Full wwPDB EM Validation Report ⓘ

Jun 17, 2025 – 01:42 pm BST

PDB ID	:	9FQ6 / pdb_00009fq6
EMDB ID	:	EMD-50644
Title	:	Structure of the complete Vaccinia DNA-dependent RNA polymerase complex assembly intermediate 4
Authors	:	Grimm, C.; Bartuli, J.; Fischer, U.
Deposited on	:	2024-06-14
Resolution	:	2.50 Å(reported)
Based on initial model	:	6rfl

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:

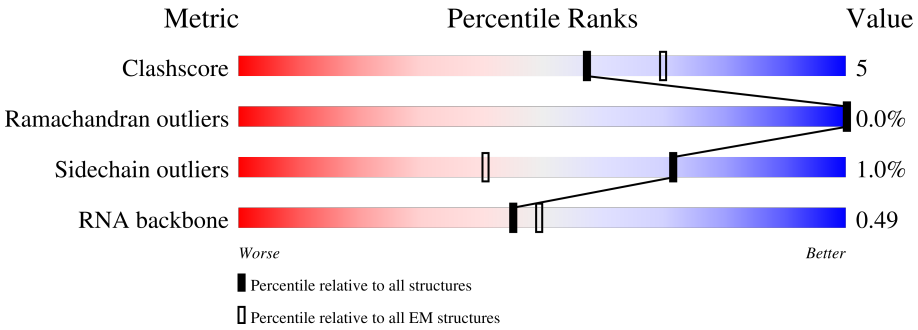
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	1286	90% 9%
2	B	1164	89% 8%
3	C	305	87% 12%
4	E	185	91% 8%
5	F	164	65% 32%
6	G	161	84% 15%
7	I	795	14% 86% 11%

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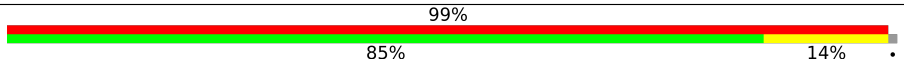
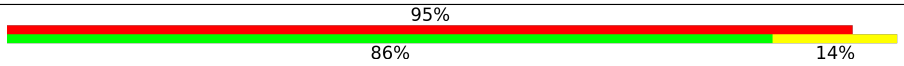
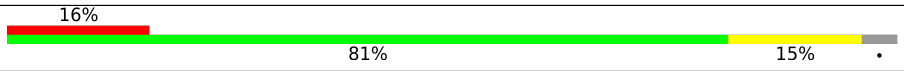
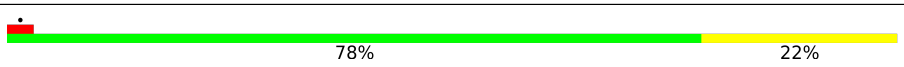
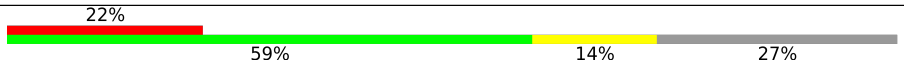
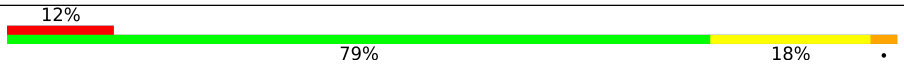
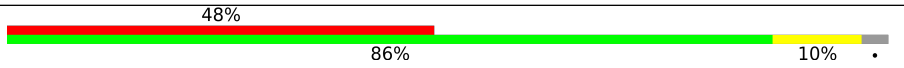
Mol	Chain	Length	Quality of chain
8	J	63	
9	L	287	
10	O	844	
11	Q	129	
11	R	129	
12	S	259	
13	U	72	
14	Y	631	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 102921 atoms, of which 51194 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 147 kDa polypeptide.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	1278	20643	6610	10368	1690	1929	46	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	THR	SER	variant	UNP P20504
A	489	GLU	LYS	variant	UNP P20504
A	1015	LYS	ARG	variant	UNP P20504

- Molecule 2 is a protein called DNA-directed RNA polymerase 133 kDa polypeptide.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	1129	18210	5794	9119	1554	1695	48	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	ASN	ASP	variant	UNP P68694
B	343	PHE	TYR	variant	UNP P68694

- Molecule 3 is a protein called DNA-directed RNA polymerase 35 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	304	4946	1608	2462	399	464	13	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	236	ASN	ASP	variant	UNP P21087

- Molecule 4 is a protein called DNA-directed RNA polymerase 22 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	184	Total	C	H	N	O	S	0	0
			3041	966	1546	248	276	5		

- Molecule 5 is a protein called DNA-directed RNA polymerase 19 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	111	Total	C	H	N	O	S	0	0
			1844	588	926	158	169	3		

- Molecule 6 is a protein called DNA-directed RNA polymerase 18 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	159	Total	C	H	N	O	S	0	0
			2460	782	1219	205	248	6		

- Molecule 7 is a protein called RNA polymerase-associated transcription-specificity factor RAP94.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	773	Total	C	H	N	O	S	0	0
			12934	4210	6488	1025	1190	21		

- Molecule 8 is a protein called DNA-directed RNA polymerase 7 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	61	Total	C	H	N	O	S	0	0
			1019	310	529	88	88	4		

- Molecule 9 is a protein called mRNA-capping enzyme regulatory subunit OPG124.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	L	284	Total	C	H	N	O	S	0	0
			4678	1492	2358	385	430	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	235	ASN	ASP	variant	UNP P20980

- Molecule 10 is a protein called mRNA-capping enzyme catalytic subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	O	844	Total	C	H	N	O	S	0	0
			13715	4399	6884	1123	1290	19		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	8	PHE	SER	variant	UNP P20979
O	202	THR	LYS	variant	UNP P20979

- Molecule 11 is a protein called Core protein OPG073.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	Q	124	Total	C	H	N	O	S	0	0
			2011	663	995	158	190	5		
11	R	129	Total	C	H	N	O	S	1	0
			2109	689	1053	165	197	5		

- Molecule 12 is a protein called DNA-directed RNA polymerase 30 kDa polypeptide.

Mol	Chain	Residues	Atoms							AltConf	Trace
12	S	189	Total	C	H	N	O	P	S	0	0
			3004	950	1473	248	325	3	5		

- Molecule 13 is a RNA chain called URQ-UUG1-1 tRNA (72-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
13	U	72	Total	C	H	N	O	P	3	0
			2405	714	808	275	533	75		

- Molecule 14 is a protein called Nucleoside triphosphatase I.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	Y	609	Total	C	H	N	O	S	0	0
			9883	3152	4966	837	903	25		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	329	ASP	ASN	variant	UNP P20637

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total Mg 1 1	0
15	U	3	Total Mg 3 3	0

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
16	A	2	Total Zn 2 2	0
16	B	1	Total Zn 1 1	0
16	I	1	Total Zn 1 1	0

- Molecule 17 is water.

