314:ARG:HH21	1.69	0.55
5:M:73:ARG:HE	10:A:585:HIS:CE1	2.24	0.55
8:R:49:VAL:HG22	8:R:51:ARG:HG2	1.88	0.55
11:B:276:ARG:NH1	16:J:141:ASP:OD2	2.39	0.55
16:J:478:GLN:NE2	16:J:479:GLU:HG3	2.22	0.55
10:A:1047:GLU:OE1	17:T:366:ARG:NH2	2.40	0.55
11:B:572:ARG:HD3	11:B:803:ARG:HH12	1.71	0.55
2:H:215:PHE:H	3:K:333:TRP:HB3	1.71	0.55
17:T:20:ILE:HG21	17:T:268:LEU:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:286:ASN:ND2	13:E:324:THR:OG1	2.35	0.55
14:F:164:ARG:HH21	14:F:192:LEU:HD13	1.72	0.55
10:A:664:TRP:H	10:A:668:ASN:ND2	2.03	0.55
13:E:161:LEU:HD21	13:E:197:VAL:HB	1.89	0.54
13:E:377:ARG:HH11	13:E:469:ASN:ND2	2.05	0.54
4:L:185:VAL:HG11	14:F:397:LEU:HD13	1.88	0.54
8:R:102:ARG:NH2	14:F:373:GLU:OE2	2.39	0.54
12:D:102:GLY:O	12:D:104:ARG:NH1	2.39	0.54
13:E:137:GLN:N	13:E:137:GLN:OE1	2.41	0.54
9:S:268:LEU:HD22	9:S:297:VAL:HG12	1.88	0.54
9:S:357:THR:HG22	9:S:363:LEU:HD22	1.88	0.54
13:E:203:ARG:HG3	13:E:203:ARG:HH11	1.73	0.54
5:M:150:LEU:HD11	9:S:107:VAL:HG21	1.90	0.54
10:A:339:THR:CG2	10:A:355:LEU:HB2	2.38	0.54
4:L:214:TRP:HZ2	14:F:532:SER:HG	1.53	0.54
11:B:105:TYR:O	11:B:109:GLU:HG2	2.07	0.54
11:B:395:ASP:OD1	11:B:396:ILE:N	2.39	0.54
9:S:81:ASP:OD1	9:S:229:LYS:NZ	2.32	0.54
3:K:333:TRP:CZ2	17:T:550:ILE:HD11	2.42	0.54
11:B:1192:LEU:HB2	13:E:752:MET:HE2	1.90	0.53
14:F:201:ASP:HA	14:F:204:LYS:HE3	1.89	0.53
17:T:546:THR:O	17:T:548:ARG:NH1	2.41	0.53
14:F:131:MET:HG3	14:F:133:ILE:H	1.73	0.53
15:I:366:SER:HB3	15:I:371:ASN:HB2	1.90	0.53
11:B:14:ILE:HG12	17:T:543:THR:HG21	1.91	0.53
11:B:975:ASN:OD1	11:B:976:SER:N	2.42	0.53
14:F:455:TYR:HD2	14:F:456:LYS:HG2	1.74	0.53
5:M:118:GLU:O	5:M:122:VAL:HG23	2.09	0.53
13:E:371:TYR:CZ	13:E:375:LEU:HD11	2.44	0.52
10:A:99:ILE:CG2	10:A:354:ASN:HB2	2.36	0.52
11:B:260:ARG:HA	16:J:150:PHE:CE2	2.44	0.52
11:B:1312:LEU:HD11	11:B:1324:ALA:HB2	1.90	0.52
14:F:447:GLU:HB3	14:F:448:ILE:HD12	1.92	0.52
6:O:625:GLU:HB2	6:O:628:LYS:NZ	2.24	0.52
5:M:102:PHE:O	5:M:150:LEU:HD22	2.10	0.52
11:B:362:ILE:HG13	11:B:410:VAL:HG11	1.92	0.52
16:J:279:ILE:HG12	16:J:304:LEU:HD13	1.92	0.52
3:K:281:LEU:HD11	17:T:623:HIS:HB3	1.91	0.52
16:J:142:ILE:HD12	16:J:142:ILE:H	1.74	0.52
16:J:277:MET:HG3	16:J:279:ILE:HD11	1.91	0.52
11:B:206:LEU:O	11:B:210:VAL:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:217:ASP:HB2	2:H:218:PRO:HD3	1.91	0.52
9:S:312:GLU:OE2	9:S:315:ARG:NH2	2.36	0.52
11:B:211:GLN:N	11:B:211:GLN:OE1	2.43	0.52
2:H:388:VAL:HG12	9:S:433:TRP:HZ3	1.75	0.51
11:B:109:GLU:O	11:B:113:GLN:HG2	2.10	0.51
15:I:451:ILE:HD11	15:I:463:TYR:HB2	1.91	0.51
17:T:181:THR:HA	17:T:184:PHE:HB3	1.92	0.51
10:A:340:ILE:HG13	10:A:355:LEU:HD13	1.92	0.51
11:B:65:ILE:H	11:B:65:ILE:HD12	1.74	0.51
17:T:200:ARG:NH1	17:T:262:GLU:O	2.43	0.51
9:S:184:LYS:HD3	9:S:185:PHE:N	2.16	0.51
11:B:492:SER:OG	14:F:381:PRO:O	2.28	0.51
3:K:284:ILE:HB	17:T:622:VAL:HG22	1.93	0.51
14:F:298:VAL:HG23	14:F:299:HIS:CD2	2.46	0.51
14:F:295:ILE:HD11	14:F:340:LEU:HD13	1.92	0.51
11:B:330:GLU:HG3	11:B:331:PRO:HD3	1.93	0.51
11:B:1326:THR:HG21	17:T:508:GLU:OE2	2.11	0.51
13:E:88:SER:O	13:E:92:GLU:HG3	2.11	0.51
14:F:375:ARG:O	14:F:379:GLY:N	2.43	0.51
15:I:474:GLY:HA3	15:I:523:ILE:HD12	1.92	0.51
16:J:298:ARG:NH1	16:J:305:GLU:OE2	2.40	0.51
13:E:494:LEU:HD21	13:E:513:VAL:HG13	1.93	0.50
4:L:182:ARG:HH22	4:L:268:ARG:HD2	1.76	0.50
11:B:205:ARG:HB3	11:B:1274:ILE:HG21	1.94	0.50
11:B:309:THR:HG23	11:B:310:HIS:CE1	2.46	0.50
11:B:1038:ASN:ND2	11:B:1053:GLN:O	2.43	0.50
11:B:458:HIS:HE1	14:F:81:TRP:CE2	2.29	0.50
13:E:203:ARG:NH1	13:E:235:GLU:OE2	2.44	0.50
16:J:295:LEU:HD22	16:J:304:LEU:HD21	1.93	0.50
16:J:283:ASP:O	20:J:501:SAM:HG1	2.12	0.50
4:L:258:LEU:O	4:L:262:MET:HG2	2.12	0.50
10:A:817:LYS:N	10:A:820:ASP:OD2	2.41	0.50
1:G:54:LYS:HG2	14:F:196:ARG:HH12	1.75	0.50
4:L:219:LEU:HD21	4:L:258:LEU:HD13	1.92	0.50
6:O:698:ARG:NH1	6:O:739:GLU:OE1	2.43	0.50
10:A:999:GLY:O	11:B:1326:THR:HG22	2.11	0.50
16:J:56:PHE:CG	16:J:57:PRO:HD2	2.47	0.50
2:H:405:ARG:HG2	10:A:635:LYS:HE2	1.93	0.50
8:R:117:TRP:O	14:F:546:ARG:NH2	2.31	0.50
8:R:132:TYR:CZ	14:F:519:ARG:HG2	2.46	0.50
11:B:192:THR:O	11:B:196:THR:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:83:THR:OG1	17:T:510:ARG:NH2	2.45	0.49
9:S:191:THR:O	9:S:214:PRO:HD2	2.12	0.49
15:I:208:SER:HB2	15:I:210:GLN:OE1	2.12	0.49
12:C:116:ILE:HD12	12:C:145:LEU:HD23	1.95	0.49
12:C:181:ASN:OD1	17:T:592:ARG:NH1	2.39	0.49
17:T:620:ILE:HD13	17:T:635:ALA:N	2.27	0.49
11:B:455:ASP:O	11:B:471:PRO:HD2	2.12	0.49
12:D:50:ARG:NH1	12:D:182:ALA:O	2.46	0.49
13:E:885:ASP:OD1	13:E:886:LYS:N	2.45	0.49
17:T:184:PHE:HA	17:T:187:PHE:CE2	2.47	0.49
10:A:440:ILE:HD11	10:A:528:ILE:HA	1.94	0.49
9:S:381:LEU:HD12	10:A:520:ILE:HG21	1.93	0.49
10:A:67:ARG:NH1	10:A:609:PRO:HG2	2.27	0.49
13:E:161:LEU:HD11	13:E:197:VAL:HG23	1.95	0.49
12:D:108:ILE:HD12	12:D:147:ILE:HD11	1.94	0.49
10:A:661:TYR:HB2	10:A:943:ILE:CG2	2.43	0.49
11:B:1163:LEU:CD1	11:B:1165:LEU:HB3	2.37	0.49
14:F:372:ASP:HA	14:F:375:ARG:HG2	1.95	0.49
4:L:215:ASP:OD1	4:L:264:ARG:NH2	2.44	0.49
8:R:73:LYS:HD3	8:R:125:ASN:HA	1.93	0.49
11:B:1312:LEU:HG	11:B:1322:ILE:HG23	1.94	0.49
12:D:119:ARG:HB2	12:D:132:ASN:HB3	1.94	0.49
12:D:221:ASN:O	12:D:225:LEU:HG	2.13	0.49
6:O:741:ARG:O	6:O:745:GLN:NE2	2.45	0.49
10:A:99:ILE:HG21	10:A:354:ASN:CB	2.38	0.49
11:B:58:GLY:H	11:B:61:ASP:HB2	1.78	0.49
16:J:425:CYS:HB2	16:J:471:ILE:HD11	1.95	0.49
11:B:205:ARG:NH2	11:B:1154:GLU:OE1	2.41	0.48
2:H:393:ASN:HD21	9:S:434:THR:HB	1.77	0.48
3:K:160:ASP:OD2	3:K:237:ARG:NH1	2.42	0.48
10:A:927:SER:HB2	10:A:944:ILE:HD12	1.94	0.48
13:E:203:ARG:HH11	13:E:203:ARG:CG	2.26	0.48
2:H:352:ASP:OD2	2:H:356:ARG:NH1	2.47	0.48
11:B:1195:VAL:HG21	13:E:757:VAL:HG21	1.95	0.48
5:N:113:MET:SD	5:N:170:LEU:HD12	2.53	0.48
17:T:139:GLY:HA2	17:T:143:CYS:SG	2.53	0.48
1:G:87:LEU:HD22	1:G:122:ALA:HA	1.95	0.48
16:J:50:SER:O	17:T:610:GLN:NE2	2.47	0.48
13:E:892:GLN:OE1	13:E:892:GLN:N	2.47	0.48
6:O:743:ALA:HA	6:O:746:TYR:CZ	2.49	0.48
10:A:664:TRP:CE3	10:A:674:LEU:HD21	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:424:GLU:O	16:J:427:LYS:HG2	2.13	0.48
2:H:252:ARG:NH1	2:H:254:ASP:OD1	2.44	0.48
2:H:277:THR:HB	3:K:327:ASP:HB3	1.95	0.48
2:H:405:ARG:NH2	5:M:75:ASP:HB3	2.29	0.48
13:E:120:GLY:HA2	13:E:150:LEU:HD11	1.94	0.48
10:A:99:ILE:HD12	10:A:356:VAL:HG21	1.95	0.48
16:J:201:THR:HG23	16:J:203:GLU:H	1.79	0.48
10:A:95:GLN:OE1	10:A:351:THR:HG23	2.14	0.48
11:B:1196:GLN:NE2	13:E:741:PHE:H	2.10	0.48
12:C:15:TRP:HA	12:C:33:ILE:O	2.13	0.48
13:E:497:GLU:OE1	13:E:614:ARG:NH2	2.44	0.48
15:I:425:THR:O	15:I:432:LYS:NZ	2.45	0.48
14:F:337:ARG:HA	14:F:363:PHE:CE2	2.49	0.47
14:F:456:LYS:O	14:F:457:LYS:HG2	2.14	0.47
10:A:826:HIS:NE2	10:A:870:GLU:OE1	2.44	0.47
13:E:140:LEU:H	13:E:140:LEU:HD23	1.80	0.47
16:J:291:PRO:HG3	16:J:323:ASN:HB2	1.95	0.47
5:M:163:ASP:N	5:M:163:ASP:OD1	2.47	0.47
7:P:93:GLU:HG3	7:P:99:PHE:CD1	2.50	0.47
10:A:67:ARG:HH12	10:A:609:PRO:HG2	1.80	0.47
13:E:822:ILE:HG23	13:E:855:LEU:HD22	1.96	0.47
15:I:241:LYS:NZ	15:I:424:ASP:OD2	2.32	0.47
5:N:112:LEU:HD13	12:D:248:LEU:HD21	1.96	0.47
5:N:165:ILE:HD12	5:N:165:ILE:H	1.77	0.47
6:O:696:VAL:O	6:O:699:VAL:HG22	2.15	0.47
9:S:351:LEU:HD21	9:S:354:LEU:HD12	1.97	0.47
10:A:336:VAL:HA	10:A:339:THR:HG22	1.96	0.47
11:B:926:ARG:HD2	11:B:941:LEU:HD11	1.95	0.47
3:K:154:ARG:HB2	3:K:168:GLU:HB2	1.97	0.47
4:L:99:GLU:HG3	4:L:212:LEU:HD13	1.96	0.47
1:G:211:LEU:HD13	1:G:233:PHE:CG	2.49	0.47
2:H:306:GLU:HB3	2:H:310:ALA:HB3	1.96	0.47
9:S:311:TYR:HA	9:S:314:ARG:HB3	1.97	0.47
11:B:455:ASP:HB2	11:B:474:SER:HB3	1.97	0.47
16:J:460:ARG:CG	16:J:464:LYS:HE3	2.44	0.47
16:J:460:ARG:HG2	16:J:464:LYS:HE3	1.96	0.47
1:G:249:ARG:HG3	11:B:991:SER:OG	2.15	0.47
16:J:118:VAL:HG22	16:J:307:MET:SD	2.55	0.47
17:T:367:PHE:HA	17:T:371:LEU:HD13	1.96	0.47
10:A:387:ILE:HD12	10:A:573:VAL:HG13	1.96	0.47
10:A:661:TYR:HB2	10:A:943:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:86:LEU:HD23	5:N:141:PHE:CE2	2.49	0.47
9:S:297:VAL:O	9:S:356:VAL:HA	2.15	0.47
11:B:55:ILE:O	11:B:55:ILE:HG22	2.15	0.47
11:B:271:ILE:HD12	11:B:271:ILE:H	1.80	0.47
12:C:16:LYS:HA	12:D:234:GLU:HA	1.97	0.46
13:E:269:GLU:HG2	13:E:273:TYR:CE2	2.50	0.46
15:I:248:GLY:N	15:I:492:ASP:OD1	2.48	0.46
3:K:208:PRO:HG3	3:K:219:LYS:HD2	1.96	0.46
4:L:185:VAL:HG13	14:F:396:GLY:HA2	1.96	0.46
11:B:1256:ARG:NH1	13:E:306:GLU:OE2	2.40	0.46
12:D:260:LEU:HD23	12:D:266:GLU:O	2.15	0.46
1:G:57:PRO:HG3	14:F:196:ARG:HH21	1.79	0.46
2:H:227:THR:OG1	11:B:415:TYR:HB2	2.16	0.46
5:M:106:TRP:CZ2	9:S:107:VAL:HG23	2.47	0.46
11:B:562:PHE:HZ	14:F:415:GLN:HE21	1.64	0.46
13:E:110:HIS:O	13:E:113:VAL:HG12	2.16	0.46
5:N:163:ASP:OD1	15:I:307:LYS:N	2.48	0.46
6:O:719:LYS:HE3	6:O:722:GLU:HB2	1.96	0.46
11:B:410:VAL:HG12	11:B:411:GLN:N	2.30	0.46
13:E:809:PRO:HD2	13:E:840:LEU:HD21	1.97	0.46
14:F:121:PRO:O	14:F:125:LYS:HG2	2.16	0.46
11:B:481:GLY:HA3	11:B:939:LEU:HD12	1.98	0.46
3:K:273:ARG:O	3:K:277:ARG:NH2	2.49	0.46
13:E:416:TRP:HZ3	13:E:791:GLU:HG3	1.81	0.46
13:E:270:ASN:HD21	17:T:2:ILE:HG22	1.79	0.46
4:L:122:TRP:CE2	4:L:212:LEU:HD11	2.51	0.46
11:B:865:LYS:HE3	14:F:436:LEU:HD22	1.96	0.46
2:H:411:GLU:OE2	5:M:76:TYR:OH	2.35	0.46
11:B:1233:LEU:HD22	11:B:1270:VAL:CG2	2.45	0.46
10:A:919:PHE:CE1	10:A:924:PRO:HB3	2.51	0.45
5:N:113:MET:O	5:N:117:LEU:HG	2.16	0.45
10:A:339:THR:HG23	10:A:355:LEU:HB2	1.98	0.45
10:A:939:GLU:OE2	11:B:53:THR:HG22	2.16	0.45
11:B:461:GLU:OE2	11:B:469:LEU:HD13	2.16	0.45
11:B:1129:LEU:CD2	11:B:1130:VAL:HG23	2.46	0.45
14:F:252:TYR:CG	14:F:253:PRO:HD2	2.51	0.45
14:F:375:ARG:HG3	14:F:376:ARG:N	2.30	0.45
15:I:406:VAL:O	15:I:454:VAL:HA	2.17	0.45
15:I:474:GLY:HA3	15:I:523:ILE:HG21	1.97	0.45
16:J:140:PRO:HB2	16:J:142:ILE:HD11	1.97	0.45
17:T:620:ILE:HD13	17:T:635:ALA:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:216:ILE:HD13	2:H:220:LYS:HE3	1.98	0.45
9:S:404:LEU:HD22	9:S:411:PHE:CZ	2.51	0.45
16:J:138:PHE:CE1	16:J:169:LEU:HD21	2.51	0.45
2:H:211:ARG:CB	2:H:212:PRO:HD2	2.45	0.45
4:L:179:LYS:HG3	4:L:216:TYR:CE1	2.52	0.45
10:A:372:HIS:CE1	10:A:374:LEU:HD12	2.52	0.45
10:A:453:PRO:O	10:A:524:GLN:NE2	2.47	0.45
11:B:153:MET:H	11:B:161:ILE:HG22	1.81	0.45
15:I:478:VAL:HG21	15:I:530:GLN:HG2	1.97	0.45
16:J:131:ARG:CG	16:J:273:GLN:HE21	2.28	0.45
2:H:279:THR:HG23	3:K:322:LEU:HD22	1.99	0.45
3:K:193:ILE:HD12	3:K:231:LYS:HD3	1.98	0.45
3:K:334:PHE:OXT	3:K:334:PHE:CG	2.69	0.45
5:M:105:THR:HG21	9:S:114:MET:H	1.81	0.45
10:A:1042:ARG:HG2	10:A:1046:ARG:HD2	1.98	0.45
11:B:455:ASP:OD2	14:F:96:ARG:NH1	2.36	0.45
11:B:1312:LEU:HD11	11:B:1324:ALA:CB	2.47	0.45
12:C:84:VAL:HA	12:C:87:ILE:HD12	1.99	0.45
14:F:171:TRP:CH2	14:F:229:TYR:HA	2.52	0.45
4:L:162:LYS:HG2	4:L:241:ILE:HG22	1.99	0.45
5:M:148:ARG:NH2	9:S:242:THR:OG1	2.50	0.45
10:A:272:LEU:HB3	10:A:274:ILE:HD12	1.98	0.45
10:A:871:CYS:HB3	10:A:945:GLY:HA3	1.99	0.45
11:B:1303:ARG:HG3	17:T:253:HIS:CD2	2.51	0.45
17:T:20:ILE:HG21	17:T:268:LEU:CB	2.46	0.45
10:A:351:THR:HA	10:A:354:ASN:HA	1.99	0.45
10:A:590:LEU:HD11	10:A:600:SER:HB2	1.98	0.45
13:E:308:LEU:HD12	13:E:328:LEU:HD22	1.98	0.45
4:L:214:TRP:CZ2	14:F:529:ARG:HA	2.52	0.45
11:B:452:TRP:O	11:B:452:TRP:CD1	2.70	0.45
11:B:926:ARG:HH12	11:B:928:PHE:HZ	1.65	0.45
12:C:175:VAL:HB	17:T:593:GLN:HE22	1.82	0.45
14:F:303:VAL:HG11	14:F:344:PHE:CD2	2.51	0.45
8:R:92:GLU:OE2	8:R:94:ARG:HD3	2.17	0.45
11:B:1314:GLU:OE1	11:B:1314:GLU:N	2.48	0.45
13:E:117:ALA:HA	13:E:150:LEU:HD22	1.98	0.45
1:G:150:GLN:HA	1:G:153:LYS:HG2	1.99	0.45
11:B:187:LYS:HG2	11:B:188:GLY:N	2.31	0.45
11:B:456:VAL:HG22	11:B:470:LEU:HG	1.99	0.45
13:E:90:VAL:O	13:E:94:ILE:HG12	2.17	0.45
1:G:126:TYR:CZ	1:G:201:LEU:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:133:TYR:HB3	10:A:306:MET:HE1	1.98	0.44
11:B:473:THR:HG21	14:F:99:LEU:HB2	1.99	0.44
12:D:58:GLU:OE1	12:D:101:TYR:OH	2.30	0.44
14:F:317:ILE:HD13	14:F:344:PHE:CE2	2.52	0.44
15:I:532:LEU:O	15:I:536:THR:HG23	2.17	0.44
16:J:174:PHE:O	16:J:182:ARG:NH1	2.49	0.44
17:T:20:ILE:HA	17:T:23:TRP:NE1	2.32	0.44
9:S:369:LYS:HG3	9:S:370:PHE:CD2	2.52	0.44
10:A:60:VAL:CG1	10:A:79:GLU:HB2	2.48	0.44
10:A:855:ASN:ND2	17:T:534:ASP:OD2	2.49	0.44
15:I:501:MET:HB2	15:I:518:THR:HG23	1.97	0.44
10:A:668:ASN:HA	10:A:672:ALA:HB3	2.00	0.44
11:B:928:PHE:O	11:B:936:GLN:HA	2.17	0.44
16:J:156:THR:HB	16:J:161:ASP:HB2	1.99	0.44
16:J:432:TYR:OH	16:J:463:ARG:HD3	2.17	0.44
2:H:216:ILE:HG13	3:K:332:ASN:OD1	2.18	0.44
3:K:296:VAL:O	3:K:299:ARG:HG2	2.17	0.44
14:F:284:THR:HG22	14:F:292:PHE:HB2	2.00	0.44
2:H:223:GLN:H	2:H:223:GLN:HG3	1.49	0.44
12:C:227:ILE:HG23	15:I:475:MET:SD	2.57	0.44
15:I:306:MET:O	15:I:307:LYS:HD2	2.18	0.44
1:G:110:TYR:CD2	1:G:202:VAL:HB	2.53	0.44
6:O:659:LEU:HD13	6:O:693:LEU:HD13	1.98	0.44
8:R:83:ASP:OD1	8:R:116:LYS:N	2.43	0.44
15:I:446:HIS:HE1	15:I:448:ASN:HB2	1.78	0.44
16:J:196:SER:HB3	16:J:255:SER:HB2	2.00	0.44
10:A:83:SER:HA	10:A:98:ARG:HA	2.00	0.44
11:B:34:TYR:O	11:B:38:ILE:HG12	2.18	0.44
11:B:572:ARG:HD3	11:B:803:ARG:NH1	2.32	0.44
1:G:54:LYS:HG2	14:F:196:ARG:NH1	2.32	0.44
5:N:121:ALA:HB2	5:N:130:ILE:HG21	2.00	0.44
9:S:235:HIS:HD2	9:S:265:PHE:CD2	2.36	0.44
12:D:39:LYS:HE2	12:D:195:LYS:HE2	2.00	0.44
16:J:475:ASP:O	16:J:478:GLN:HG3	2.17	0.44
1:G:213:VAL:HG12	1:G:213:VAL:O	2.18	0.43
10:A:43:ASP:OD1	10:A:46:HIS:N	2.51	0.43
11:B:473:THR:HG22	11:B:1111:PRO:HD3	2.00	0.43
12:D:52:ALA:HA	12:D:56:GLU:HG2	2.00	0.43
10:A:56:THR:O	10:A:58:GLN:HG3	2.18	0.43
10:A:372:HIS:HE1	10:A:374:LEU:HD12	1.82	0.43
16:J:205:LEU:HD13	16:J:214:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:96:ARG:N	11:B:315:GLU:OE2	2.52	0.43
11:B:92:HIS:CE1	11:B:95:GLU:HG3	2.53	0.43
11:B:995:LEU:HD12	11:B:995:LEU:O	2.19	0.43
11:B:1082:LYS:HB3	11:B:1084:PRO:HD2	2.01	0.43
15:I:226:TYR:HA	15:I:230:GLU:HB3	2.00	0.43
4:L:185:VAL:HG12	4:L:187:ASN:H	1.83	0.43
15:I:307:LYS:HA	15:I:317:THR:HB	2.01	0.43
2:H:319:TRP:CG	2:H:346:MET:HG3	2.53	0.43
11:B:49:GLN:HE22	17:T:541:VAL:HG12	1.84	0.43
11:B:1232:VAL:HG12	11:B:1269:ALA:HA	1.99	0.43
14:F:505:ARG:NH1	14:F:508:GLU:OE1	2.52	0.43
15:I:307:LYS:HE3	15:I:317:THR:O	2.19	0.43
10:A:943:ILE:H	11:B:56:SER:HB3	1.82	0.43
14:F:358:ASP:N	14:F:358:ASP:OD1	2.51	0.43
2:H:233:SER:HA	11:B:411:GLN:HE22	1.83	0.43
2:H:313:SER:OG	2:H:323:THR:HG21	2.19	0.43
10:A:664:TRP:HZ3	10:A:667:TYR:CD2	2.37	0.43
12:C:172:ILE:O	12:C:173:ASP:OD1	2.37	0.43
13:E:323:LYS:HE3	13:E:327:LEU:HD11	2.01	0.43
3:K:323:ARG:NH2	11:B:395:ASP:OD2	2.52	0.43
10:A:917:TRP:O	10:A:927:SER:OG	2.31	0.43
11:B:980:LEU:HD22	11:B:1040:VAL:HG11	2.01	0.43
2:H:220:LYS:O	2:H:221:LYS:HB2	2.19	0.43
4:L:192:LEU:N	4:L:193:PRO:HD3	2.34	0.43
8:R:116:LYS:HE2	8:R:117:TRP:NE1	2.34	0.43
10:A:547:SER:HB2	10:A:825:ARG:O	2.19	0.43
10:A:1049:ARG:HD2	17:T:23:TRP:CZ3	2.54	0.43
11:B:1322:ILE:C	11:B:1324:ALA:H	2.22	0.43
15:I:451:ILE:HD13	15:I:515:LEU:HD13	2.01	0.43
17:T:452:LEU:O	17:T:463:ILE:HD12	2.18	0.43
8:R:79:ASP:OD1	8:R:79:ASP:N	2.52	0.42
9:S:265:PHE:CE2	9:S:397:VAL:HG13	2.54	0.42