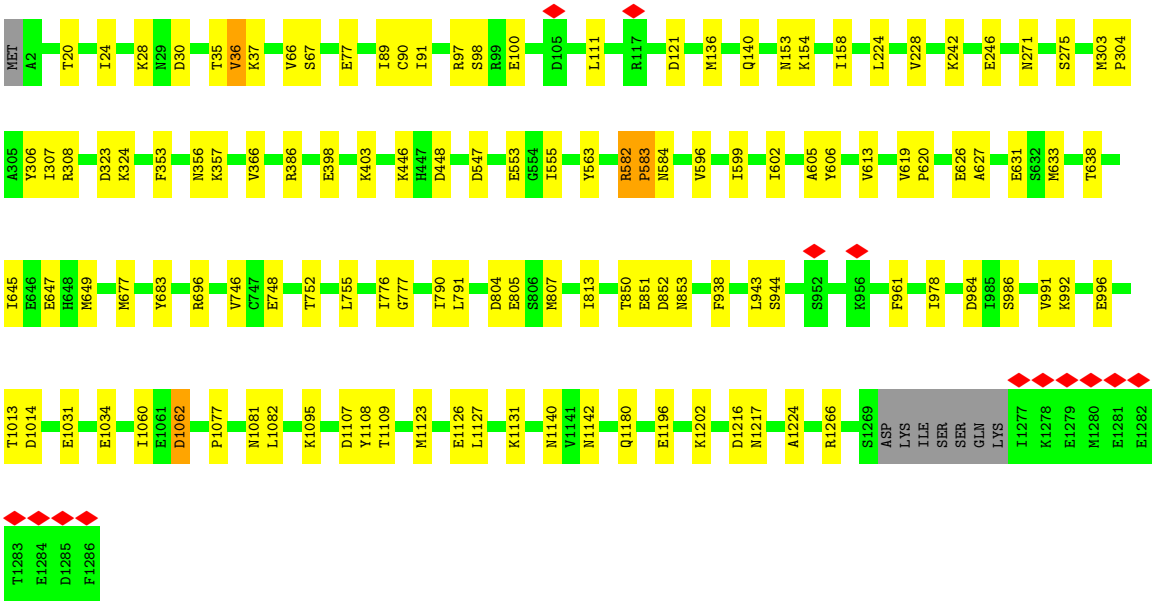
Mol	Chain	Residues	Atoms	AltConf
17	A	2	Total O 2 2	0
17	B	2	Total O 2 2	0
17	F	1	Total O 1 1	0
17	I	1	Total O 1 1	0
17	L	2	Total O 2 2	0
17	S	2	Total O 2 2	0
17	Y	1	Total O 1 1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

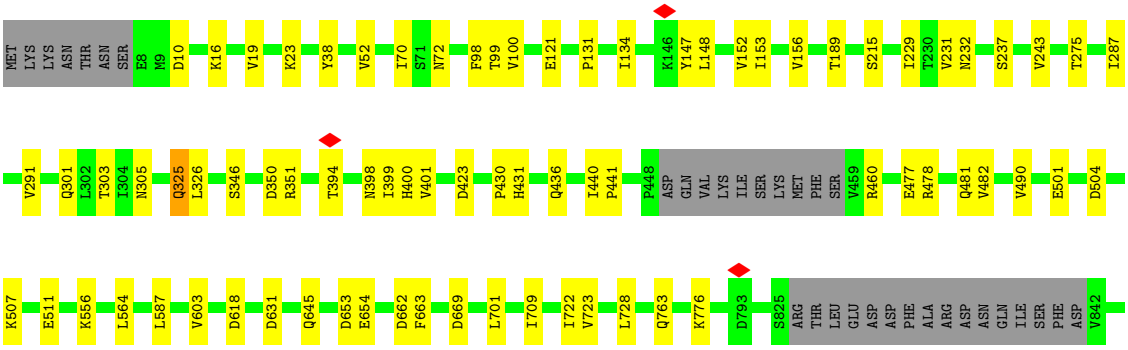
• Molecule 1: DNA-directed RNA polymerase 147 kDa polypeptide

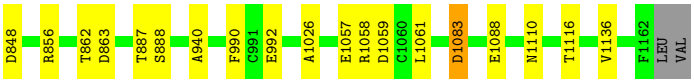
Chain A:



• Molecule 2: DNA-directed RNA polymerase 133 kDa polypeptide

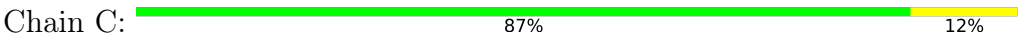
Chain B:

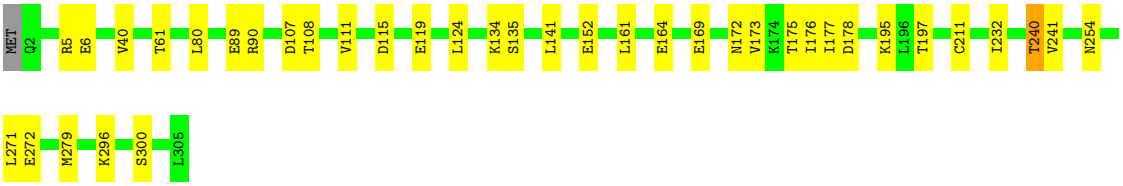




• Molecule 3: DNA-directed RNA polymerase 35 kDa subunit

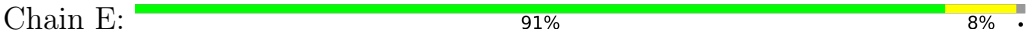
Chain C:

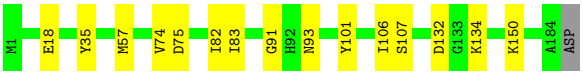




• Molecule 4: DNA-directed RNA polymerase 22 kDa subunit

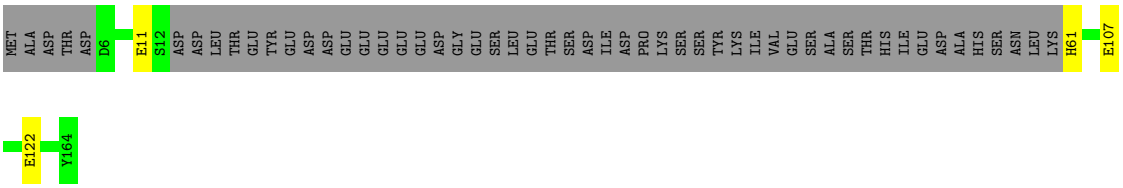
Chain E:





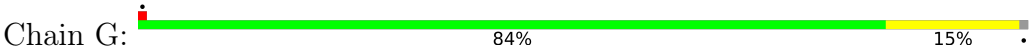
• Molecule 5: DNA-directed RNA polymerase 19 kDa subunit

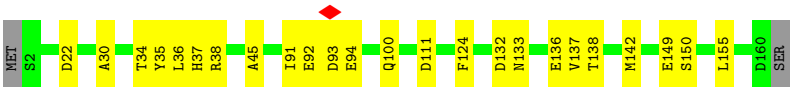
Chain F:



• Molecule 6: DNA-directed RNA polymerase 18 kDa subunit

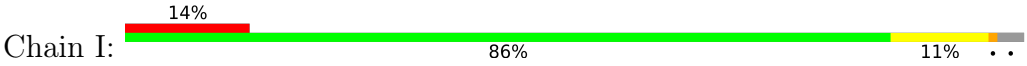
Chain G:

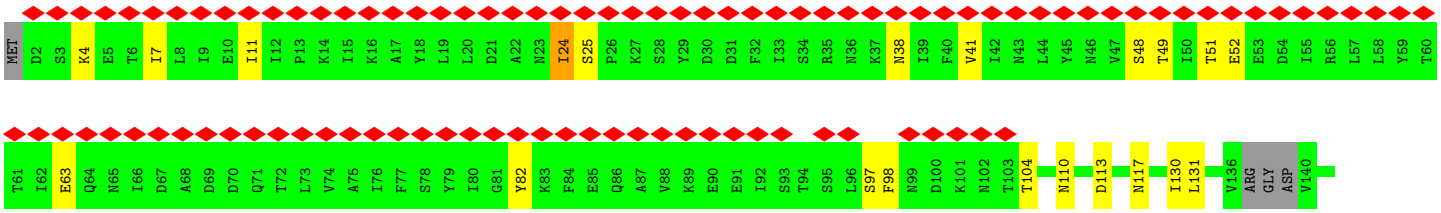


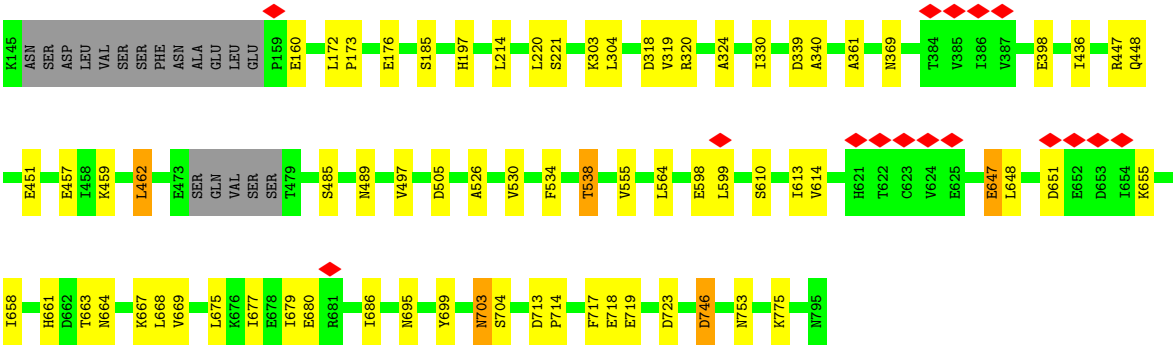


• Molecule 7: RNA polymerase-associated transcription-specificity factor RAP94

Chain I:

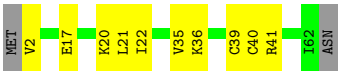






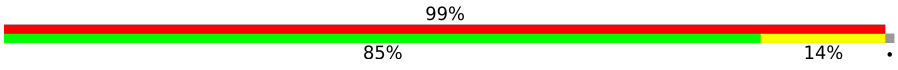
• Molecule 8: DNA-directed RNA polymerase 7 kDa subunit

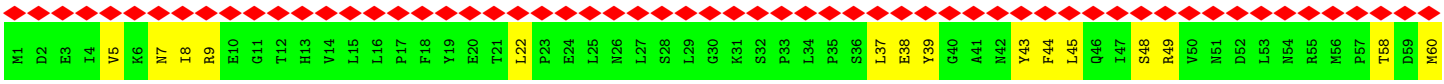
Chain J:

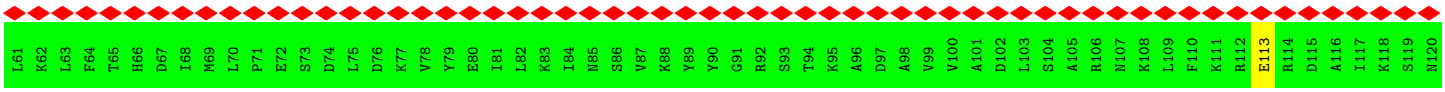


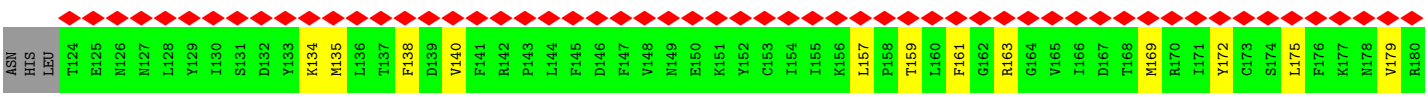
• Molecule 9: mRNA-capping enzyme regulatory subunit OPG124

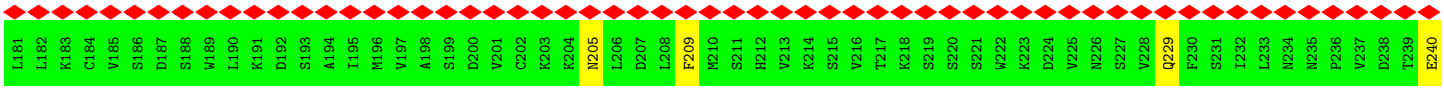
Chain L:

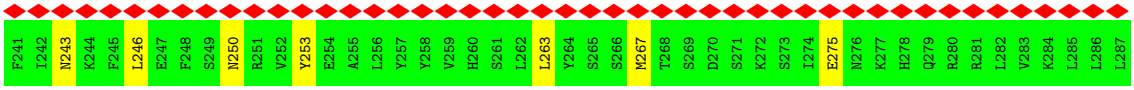






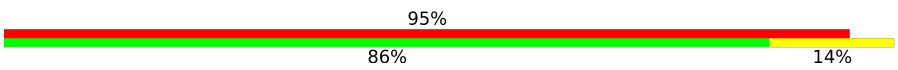


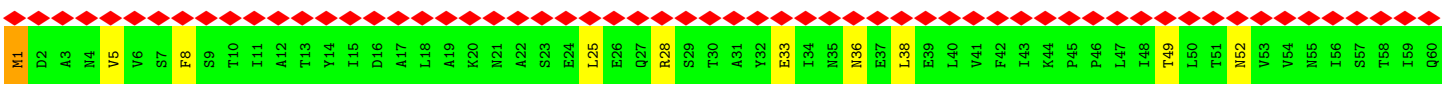


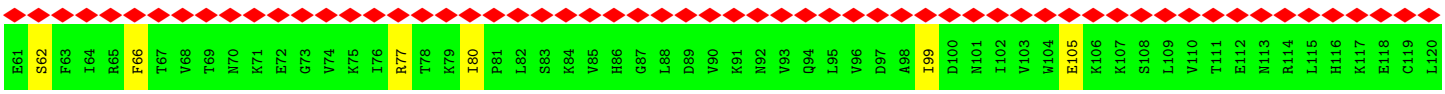


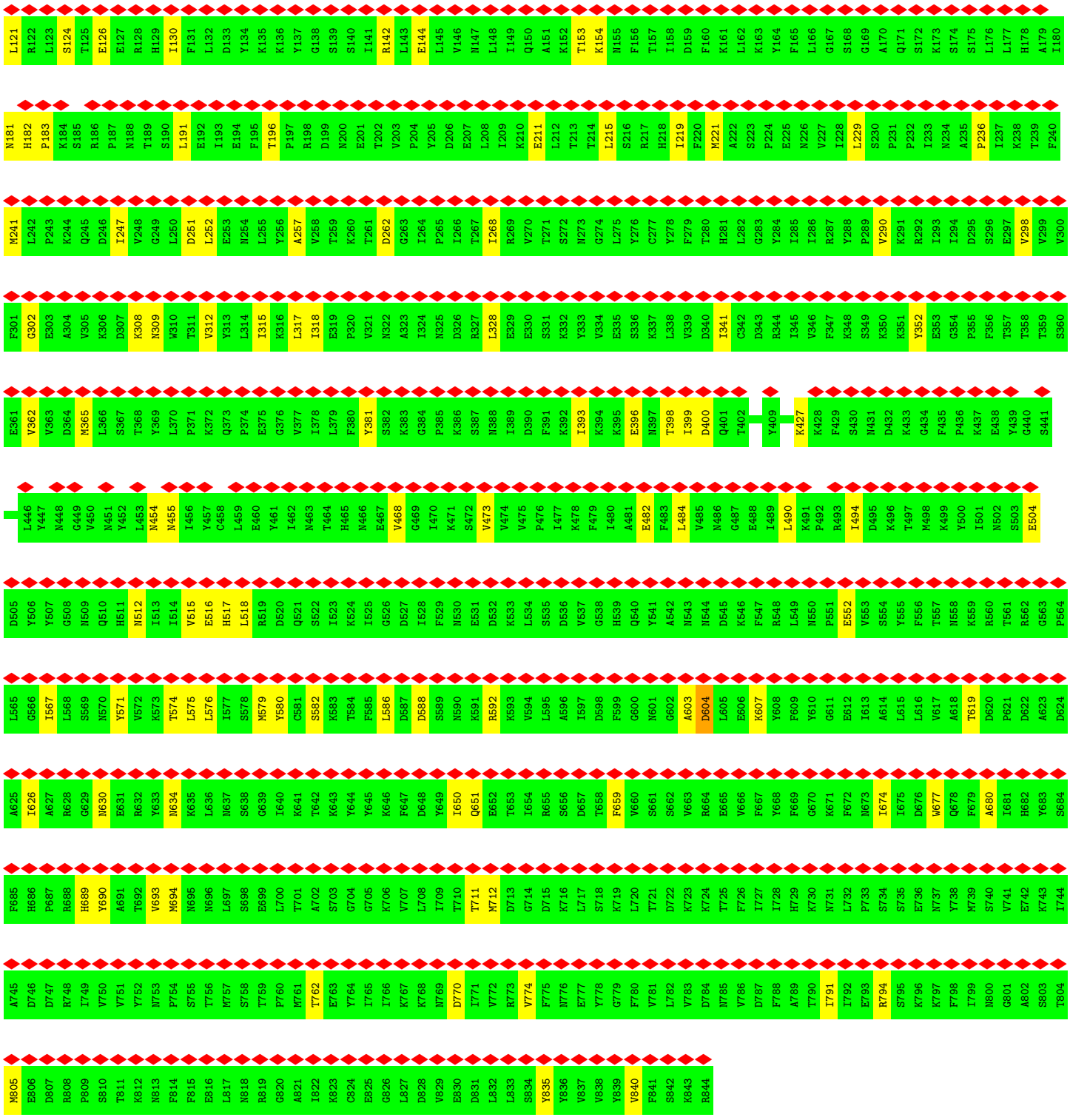
• Molecule 10: mRNA-capping enzyme catalytic subunit

Chain O:



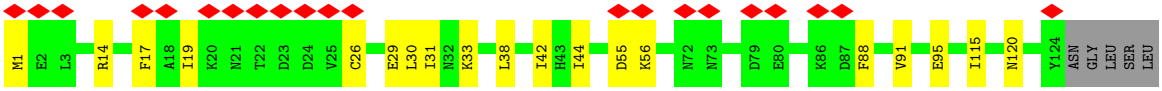






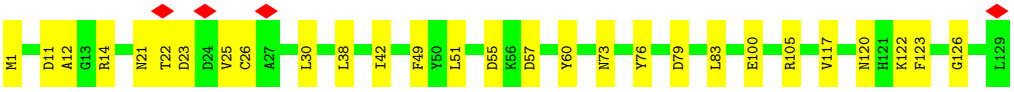
• Molecule 11: Core protein OPG073

Chain Q:



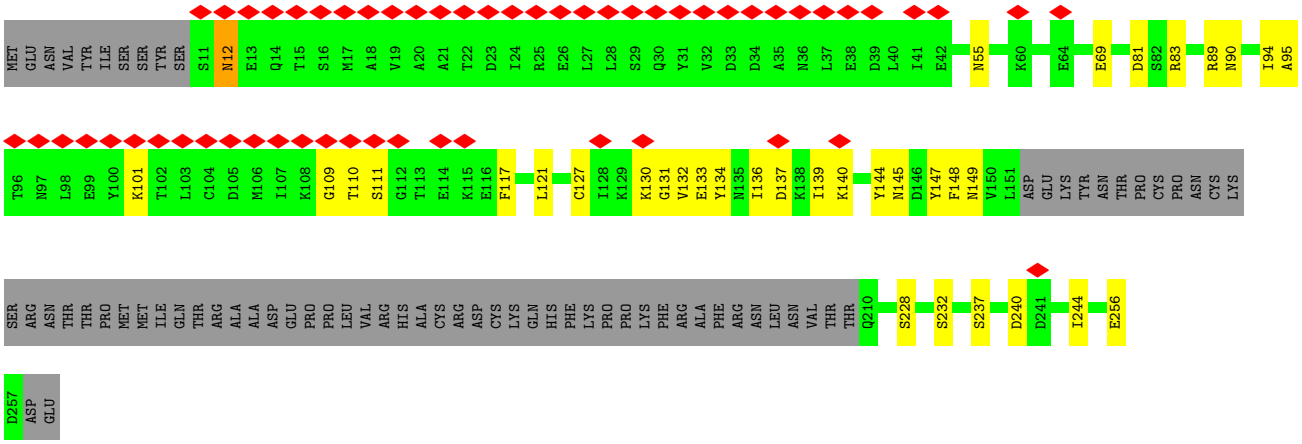
• Molecule 11: Core protein OPG073

Chain R:



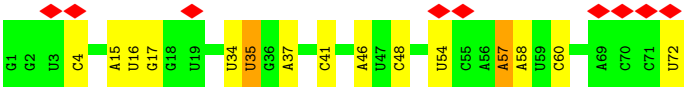
• Molecule 12: DNA-directed RNA polymerase 30 kDa polypeptide

Chain S:



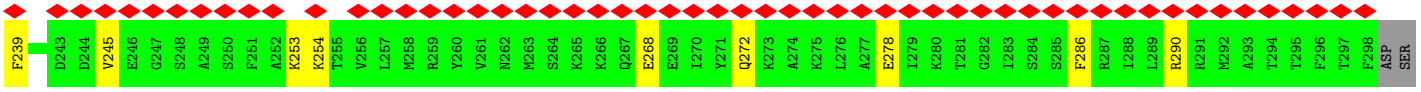
• Molecule 13: URQ-UUG1-1 tRNA (72-MER)

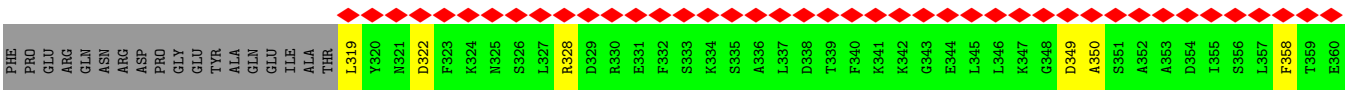
Chain U:

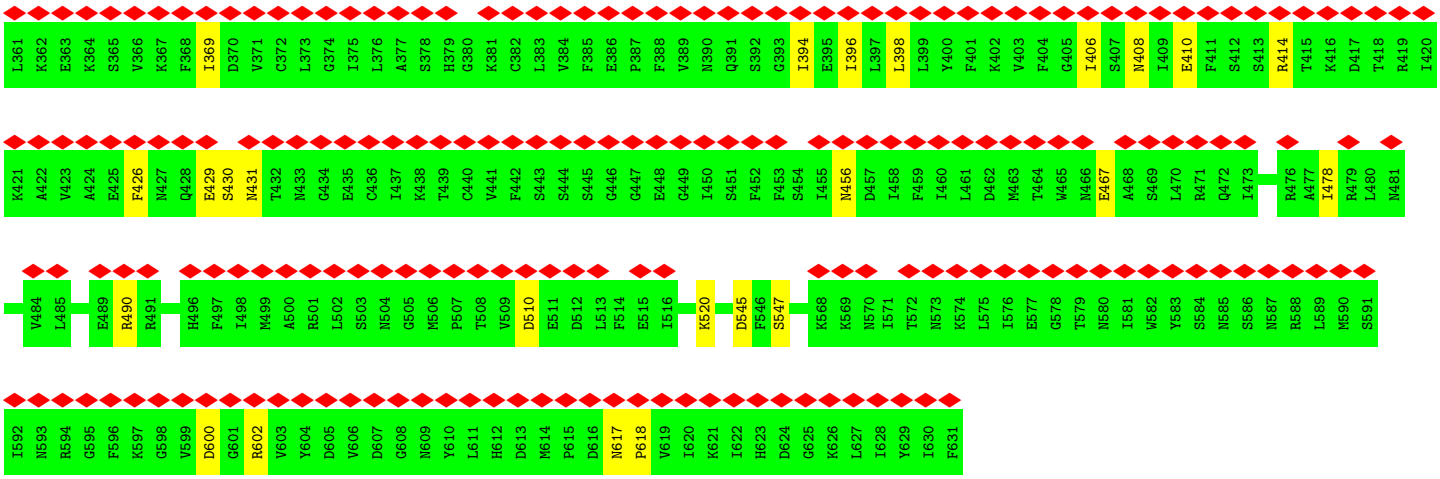


• Molecule 14: Nucleoside triphosphatase I

Chain Y:






L361 K362 E363 K364 S365 V366 K367 F368 I369 D370 V371 C372 L373 G374 I375 L376 A377 S378 H379 G380 K381 C382 L383 V384 F385 E386 P387 F388 V389 N390 Q391 S392 G393 I394 E395 I396 L397 L398 L399 Y400 F401 K402 V403 F404 G405 I406 S407 N408 I409 E410 F411 S412 S413 R414 T415 K416 D417 T418 R419 I420
K421 A422 V423 A424 E425 F426 N427 Q428 E429 S430 N431 T432 N433 G434 E435 C436 I437 K438 T439 C440 V441 F442 S443 S444 S445 G446 G447 E448 G449 I450 S451 F452 F453 S454 I455 N456 D457 I458 F459 I460 L461 D462 M463 T464 W465 N466 E467 A468 S469 L470 R471 Q472 I473 R476 A477 I478 R479 L480 N481
V484 L485 E489 R490 R491 H496 F497 I498 M499 A500 R501 L502 S503 N504 G505 M506 P507 T508 V509 D510 E511 D512 L513 F514 E515 I516 K520 D545 F546 S547 K568 K569 N570 I571 T572 N573 K574 L575 I576 E577 G578 T579 N580 I581 W582 Y583 S584 N585 S586 N587 R588 L589 M590 S591
I592 N593 R594 G595 F596 K597 G598 V599 D600 G601 R602 V603 Y604 D605 V606 D607 G608 N609 Y610 L611 H612 D613 M614 P615 D616 N617 P618 V619 I620 K621 I622 H623 D624 G625 K626 L627 I628 Y629 I630 F631

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171057	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	70	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.948	Depositor
Minimum map value	-0.487	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	308.47998, 308.47998, 308.47998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9639999, 0.9639999, 0.9639999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, ZN, 1MA, 5MU, OMC, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.15	0/10481	0.31	0/14166
2	B	0.14	0/9281	0.29	0/12537
3	C	0.16	0/2540	0.33	0/3440
4	E	0.14	0/1522	0.30	0/2069
5	F	0.16	0/933	0.35	0/1252
6	G	0.15	0/1260	0.30	0/1709
7	I	0.13	0/6590	0.28	0/8918
8	J	0.17	0/494	0.35	0/663
9	L	0.15	0/2365	0.28	0/3189
10	O	0.10	0/6973	0.27	0/9433
11	Q	0.10	0/1038	0.28	0/1406
11	R	0.12	0/1081	0.33	0/1463
12	S	0.12	0/1524	0.31	0/2050
13	U	0.09	0/1710	0.20	0/2661
14	Y	0.11	0/5013	0.26	0/6750
All	All	0.13	0/52805	0.29	0/71706