11:B:211:GLN:HE22	11:B:1281:THR:HG21	1.84	0.42
8:R:80:TRP:O	8:R:117:TRP:N	2.45	0.42
11:B:254:ASP:OD1	11:B:265:ARG:N	2.50	0.42
14:F:303:VAL:HG22	14:F:342:LEU:HB2	2.01	0.42
15:I:487:MET:O	15:I:487:MET:HG3	2.19	0.42
15:I:507:ASP:OD1	15:I:507:ASP:N	2.50	0.42
4:L:183:LEU:HB2	4:L:188:ALA:CB	2.49	0.42
8:R:59:ASP:OD1	8:R:60:GLU:N	2.53	0.42
8:R:86:VAL:HG13	8:R:130:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:446:ASP:N	10:A:446:ASP:OD1	2.51	0.42
13:E:455:LYS:NZ	17:T:260:GLU:OE2	2.37	0.42
16:J:71:GLU:OE1	16:J:71:GLU:N	2.52	0.42
1:G:161:PHE:CE1	1:G:180:LEU:HD13	2.53	0.42
3:K:172:THR:HG22	3:K:173:PRO:O	2.19	0.42
12:C:104:ARG:HH22	15:I:505:GLN:NE2	2.16	0.42
12:D:34:LEU:HD23	12:D:37:LEU:HD11	2.01	0.42
12:D:263:LYS:HE2	12:D:265:LYS:HE3	2.01	0.42
15:I:307:LYS:HG3	15:I:317:THR:O	2.19	0.42
15:I:483:PHE:CZ	15:I:540:PRO:HG3	2.55	0.42
16:J:287:HIS:HB2	16:J:324:TYR:CE2	2.54	0.42
4:L:58:ASP:OD1	4:L:66:ARG:HD2	2.20	0.42
5:M:178:ASP:OD1	5:M:182:ASN:ND2	2.37	0.42
6:O:613:ARG:NH2	6:O:709:GLU:OE1	2.51	0.42
6:O:635:ILE:HG23	6:O:639:LYS:HD3	2.00	0.42
10:A:159:GLU:OE1	10:A:171:ARG:NH1	2.49	0.42
14:F:86:GLU:O	14:F:146:ARG:NH2	2.52	0.42
16:J:409:PRO:HB2	16:J:414:GLU:HG3	2.02	0.42
2:H:231:ASP:HB2	14:F:121:PRO:HB2	2.01	0.42
2:H:257:THR:HG22	2:H:281:THR:HG21	2.00	0.42
3:K:267:VAL:HG22	3:K:293:ILE:HD12	2.02	0.42
5:N:142:ALA:HB1	5:N:147:VAL:HG21	2.02	0.42
6:O:735:ASP:OD2	6:O:737:ARG:NH2	2.51	0.42
11:B:1314:GLU:H	11:B:1314:GLU:CD	2.23	0.42
16:J:157:ASP:O	16:J:165:ARG:NH1	2.49	0.42
4:L:211:PRO:HA	4:L:214:TRP:HE3	1.83	0.42
5:N:154:PHE:CD1	5:N:166:ARG:HB2	2.55	0.42
7:P:118:TYR:CE1	7:P:122:LYS:HE3	2.55	0.42
11:B:615:PHE:CE1	11:B:810:LEU:HD22	2.54	0.42
11:B:1026:GLU:HA	14:F:164:ARG:NH2	2.35	0.42
13:E:79:MET:SD	16:J:410:ILE:HD13	2.60	0.42
1:G:175:SER:HB3	1:G:214:TRP:CD2	2.55	0.42
10:A:162:ILE:HD11	10:A:168:ILE:HG12	2.02	0.42
10:A:292:HIS:O	10:A:296:MET:HG2	2.20	0.42
12:D:220:ARG:NH1	15:I:229:GLN:HE22	2.17	0.42
13:E:885:ASP:HA	13:E:888:ILE:HG12	2.01	0.42
15:I:533:LEU:HD12	15:I:533:LEU:HA	1.87	0.42
6:O:614:ILE:HG23	6:O:640:SER:HA	2.02	0.42
10:A:352:PRO:O	10:A:354:ASN:N	2.52	0.42
10:A:440:ILE:HG12	10:A:526:PHE:O	2.19	0.42
14:F:418:LEU:HD13	14:F:481:ARG:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:109:PRO:HB2	5:M:151:PRO:HD3	2.02	0.41
5:N:106:TRP:HA	15:I:485:ARG:HD3	2.01	0.41
11:B:149:MET:HG2	11:B:151:GLY:H	1.85	0.41
11:B:247:ILE:HD12	11:B:271:ILE:HG13	2.01	0.41
12:D:100:LEU:O	12:D:104:ARG:NH2	2.53	0.41
5:M:90:VAL:O	5:M:94:ARG:NH1	2.52	0.41
11:B:1284:PHE:CD2	11:B:1307:ASP:HB2	2.54	0.41
15:I:481:THR:HG22	15:I:539:TYR:CZ	2.55	0.41
6:O:625:GLU:O	6:O:628:LYS:HG2	2.21	0.41
6:O:648:ASP:HB2	6:O:697:ARG:HH21	1.84	0.41
6:O:698:ARG:HG2	6:O:734:TYR:HE2	1.84	0.41
7:P:118:TYR:CE1	7:P:122:LYS:HG3	2.55	0.41
11:B:1158:ILE:O	11:B:1273:GLY:HA3	2.20	0.41
14:F:67:THR:HG23	14:F:70:GLU:HB3	2.01	0.41
5:N:166:ARG:HG2	15:I:307:LYS:HZ3	1.84	0.41
6:O:695:ASP:N	6:O:695:ASP:OD1	2.54	0.41
10:A:295:GLY:O	10:A:300:MET:N	2.52	0.41
11:B:119:PHE:HB3	11:B:129:HIS:CG	2.56	0.41
11:B:861:GLU:HG3	11:B:868:ILE:HG23	2.02	0.41
2:H:295:ARG:NH1	2:H:368:ASP:OD2	2.53	0.41
14:F:334:TYR:CZ	14:F:365:ARG:HD3	2.55	0.41
17:T:583:ASN:OD1	17:T:585:TYR:N	2.51	0.41
12:C:104:ARG:HH12	15:I:505:GLN:NE2	2.15	0.41
12:D:63:THR:HG21	12:D:152:GLU:HB3	2.03	0.41
13:E:288:VAL:HG13	13:E:307:LEU:HD23	2.02	0.41
13:E:748:ALA:O	13:E:752:MET:HG3	2.21	0.41
14:F:331:ARG:HB3	14:F:336:PHE:CD2	2.56	0.41
14:F:476:ALA:O	14:F:480:GLU:OE1	2.38	0.41
15:I:199:TRP:CG	15:I:200:PRO:HA	2.55	0.41
16:J:57:PRO:HB3	16:J:102:PHE:CZ	2.51	0.41
3:K:282:LEU:HD21	3:K:284:ILE:HD11	2.03	0.41
11:B:330:GLU:N	11:B:331:PRO:HD2	2.36	0.41
14:F:276:MET:HB2	14:F:327:ILE:HD12	2.02	0.41
1:G:183:LYS:HB2	1:G:186:GLU:O	2.20	0.41
2:H:269:VAL:HG11	3:K:334:PHE:CD1	2.56	0.41
3:K:323:ARG:HE	11:B:358:TYR:HD1	1.69	0.41
5:M:170:LEU:HB2	9:S:101:LYS:HE3	2.02	0.41
16:J:51:LEU:HG	16:J:52:GLU:HG3	2.01	0.41
1:G:150:GLN:OE1	1:G:256:LEU:HD13	2.21	0.41
7:P:118:TYR:HE2	7:P:124:ALA:HA	1.86	0.41
8:R:90:GLU:HG2	8:R:129:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:132:SER:HB3	11:B:143:VAL:HG21	2.02	0.41
14:F:128:ILE:HG23	14:F:133:ILE:O	2.21	0.41
14:F:284:THR:CG2	14:F:292:PHE:HB2	2.50	0.41
14:F:331:ARG:HB2	14:F:339:PRO:HA	2.03	0.41
6:O:702:ARG:HA	6:O:705:VAL:HG22	2.02	0.41
10:A:860:PRO:HG3	11:B:131:MET:SD	2.61	0.41
11:B:473:THR:HG22	11:B:1110:THR:HA	2.03	0.41
11:B:1092:LEU:HG	11:B:1102:ARG:HB2	2.02	0.41
12:C:63:THR:HG21	12:C:152:GLU:HB2	2.02	0.41
14:F:284:THR:HG23	14:F:292:PHE:HD2	1.86	0.41
16:J:248:GLU:HA	16:J:251:ILE:HG22	2.03	0.41
16:J:365:VAL:HG11	16:J:477:TYR:HA	2.03	0.41
4:L:185:VAL:HG11	14:F:397:LEU:CD1	2.51	0.40
5:N:86:LEU:HD23	5:N:141:PHE:HE2	1.86	0.40
10:A:41:ILE:HG13	10:A:336:VAL:HG21	2.02	0.40
11:B:30:PHE:HB3	11:B:34:TYR:HB2	2.04	0.40
11:B:928:PHE:HE2	11:B:1122:ILE:HD11	1.86	0.40
11:B:1179:ILE:HG22	11:B:1180:LEU:HD22	2.03	0.40
12:D:18:VAL:HG21	12:D:33:ILE:HB	2.03	0.40
16:J:163:ASP:OD1	16:J:163:ASP:N	2.54	0.40
5:M:117:LEU:HD11	5:M:153:LEU:HD21	2.03	0.40
5:N:86:LEU:HD21	5:N:100:VAL:HG21	2.03	0.40
6:O:614:ILE:HD11	6:O:715:VAL:HG13	2.02	0.40
7:P:138:PHE:HB3	7:P:140:ARG:NH1	2.36	0.40
8:R:92:GLU:OE2	8:R:105:GLN:HG3	2.20	0.40
14:F:207:LYS:HD2	14:F:211:ASP:OD2	2.20	0.40
14:F:302:TRP:O	14:F:342:LEU:N	2.50	0.40
10:A:869:PHE:HD1	10:A:902:VAL:HG21	1.86	0.40
15:I:267:MET:HE1	15:I:337:LEU:HD21	2.03	0.40
15:I:451:ILE:HD12	15:I:464:TYR:O	2.22	0.40
15:I:487:MET:HG3	15:I:490:SER:OG	2.21	0.40
17:T:249:GLU:O	17:T:253:HIS:ND1	2.39	0.40
5:M:113:MET:HE2	5:M:170:LEU:HD23	2.02	0.40
9:S:321:TYR:CE2	14:F:252:TYR:HB2	2.57	0.40
10:A:331:ARG:O	10:A:335:VAL:HG23	2.21	0.40
10:A:339:THR:HG21	10:A:355:LEU:HB2	2.03	0.40
10:A:675:ILE:HG22	10:A:852:MET:HG2	2.03	0.40
10:A:894:GLU:OE2	10:A:900:LYS:NZ	2.37	0.40
11:B:923:GLY:HA3	11:B:941:LEU:O	2.21	0.40
1:G:179:TRP:CE3	1:G:210:SER:HB3	2.57	0.40
4:L:182:ARG:NH2	4:L:268:ARG:HD2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:196:GLU:H	4:L:196:GLU:HG3	1.69	0.40
9:S:90:PRO:HA	9:S:91:PRO:HD3	1.97	0.40
10:A:32:ILE:HD11	10:A:57:TYR:CE1	2.57	0.40
10:A:675:ILE:HB	10:A:679:LEU:HD12	2.03	0.40
13:E:241:ARG:HH11	13:E:241:ARG:HG2	1.86	0.40
15:I:306:MET:HB2	15:I:319:VAL:HB	2.02	0.40
17:T:101:ARG:HD3	17:T:275:GLU:OE2	2.21	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	G	212/264 (80%)	207 (98%)	5 (2%)	0	100	100
2	H	222/529 (42%)	211 (95%)	10 (4%)	1 (0%)	25	59
3	K	198/334 (59%)	189 (96%)	8 (4%)	1 (0%)	25	59
4	L	220/297 (74%)	213 (97%)	5 (2%)	2 (1%)	14	49
5	M	112/184 (61%)	109 (97%)	3 (3%)	0	100	100
5	N	106/184 (58%)	99 (93%)	7 (7%)	0	100	100
6	O	192/768 (25%)	181 (94%)	11 (6%)	0	100	100
7	P	63/162 (39%)	61 (97%)	2 (3%)	0	100	100
8	R	98/140 (70%)	95 (97%)	3 (3%)	0	100	100
9	S	382/460 (83%)	367 (96%)	14 (4%)	1 (0%)	37	68
10	A	773/1072 (72%)	740 (96%)	32 (4%)	1 (0%)	48	79
11	B	901/1373 (66%)	860 (95%)	39 (4%)	2 (0%)	44	75
12	C	204/327 (62%)	195 (96%)	8 (4%)	1 (0%)	25	59
12	D	272/327 (83%)	253 (93%)	18 (7%)	1 (0%)	30	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	E	624/911 (68%)	602 (96%)	20 (3%)	2 (0%)	37	68
14	F	479/675 (71%)	464 (97%)	15 (3%)	0	100	100
15	I	334/611 (55%)	315 (94%)	18 (5%)	1 (0%)	37	68
16	J	420/483 (87%)	400 (95%)	19 (4%)	1 (0%)	44	75
17	T	487/680 (72%)	470 (96%)	17 (4%)	0	100	100
All	All	6299/9781 (64%)	6031 (96%)	254 (4%)	14 (0%)	45	75

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	212	PRO
4	L	198	LYS
12	D	36	PRO
4	L	186	ALA
15	I	447	GLU
3	K	299	ARG
16	J	51	LEU
11	B	1322	ILE
12	C	55	GLY
11	B	1159	ASP
10	A	1000	VAL
13	E	827	PRO
9	S	380	VAL
13	E	105	GLY

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	G	187/231 (81%)	186 (100%)	1 (0%)	86	93
2	H	204/469 (44%)	201 (98%)	3 (2%)	60	77
3	K	191/299 (64%)	187 (98%)	4 (2%)	48	71
4	L	190/259 (73%)	187 (98%)	3 (2%)	58	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	M	103/168 (61%)	101 (98%)	2 (2%)	52	73
5	N	97/168 (58%)	97 (100%)	0	100	100
6	O	167/661 (25%)	166 (99%)	1 (1%)	84	91
7	P	57/144 (40%)	57 (100%)	0	100	100
8	R	91/127 (72%)	89 (98%)	2 (2%)	47	70
9	S	338/401 (84%)	334 (99%)	4 (1%)	67	82
10	A	688/931 (74%)	685 (100%)	3 (0%)	89	95
11	B	823/1230 (67%)	810 (98%)	13 (2%)	58	76
12	C	185/301 (62%)	185 (100%)	0	100	100
12	D	252/301 (84%)	247 (98%)	5 (2%)	50	72
13	E	541/782 (69%)	540 (100%)	1 (0%)	92	97
14	F	431/609 (71%)	430 (100%)	1 (0%)	92	97
15	I	291/532 (55%)	290 (100%)	1 (0%)	91	96
16	J	378/431 (88%)	377 (100%)	1 (0%)	91	96
17	T	458/608 (75%)	457 (100%)	1 (0%)	92	97
All	All	5672/8652 (66%)	5626 (99%)	46 (1%)	77	88