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	582	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10275	10368	10388	81	0
2	B	9091	9119	9146	56	0
3	C	2484	2462	2470	27	0
4	E	1495	1546	1548	13	0
5	F	918	926	930	5	0
6	G	1241	1219	1222	18	0
7	I	6446	6488	6502	69	0
8	J	490	529	530	7	0
9	L	2320	2358	2363	34	0
10	O	6831	6884	6899	86	0
11	Q	1016	995	1007	15	0
11	R	1056	1053	1056	25	0
12	S	1531	1473	1473	29	0
13	U	1597	808	808	4	0
14	Y	4917	4966	4981	43	0
15	A	1	0	0	0	0
15	U	3	0	0	0	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	I	1	0	0	0	0
17	A	2	0	0	0	0
17	B	2	0	0	0	0
17	F	1	0	0	0	0
17	I	1	0	0	0	0
17	L	2	0	0	0	0
17	S	2	0	0	2	0
17	Y	1	0	0	0	0
All	All	51727	51194	51323	473	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (473) 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)
9:L:43:TYR:OH	10:O:579:MET:N	1.98	0.97
6:G:136:GLU:OE2	6:G:136:GLU:N	2.07	0.88
10:O:588:ASP:O	10:O:592:ARG:NH2	2.08	0.86
1:A:446:LYS:NZ	1:A:547:ASP:OD1	2.07	0.86
14:Y:56:GLU:O	14:Y:61:LYS:NZ	2.12	0.81
10:O:130:ILE:HD12	10:O:130:ILE:O	1.80	0.81
10:O:28:ARG:NH1	10:O:36:ASN:O	2.13	0.81
13:U:35:U:O2'	14:Y:120:ARG:NH1	2.14	0.81
10:O:251:ASP:OD1	10:O:381:TYR:OH	2.01	0.78
2:B:1058:ARG:NH2	2:B:1059:ASP:OD1	2.17	0.78
2:B:477:GLU:N	2:B:477:GLU:OE1	2.17	0.77
7:I:339:ASP:OD2	7:I:340:ALA:N	2.18	0.77
14:Y:406:ILE:O	14:Y:408:ASN:ND2	2.18	0.77
10:O:582:SER:O	10:O:592:ARG:NH1	2.18	0.77
2:B:776:LYS:NZ	2:B:848:ASP:OD2	2.16	0.76
14:Y:600:ASP:OD2	14:Y:602:ARG:NH1	2.19	0.76
10:O:80:ILE:HD12	10:O:80:ILE:O	1.87	0.75
10:O:579:MET:O	10:O:586:LEU:HD11	1.87	0.75
9:L:43:TYR:HH	10:O:579:MET:N	1.84	0.75
14:Y:92:ASP:O	14:Y:96:ASN:ND2	2.19	0.75
6:G:93:ASP:OD1	6:G:94:GLU:N	2.21	0.73
13:U:35:U:N3	14:Y:163:SER:OG	2.22	0.73
11:R:14:ARG:NH1	11:R:83:LEU:O	2.23	0.72
11:Q:19:ILE:HD11	11:Q:30:LEU:HD22	1.72	0.72
4:E:18:GLU:OE1	4:E:35:TYR:OH	2.06	0.72
11:Q:19:ILE:CD1	11:Q:30:LEU:HD22	2.20	0.72
1:A:1131:LYS:NZ	4:E:101:TYR:OH	2.22	0.71
6:G:30:ALA:O	6:G:34:THR:HG22	1.90	0.71
12:S:69:GLU:N	12:S:69:GLU:OE1	2.24	0.71
11:Q:14:ARG:NH1	11:Q:95:GLU:OE2	2.23	0.71
1:A:606:TYR:OH	1:A:626:GLU:OE2	2.08	0.70
2:B:325:GLN:OE1	2:B:326:LEU:N	2.24	0.70
2:B:431:HIS:HB3	2:B:701:LEU:HD21	1.72	0.70
12:S:94:ILE:HG22	12:S:95:ALA:H	1.57	0.70
12:S:81:ASP:OD2	12:S:83:ARG:NH1	2.25	0.69
12:S:101:LYS:O	17:S:301:HOH:O	2.10	0.69
2:B:460:ARG:NH2	2:B:482:VAL:O	2.26	0.69
10:O:484:LEU:HG	10:O:490:LEU:HD11	1.75	0.69
14:Y:116:ASP:OD1	14:Y:117:GLN:N	2.26	0.68
7:I:703:ASN:O	7:I:704:SER:OG	2.09	0.68
3:C:89:GLU:OE2	3:C:89:GLU:N	2.27	0.68
10:O:630:ASN:O	10:O:634:ASN:ND2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LYS:HE3	1:A:154:LYS:HA	1.75	0.68
2:B:350:ASP:OD1	2:B:351:ARG:N	2.27	0.68
9:L:37:LEU:HD13	10:O:579:MET:SD	2.34	0.67
10:O:153:THR:HG21	10:O:215:LEU:HD21	1.77	0.67
1:A:992:LYS:NZ	1:A:1031:GLU:OE1	2.25	0.67
7:I:459:LYS:O	11:R:73:ASN:ND2	2.27	0.66
3:C:173:VAL:O	3:C:176:ILE:N	2.28	0.66
6:G:92:GLU:N	6:G:92:GLU:OE1	2.29	0.66
1:A:1060:ILE:O	12:S:130:LYS:NZ	2.28	0.66
9:L:246:LEU:O	9:L:250:ASN:ND2	2.29	0.65
1:A:357:LYS:NZ	7:I:324:ALA:O	2.26	0.65
2:B:1110:ASN:ND2	7:I:110:ASN:OD1	2.30	0.65
7:I:4:LYS:NZ	7:I:49:THR:O	2.29	0.65
14:Y:268:GLU:O	14:Y:272:GLN:NE2	2.29	0.65
1:A:356:ASN:O	7:I:320:ARG:NH2	2.29	0.65
11:Q:55:ASP:OD1	11:Q:56:LYS:N	2.26	0.65
9:L:43:TYR:HH	10:O:579:MET:H	1.42	0.65
1:A:91:ILE:O	1:A:91:ILE:HG23	1.96	0.64
1:A:1062:ASP:N	1:A:1062:ASP:OD1	2.30	0.64
7:I:719:GLU:OE1	7:I:719:GLU:O	2.15	0.64
7:I:667:LYS:O	7:I:677:ILE:HD12	1.97	0.64
14:Y:286:PHE:O	14:Y:290:ARG:NH2	2.31	0.64
10:O:25:LEU:HD21	10:O:38:LEU:HD12	1.80	0.64
2:B:16:LYS:O	2:B:19:VAL:HG22	1.98	0.63
3:C:107:ASP:OD1	3:C:108:THR:N	2.30	0.63
14:Y:278:GLU:OE1	14:Y:290:ARG:NE	2.30	0.63
7:I:318:ASP:OD1	7:I:319:VAL:N	2.30	0.63
2:B:423:ASP:OD1	2:B:423:ASP:N	2.32	0.63
7:I:398:GLU:O	14:Y:547:SER:OG	2.17	0.63
1:A:323:ASP:OD1	1:A:324:LYS:N	2.32	0.62
11:Q:26:CYS:N	11:Q:29:GLU:OE2	2.33	0.62
7:I:361:ALA:O	7:I:369:ASN:ND2	2.32	0.62
11:R:21:ASN:OD1	11:R:22:THR:N	2.32	0.62
1:A:1034:GLU:OE1	1:A:1034:GLU:N	2.33	0.62
3:C:164:GLU:N	3:C:164:GLU:OE1	2.31	0.62
10:O:77:ARG:NH1	10:O:105:GLU:OE2	2.32	0.62
4:E:91:GLY:O	4:E:150:LYS:NZ	2.33	0.62
1:A:582:ARG:O	1:A:584:ASN:N	2.33	0.61
9:L:60:MET:SD	9:L:267:MET:HB3	2.40	0.61
9:L:134:LYS:O	9:L:229:GLN:NE2	2.33	0.61
14:Y:426:PHE:O	14:Y:431:ASN:ND2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Y:319:LEU:N	14:Y:322:ASP:OD2	2.33	0.61
6:G:34:THR:HG23	6:G:35:TYR:CD2	2.36	0.61
14:Y:131:ASN:OD1	14:Y:132:SER:N	2.33	0.60
1:A:271:ASN:O	1:A:275:SER:OG	2.17	0.60
6:G:149:GLU:O	6:G:149:GLU:HG3	2.01	0.60
9:L:157:LEU:HD23	9:L:157:LEU:H	1.66	0.60
14:Y:239:PHE:CD1	14:Y:245:VAL:HG22	2.36	0.60
7:I:448:GLN:N	7:I:448:GLN:OE1	2.34	0.60
12:S:89:ARG:NH1	12:S:90:ASN:O	2.34	0.60
1:A:1266:ARG:NH2	6:G:22:ASP:OD1	2.35	0.60
7:I:24:ILE:HD12	7:I:25:SER:H	1.66	0.60