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	187	ARG
2	H	222	LYS
2	H	223	GLN
2	H	226	THR
3	K	281	LEU
3	K	294	ILE
3	K	295	HIS
3	K	299	ARG
4	L	194	LYS
4	L	196	GLU
4	L	197	ASP
5	M	148	ARG
5	M	150	LEU
6	O	731	LYS
8	R	53	VAL
8	R	121	ASP
9	S	127	TRP

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Mol	Chain	Res	Type
9	S	129	PRO
9	S	181	ARG
9	S	344	LYS
10	A	354	ASN
10	A	355	LEU
10	A	377	VAL
11	B	175	LEU
11	B	179	ILE
11	B	182	CYS
11	B	183	TYR
11	B	186	ARG
11	B	187	LYS
11	B	195	ARG
11	B	201	TYR
11	B	470	LEU
11	B	1096	ARG
11	B	1163	LEU
11	B	1164	ASN
11	B	1318	LEU
12	D	36	PRO
12	D	103	THR
12	D	104	ARG
12	D	105	ASN
12	D	249	PRO
13	E	753	ARG
14	F	318	ARG
15	I	443	PRO
16	J	56	PHE
17	T	101	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	223	GLN
2	H	349	HIS
4	L	187	ASN
9	S	147	HIS
9	S	235	HIS
9	S	432	GLN
10	A	292	HIS
10	A	307	ASN
10	A	354	ASN

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Mol	Chain	Res	Type
10	A	1002	HIS
10	A	1057	HIS
11	B	92	HIS
11	B	398	HIS
11	B	494	HIS
11	B	1196	GLN
11	B	1315	ASN
12	D	276	GLN
13	E	270	ASN
13	E	469	ASN
14	F	355	ASN
14	F	364	HIS
14	F	370	ASN
14	F	401	HIS
14	F	415	GLN
15	I	505	GLN
16	J	273	GLN
16	J	438	GLN
17	T	128	ASN
17	T	593	GLN
17	T	610	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 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
20	SAM	J	501	-	24,29,29	0.67	0	23,42,42	0.88	1 (4%)

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
20	SAM	J	501	-	-	7/12/33/33	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	501	SAM	C5-C6-N6	2.25	123.77	120.35

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	J	501	SAM	O4'-C4'-C5'-SD
20	J	501	SAM	C3'-C4'-C5'-SD
20	J	501	SAM	CB-CG-SD-CE
20	J	501	SAM	CB-CG-SD-C5'
20	J	501	SAM	CA-CB-CG-SD
20	J	501	SAM	O-C-CA-CB
20	J	501	SAM	OXT-C-CA-CB

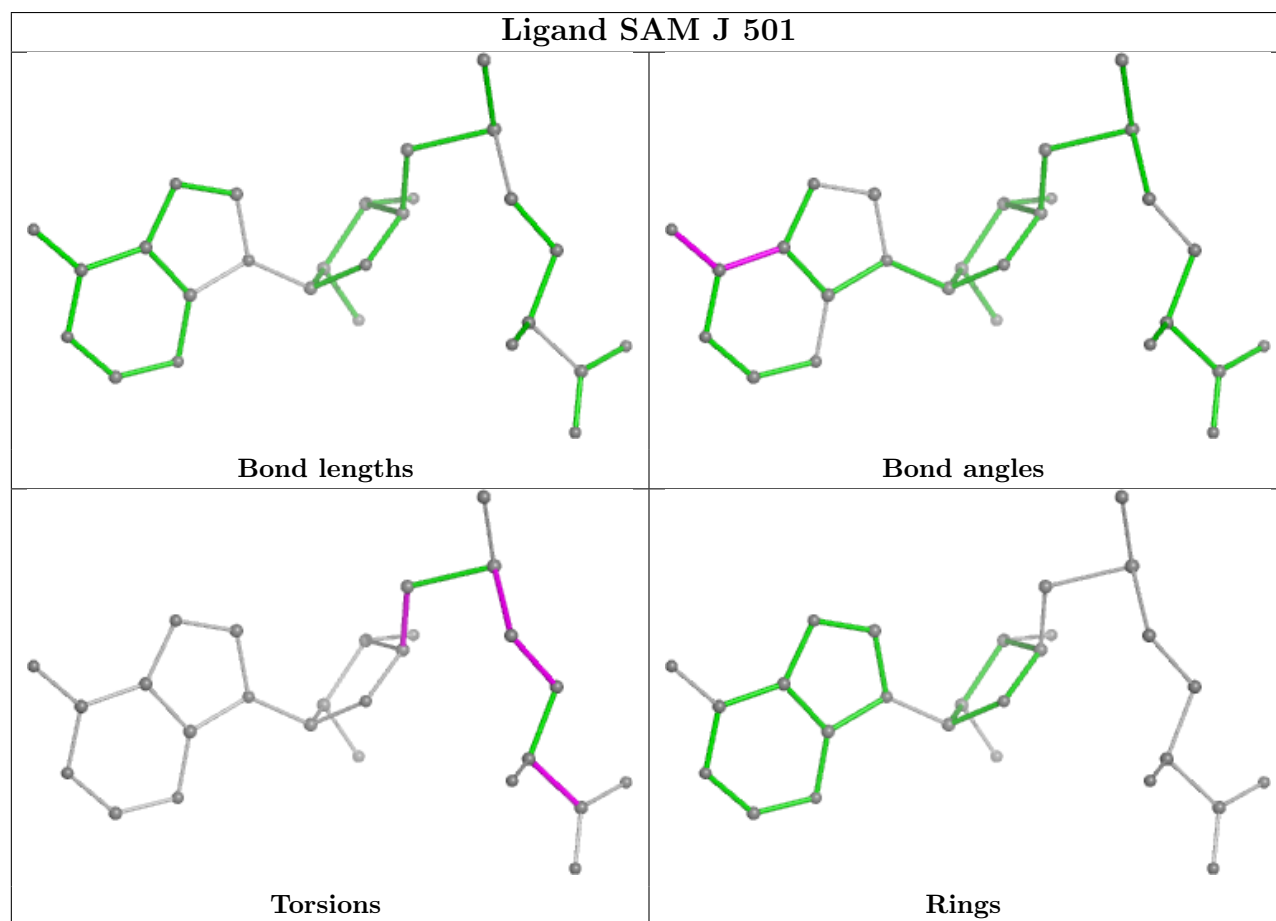
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	J	501	SAM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

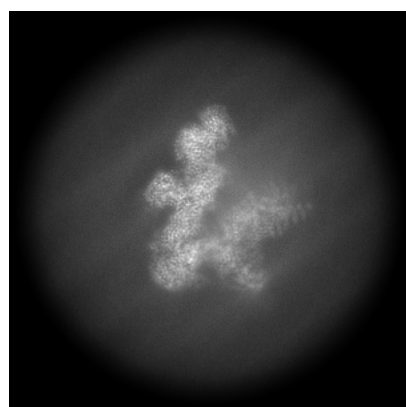
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18496. These allow visual inspection of the internal detail of the map and identification of artifacts.

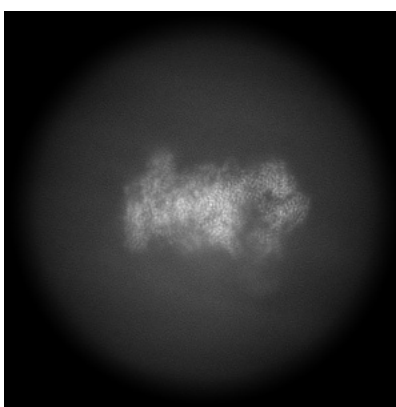
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

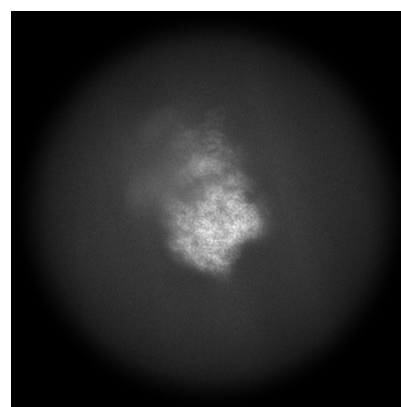
6.1.1 Primary map



X



Y

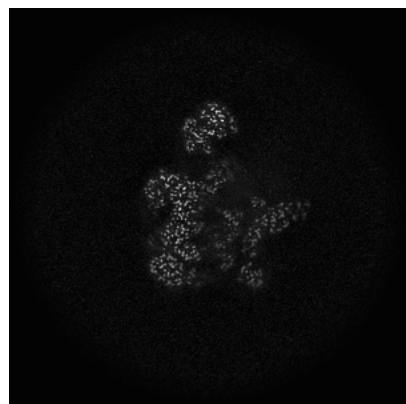


Z

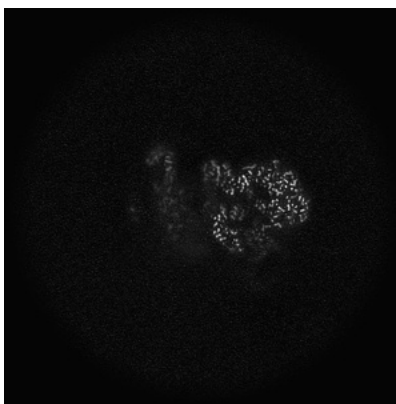
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

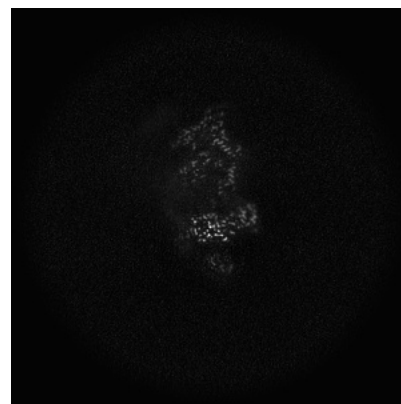
6.2.1 Primary map



X Index: 220



Y Index: 220

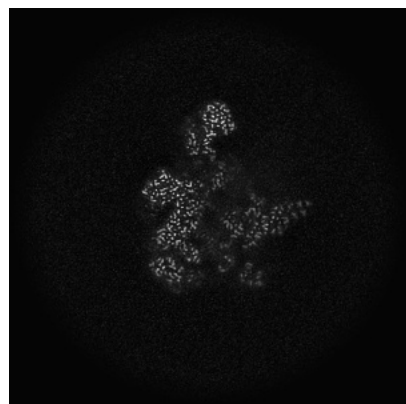


Z Index: 220

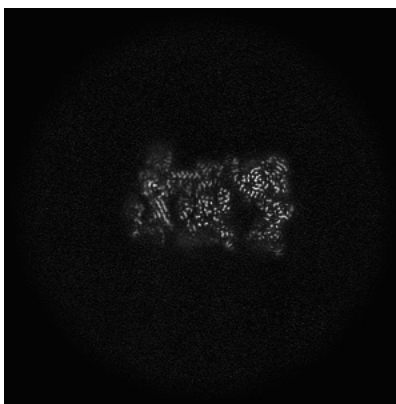
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

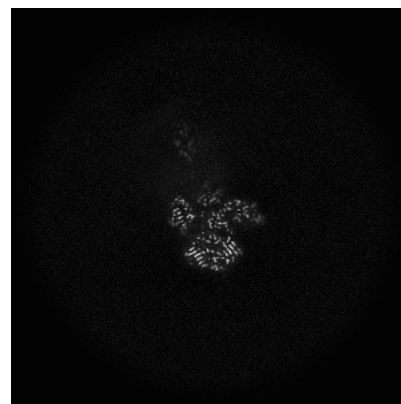
6.3.1 Primary map



X Index: 224



Y Index: 202

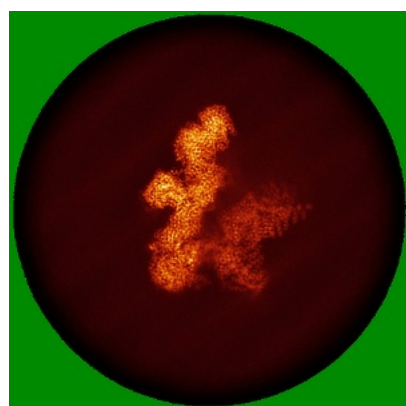


Z Index: 246

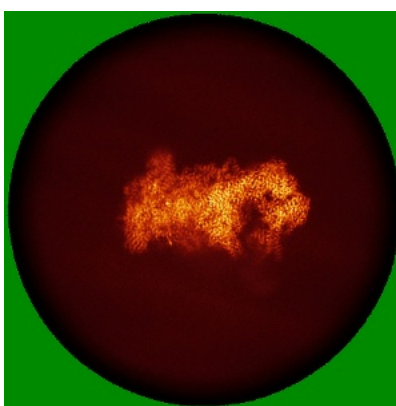
The images above show the largest variance slices of the map in three orthogonal directions.