4:E:57:MET:HA	4:E:57:MET:HE3	1.83	0.60
10:O:1:MET:SD	10:O:5:VAL:HG21	2.42	0.59
9:L:135:MET:HE3	9:L:135:MET:HA	1.83	0.59
10:O:454:ASN:ND2	10:O:455:ASN:OD1	2.35	0.59
9:L:43:TYR:OH	10:O:579:MET:CA	2.50	0.59
7:I:598:GLU:C	7:I:599:LEU:HD22	2.27	0.59
1:A:553:GLU:N	1:A:553:GLU:OE1	2.35	0.59
2:B:1057:GLU:OE1	2:B:1057:GLU:N	2.33	0.59
2:B:556:LYS:NZ	2:B:564:LEU:O	2.36	0.59
10:O:770:ASP:O	10:O:774:VAL:HG12	2.03	0.59
14:Y:165:TYR:OH	14:Y:196:MET:O	2.18	0.59
1:A:804:ASP:H	1:A:807:MET:HE2	1.67	0.58
2:B:1083:ASP:OD1	2:B:1083:ASP:N	2.35	0.58
9:L:159:THR:HG22	9:L:161:PHE:H	1.67	0.58
1:A:563:TYR:OH	3:C:272:GLU:OE1	2.21	0.58
1:A:943:LEU:O	1:A:944:SER:OG	2.18	0.58
10:O:399:ILE:HG22	10:O:517:HIS:CD2	2.39	0.58
10:O:504:GLU:OE1	10:O:504:GLU:N	2.36	0.58
1:A:647:GLU:OE1	1:A:647:GLU:O	2.22	0.58
2:B:940:ALA:O	8:J:41:ARG:NH2	2.37	0.58
3:C:152:GLU:OE1	3:C:152:GLU:O	2.22	0.58
14:Y:21:VAL:HG22	14:Y:21:VAL:O	2.03	0.58
10:O:690:TYR:O	10:O:694:MET:HG2	2.04	0.57
11:R:1:MET:HE2	11:R:1:MET:HA	1.87	0.57
1:A:1196:GLU:OE2	1:A:1202:LYS:N	2.37	0.57
7:I:598:GLU:O	7:I:599:LEU:HD22	2.04	0.57
10:O:468:VAL:HG12	10:O:468:VAL:O	2.04	0.57
11:R:100:GLU:OE1	11:R:100:GLU:C	2.47	0.57
3:C:6:GLU:N	3:C:6:GLU:OE1	2.37	0.57
7:I:614:VAL:HG12	7:I:614:VAL:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:THR:OG1	2:B:121:GLU:OE2	2.21	0.56
10:O:252:LEU:HD23	10:O:252:LEU:H	1.70	0.56
10:O:619:THR:HG23	10:O:619:THR:O	2.06	0.56
3:C:232:ILE:HG21	3:C:279:MET:HE2	1.88	0.56
7:I:614:VAL:O	7:I:614:VAL:CG1	2.54	0.56
2:B:398:ASN:O	2:B:401:VAL:HG22	2.06	0.56
10:O:236:PRO:HG3	10:O:318:ILE:HD11	1.87	0.56
11:R:60:TYR:OH	11:R:76:TYR:O	2.24	0.56
9:L:169:MET:HE1	9:L:179:VAL:HG11	1.87	0.55
9:L:169:MET:CE	9:L:179:VAL:HG11	2.36	0.55
1:A:398:GLU:O	1:A:403:LYS:NZ	2.36	0.55
1:A:776:ILE:HG23	1:A:777:GLY:H	1.72	0.55
7:I:451:GLU:OE1	11:R:123:PHE:CE2	2.59	0.55
10:O:142:ARG:NH1	10:O:144:GLU:OE2	2.39	0.55
2:B:72:ASN:OD1	2:B:72:ASN:O	2.24	0.55
11:Q:38:LEU:O	11:Q:42:ILE:N	2.36	0.55
7:I:613:ILE:HD12	7:I:613:ILE:O	2.07	0.55
7:I:214:LEU:HD11	7:I:221:SER:HB3	1.89	0.55
10:O:196:THR:O	10:O:196:THR:OG1	2.25	0.54
10:O:580:TYR:O	10:O:674:ILE:HD11	2.06	0.54
7:I:534:PHE:O	7:I:538:THR:OG1	2.24	0.54
10:O:247:ILE:HD13	10:O:393:ILE:HD11	1.88	0.54
1:A:303:MET:O	1:A:308:ARG:NH1	2.40	0.54
8:J:2:VAL:HG12	8:J:2:VAL:O	2.07	0.54
11:R:55:ASP:OD1	11:R:55:ASP:O	2.25	0.54
12:S:132:VAL:HG12	12:S:133:GLU:H	1.73	0.54
12:S:145:ASN:O	12:S:149:ASN:ND2	2.41	0.54
11:Q:120:ASN:OD1	11:R:120:ASN:ND2	2.41	0.54
1:A:158:ILE:HG23	7:I:176:GLU:OE1	2.08	0.54
1:A:242:LYS:O	1:A:246:GLU:HG3	2.07	0.54
10:O:268:ILE:HD12	10:O:312:VAL:HG11	1.90	0.54
3:C:195:LYS:NZ	3:C:197:THR:OG1	2.41	0.54
9:L:140:VAL:O	9:L:172:TYR:OH	2.25	0.54
14:Y:95:MET:HE3	14:Y:95:MET:HA	1.90	0.54
9:L:138:PHE:O	9:L:138:PHE:CD1	2.61	0.53
12:S:256:GLU:O	12:S:256:GLU:HG3	2.07	0.53
1:A:627:ALA:O	1:A:631:GLU:HG2	2.08	0.53
9:L:263:LEU:O	9:L:267:MET:HG3	2.08	0.53
6:G:111:ASP:OD1	6:G:111:ASP:O	2.27	0.53
10:O:262:ASP:O	10:O:262:ASP:OD1	2.27	0.53
1:A:36:VAL:HG21	1:A:224:LEU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:132:ASP:O	4:E:132:ASP:OD2	2.26	0.53
14:Y:394:ILE:O	14:Y:398:LEU:HD23	2.09	0.53
9:L:44:PHE:O	9:L:48:SER:OG	2.17	0.52
1:A:98:SER:OG	1:A:100:GLU:OE1	2.27	0.52
1:A:121:ASP:C	1:A:121:ASP:OD1	2.52	0.52
2:B:1088:GLU:OE2	2:B:1116:THR:OG1	2.27	0.52
10:O:181:ASN:OD1	10:O:427:LYS:NZ	2.39	0.52
1:A:37:LYS:CG	1:A:37:LYS:O	2.58	0.52
12:S:256:GLU:O	12:S:256:GLU:CG	2.57	0.52
14:Y:33:ASP:OD1	14:Y:33:ASP:N	2.43	0.52
14:Y:104:GLU:OE1	14:Y:104:GLU:N	2.42	0.52
7:I:485:SER:O	7:I:489:ASN:ND2	2.38	0.52
1:A:89:ILE:O	1:A:97:ARG:NE	2.41	0.52
1:A:984:ASP:O	1:A:986:SER:N	2.43	0.52
8:J:39:CYS:SG	8:J:40:CYS:N	2.82	0.52
2:B:662:ASP:OD1	2:B:663:PHE:N	2.43	0.51
6:G:100:GLN:N	6:G:100:GLN:OE1	2.44	0.51
2:B:303:THR:OG1	2:B:305:ASN:O	2.28	0.51
9:L:58:THR:HG21	9:L:113:GLU:CG	2.41	0.51
10:O:576:LEU:O	10:O:579:MET:HG2	2.11	0.51
2:B:763:GLN:OE1	2:B:763:GLN:N	2.43	0.51
10:O:38:LEU:HD22	10:O:121:LEU:HD11	1.93	0.51
10:O:396:GLU:O	10:O:396:GLU:HG2	2.10	0.51
12:S:244:ILE:HD12	12:S:244:ILE:O	2.10	0.51
9:L:38:GLU:O	10:O:794:ARG:NH1	2.44	0.51
11:R:11:ASP:OD2	11:R:11:ASP:C	2.54	0.51
2:B:478:ARG:HG2	2:B:478:ARG:HH11	1.76	0.50
2:B:645:GLN:NE2	7:I:610:SER:O	2.44	0.50
7:I:675:LEU:HD11	7:I:686:ILE:HD12	1.92	0.50
14:Y:545:ASP:O	14:Y:545:ASP:OD2	2.29	0.50
3:C:5:ARG:NH2	8:J:17:GLU:OE1	2.44	0.50
7:I:679:ILE:HD12	7:I:680:GLU:N	2.26	0.50
1:A:645:ILE:O	1:A:649:MET:HG3	2.10	0.50
7:I:668:LEU:HD23	7:I:669:VAL:N	2.26	0.50
11:R:11:ASP:OD2	11:R:12:ALA:N	2.45	0.50
1:A:140:GLN:OE1	1:A:153:ASN:ND2	2.45	0.50
11:Q:1:MET:SD	11:Q:1:MET:N	2.80	0.50
10:O:80:ILE:HD12	10:O:80:ILE:C	2.36	0.50
14:Y:456:ASN:OD1	14:Y:490:ARG:NH1	2.44	0.50
9:L:169:MET:HE3	9:L:169:MET:HA	1.94	0.50