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

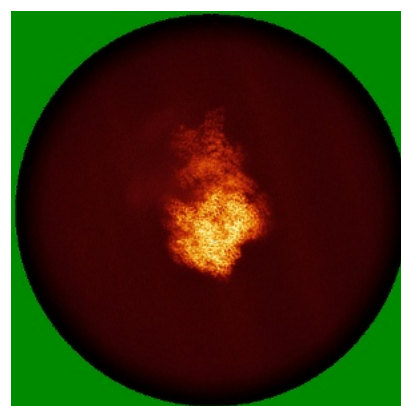
6.4.1 Primary map



X



Y

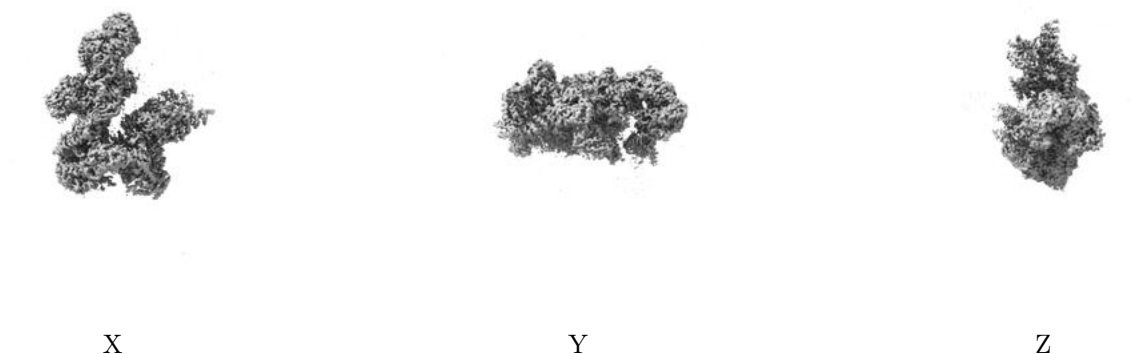


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

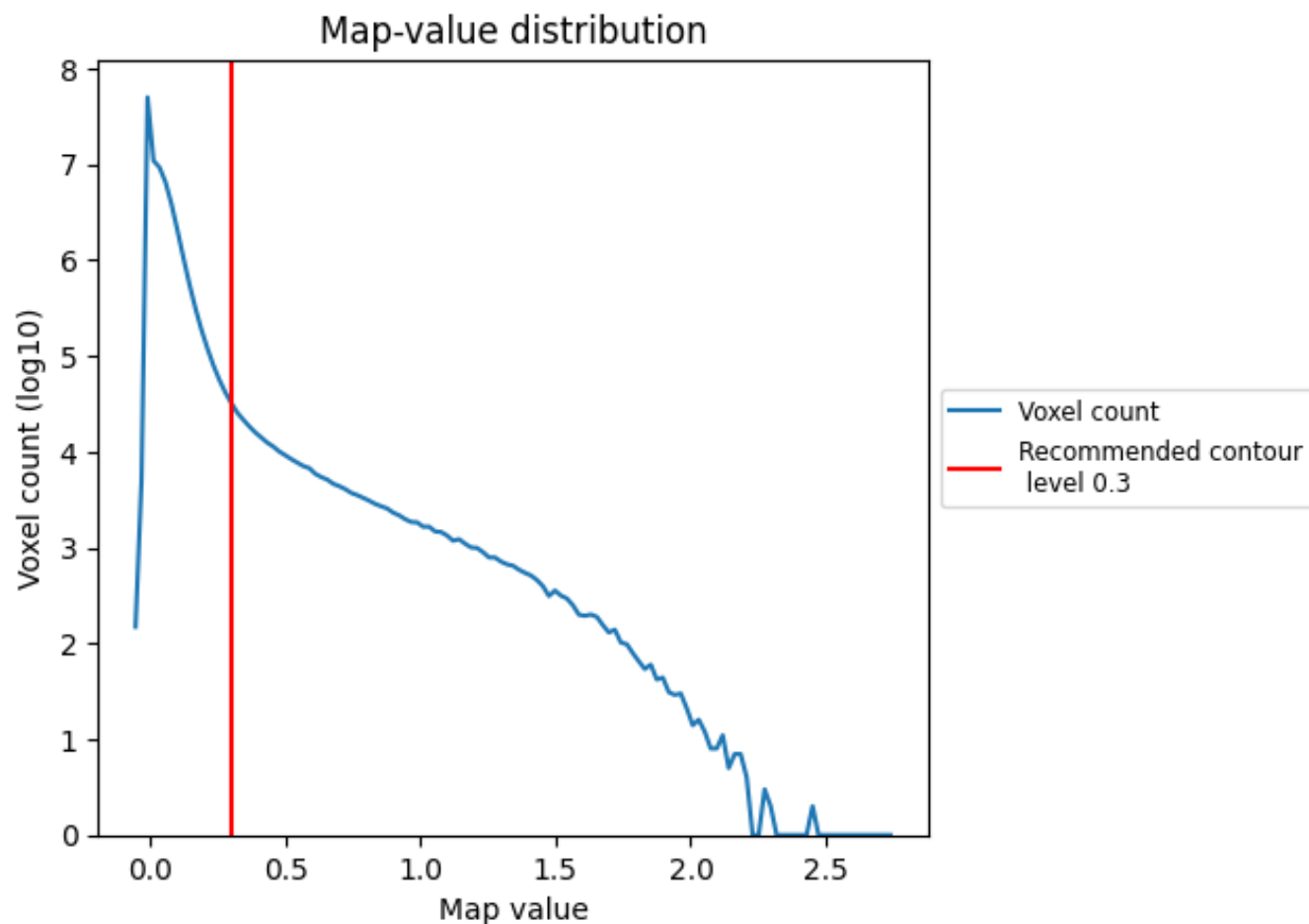
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

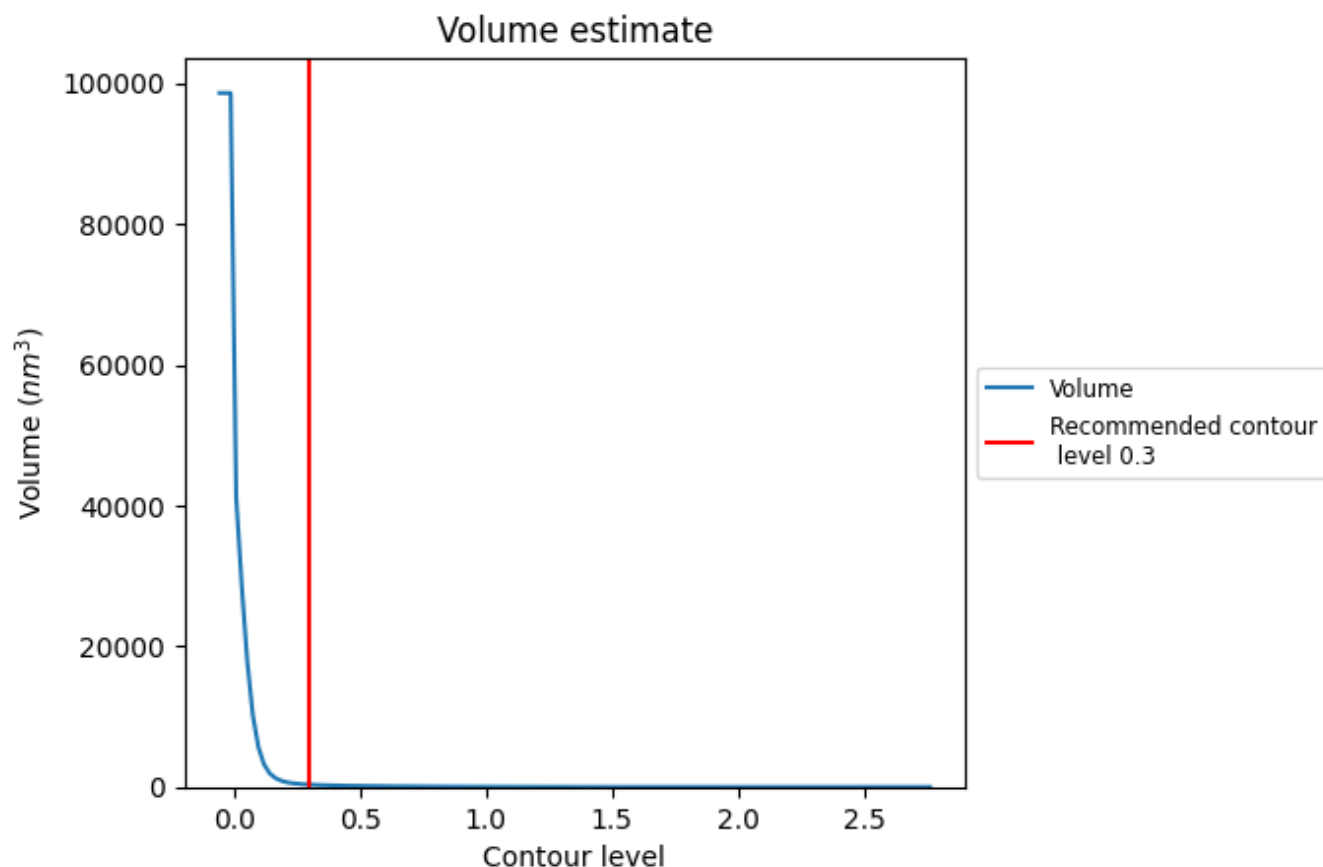
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

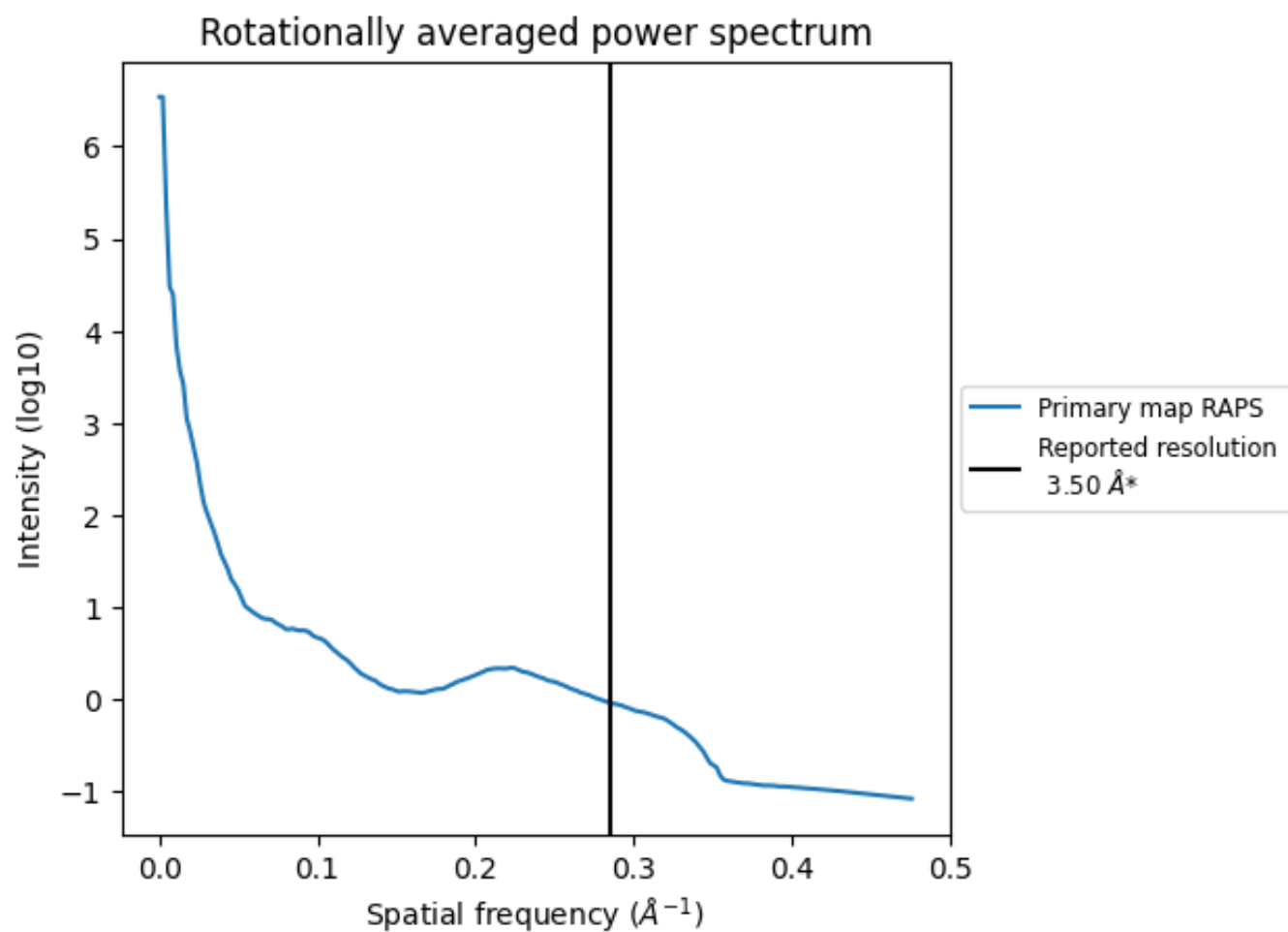
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 330 nm^3 ; this corresponds to an approximate mass of 298 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 0.286 Å⁻¹

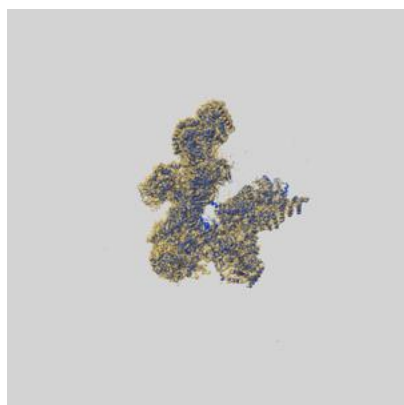
8 Fourier-Shell correlation

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

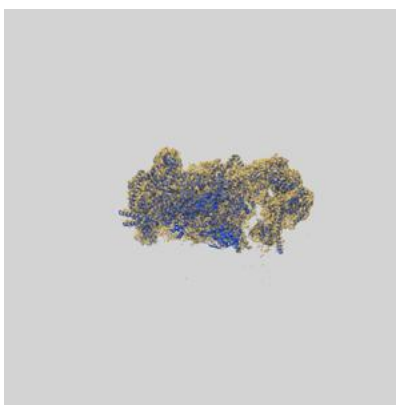
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18496 and PDB model 8QMA. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

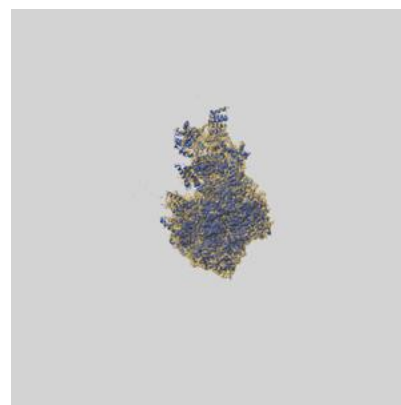
9.1 Map-model overlay [i](#)



X



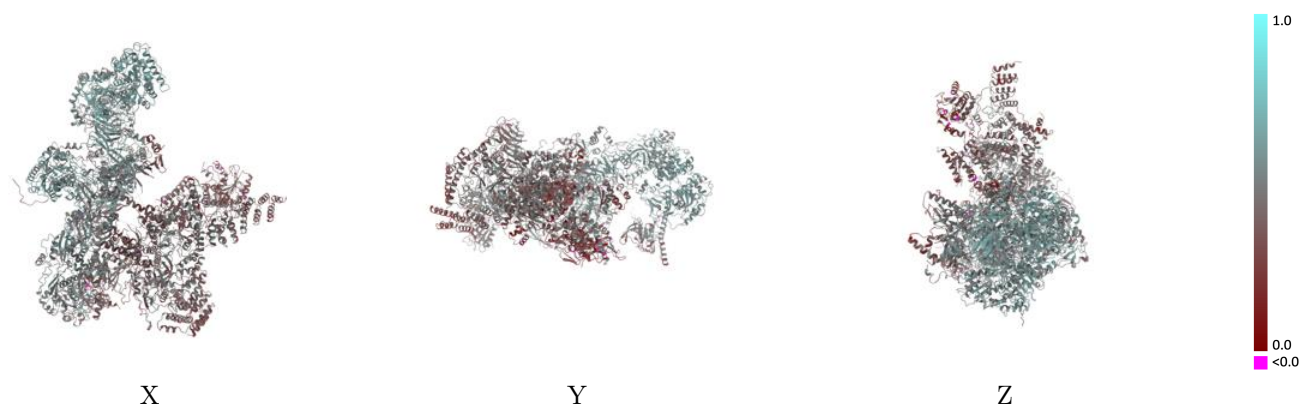
Y



Z

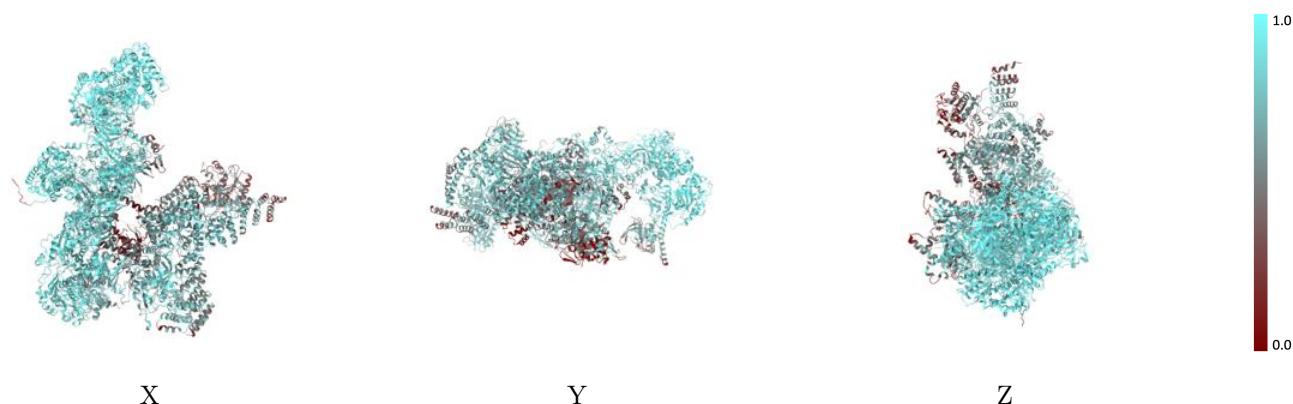
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



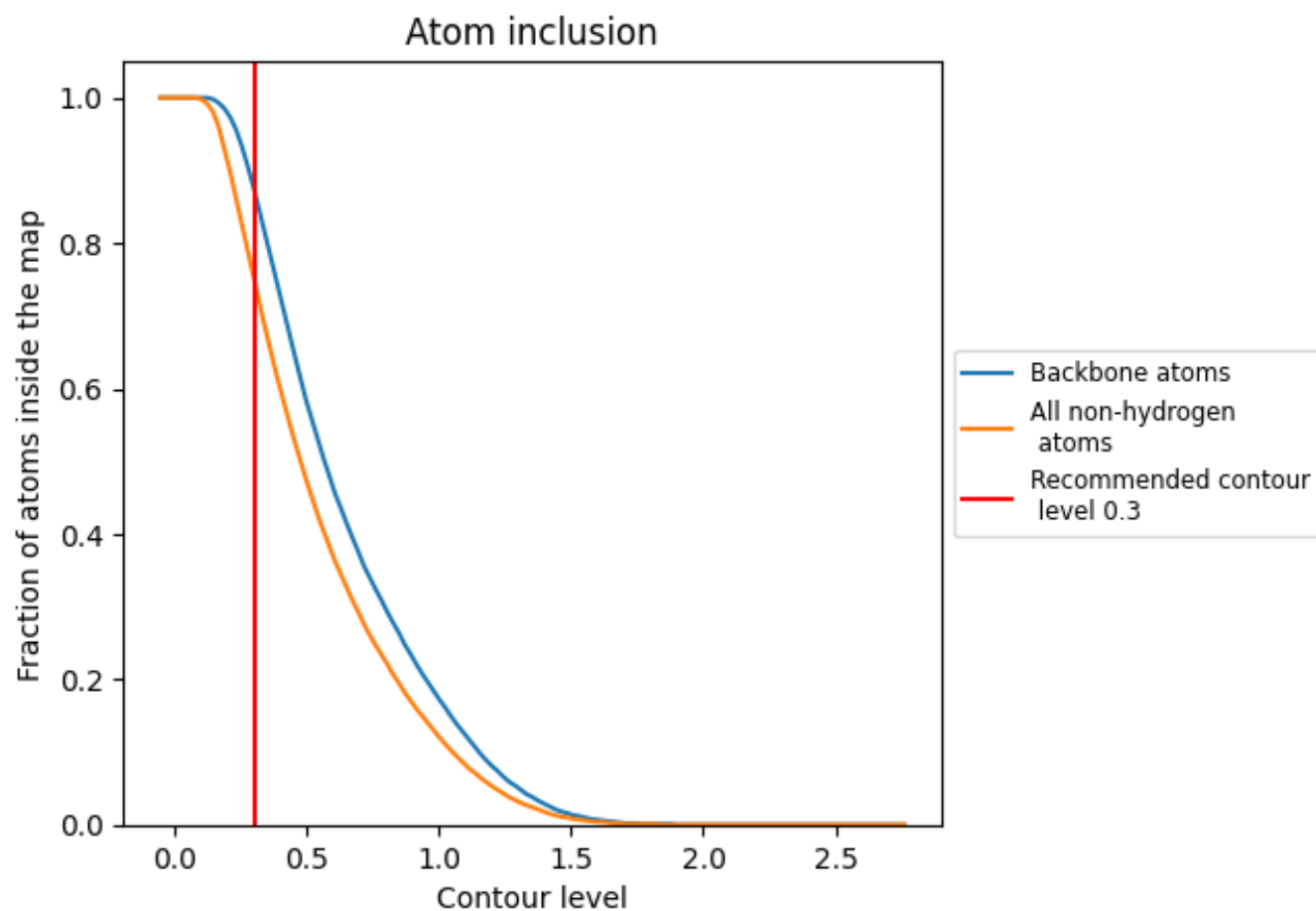
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).









































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 75% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7480	 0.4610
A	 0.7720	 0.4740
B	 0.7140	 0.4630
C	 0.8410	 0.4650
D	 0.7880	 0.4570
E	 0.6290	 0.3910
F	 0.8230	 0.5210
G	 0.9470	 0.5820
H	 0.8900	 0.5200
I	 0.8950	 0.4900
J	 0.7330	 0.4160
K	 0.6930	 0.4000
L	 0.9250	 0.5620
M	 0.9050	 0.5460
N	 0.7800	 0.4330
O	 0.3140	 0.2910
P	 0.4840	 0.3120
R	 0.9340	 0.5890
S	 0.9210	 0.5640
T	 0.4820	 0.3490