10:O:211:GLU:O	10:O:215:LEU:HD23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Y:410:GLU:OE1	14:Y:414:ARG:NH2	2.45	0.50
14:Y:467:GLU:CD	14:Y:467:GLU:H	2.20	0.50
7:I:82:TYR:HH	10:O:762:THR:HG1	1.59	0.50
7:I:613:ILE:HD12	7:I:613:ILE:C	2.37	0.50
10:O:241:MET:HE2	10:O:516:GLU:OE1	2.11	0.49
10:O:689:HIS:O	10:O:693:VAL:HG12	2.12	0.49
1:A:111:LEU:HD12	1:A:111:LEU:O	2.12	0.49
1:A:1077:PRO:O	1:A:1081:ASN:ND2	2.44	0.49
1:A:851:GLU:OE2	1:A:851:GLU:O	2.31	0.49
3:C:169:GLU:O	3:C:173:VAL:HG22	2.13	0.49
10:O:290:VAL:HG13	10:O:341:ILE:HG22	1.93	0.49
2:B:152:VAL:O	2:B:152:VAL:HG13	2.13	0.49
5:F:107:GLU:OE2	5:F:107:GLU:O	2.30	0.49
1:A:1082:LEU:C	1:A:1082:LEU:HD23	2.38	0.49
7:I:447:ARG:O	7:I:451:GLU:HG2	2.12	0.49
7:I:713:ASP:N	7:I:713:ASP:OD1	2.43	0.49
1:A:602:ILE:HG23	1:A:633:MET:SD	2.53	0.49
3:C:40:VAL:HG22	3:C:141:LEU:CD2	2.43	0.49
7:I:651:ASP:O	7:I:655:LYS:NZ	2.45	0.49
9:L:275:GLU:N	9:L:275:GLU:OE1	2.45	0.49
1:A:353:PHE:CD1	1:A:353:PHE:C	2.91	0.48
2:B:10:ASP:OD1	2:B:10:ASP:N	2.41	0.48
1:A:66:VAL:HG21	1:A:228:VAL:HG22	1.95	0.48
7:I:104:THR:O	7:I:104:THR:OG1	2.26	0.48
2:B:38:TYR:OH	2:B:131:PRO:O	2.31	0.48
9:L:49:ARG:NH2	10:O:805:MET:O	2.46	0.48
10:O:49:THR:HG21	10:O:191:LEU:HD22	1.96	0.48
1:A:30:ASP:OD1	1:A:30:ASP:N	2.46	0.48
2:B:887:THR:O	2:B:888:SER:OG	2.20	0.48
6:G:36:LEU:O	6:G:45:ALA:O	2.31	0.48
7:I:699:TYR:OH	7:I:714:PRO:O	2.24	0.48
11:Q:33:LYS:HD2	11:Q:33:LYS:N	2.28	0.48
1:A:991:VAL:CG1	1:A:1123:MET:HE1	2.44	0.48
2:B:490:VAL:HG13	2:B:669:ASP:O	2.13	0.48
9:L:240:GLU:O	9:L:243:ASN:OD1	2.31	0.48
10:O:262:ASP:OD1	10:O:262:ASP:C	2.55	0.48
5:F:122:GLU:OE1	5:F:122:GLU:HA	2.13	0.48
12:S:131:GLY:O	17:S:302:HOH:O	2.20	0.48
2:B:23:LYS:NZ	2:B:618:ASP:OD2	2.47	0.47
3:C:172:ASN:O	3:C:175:THR:HB	2.14	0.47
9:L:39:TYR:OH	9:L:163:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:473:VAL:HG11	10:O:494:ILE:HD11	1.96	0.47
10:O:518:LEU:O	10:O:518:LEU:HD13	2.14	0.47
10:O:580:TYR:CE1	10:O:840:VAL:HG11	2.48	0.47
1:A:306:TYR:OH	2:B:1026:ALA:HB1	2.15	0.47
2:B:301:GLN:N	2:B:301:GLN:OE1	2.47	0.47
1:A:851:GLU:O	1:A:851:GLU:CD	2.57	0.47
4:E:74:VAL:HG12	4:E:75:ASP:N	2.29	0.47
7:I:436:ILE:HG13	7:I:497:VAL:HG11	1.97	0.47
10:O:25:LEU:HD21	10:O:38:LEU:CD1	2.44	0.47
3:C:111:VAL:HG23	3:C:111:VAL:O	2.13	0.47
1:A:633:MET:HE2	12:S:148:PHE:HA	1.97	0.47
11:R:1:MET:HE2	11:R:1:MET:CA	2.45	0.47
6:G:111:ASP:OD1	6:G:111:ASP:C	2.58	0.47
6:G:91:ILE:HD11	6:G:124:PHE:HB2	1.96	0.47
10:O:298:VAL:CG2	10:O:317:LEU:HD11	2.45	0.47
9:L:209:PHE:CD1	9:L:209:PHE:C	2.93	0.46
10:O:603:ALA:O	10:O:607:LYS:NZ	2.48	0.46
11:Q:115:ILE:HD12	11:R:105:ARG:HG3	1.97	0.46
13:U:15:A:H2'	13:U:58:A:H61	1.80	0.46
1:A:776:ILE:HG23	1:A:777:GLY:N	2.31	0.46
2:B:70:ILE:HG23	2:B:98:PHE:CD2	2.51	0.46
2:B:990:PHE:O	2:B:992:GLU:N	2.47	0.46
7:I:51:THR:HG22	7:I:52:GLU:N	2.30	0.46
7:I:675:LEU:HD12	7:I:675:LEU:O	2.16	0.46
10:O:308:LYS:O	10:O:309:ASN:OD1	2.34	0.46
14:Y:358:PHE:CE2	14:Y:369:ILE:HD11	2.51	0.46
9:L:22:LEU:HD11	9:L:205:ASN:HA	1.97	0.46
9:L:58:THR:HG21	9:L:113:GLU:HG3	1.97	0.46
10:O:604:ASP:OD1	10:O:604:ASP:N	2.48	0.46
5:F:107:GLU:OE2	5:F:107:GLU:C	2.58	0.46
7:I:695:ASN:OD1	7:I:695:ASN:N	2.49	0.46
10:O:518:LEU:HD13	10:O:518:LEU:C	2.41	0.46
14:Y:253:LYS:HD3	14:Y:253:LYS:C	2.41	0.46
2:B:134:ILE:HD12	2:B:156:VAL:HG23	1.98	0.46
3:C:195:LYS:CG	3:C:195:LYS:O	2.63	0.46
11:R:79:ASP:OD2	11:R:126:GLY:N	2.43	0.46
9:L:138:PHE:CD1	9:L:138:PHE:C	2.94	0.46
10:O:468:VAL:O	10:O:468:VAL:CG1	2.64	0.46
3:C:90:ARG:HE	3:C:90:ARG:HA	1.80	0.46
2:B:399:ILE:HG22	2:B:400:HIS:H	1.81	0.46
6:G:142:MET:N	6:G:155:LEU:O	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:658:ILE:HD11	7:I:717:PHE:CZ	2.50	0.46
10:O:490:LEU:HD12	10:O:490:LEU:N	2.31	0.46
1:A:996:GLU:O	1:A:1095:LYS:NZ	2.49	0.45
7:I:648:LEU:HD13	7:I:775:LYS:HE2	1.97	0.45
10:O:835:TYR:N	10:O:835:TYR:CD2	2.84	0.45
13:U:54:U:N3	13:U:57:1MA:OP2	2.41	0.45
3:C:152:GLU:OE1	3:C:152:GLU:C	2.59	0.45
3:C:40:VAL:HG22	3:C:141:LEU:HD22	1.99	0.45
7:I:675:LEU:HD12	7:I:675:LEU:C	2.41	0.45
14:Y:104:GLU:H	14:Y:104:GLU:CD	2.24	0.45
7:I:7:ILE:HG22	7:I:11:ILE:HD12	1.98	0.45
2:B:72:ASN:OD1	2:B:72:ASN:C	2.60	0.45
2:B:394:THR:O	2:B:394:THR:HG22	2.16	0.45
10:O:5:VAL:HA	10:O:8:PHE:CD1	2.50	0.45
10:O:626:ILE:HD11	10:O:651:GLN:HB2	1.99	0.45
6:G:132:ASP:OD1	6:G:133:ASN:N	2.49	0.45
2:B:399:ILE:HG22	2:B:400:HIS:N	2.32	0.45
12:S:110:THR:O	12:S:111:SER:C	2.59	0.45
1:A:852:ASP:OD1	1:A:853:ASN:N	2.50	0.45
2:B:709:ILE:HD11	2:B:856:ARG:HG3	1.99	0.45
4:E:134:LYS:HE2	4:E:134:LYS:HA	1.98	0.45
11:R:23:ASP:OD1	11:R:23:ASP:O	2.34	0.45
14:Y:253:LYS:HD3	14:Y:254:LYS:N	2.32	0.45
2:B:862:THR:O	7:I:505:ASP:CB	2.65	0.45
5:F:11:GLU:N	5:F:11:GLU:OE1	2.49	0.45
10:O:398:THR:HG21	10:O:482:GLU:OE1	2.17	0.45
7:I:526:ALA:O	7:I:530:VAL:HG23	2.17	0.45
9:L:175:LEU:HD21	9:L:209:PHE:HD2	1.82	0.45
10:O:619:THR:HG21	10:O:659:PHE:HE1	1.82	0.45
1:A:28:LYS:O	1:A:28:LYS:HG3	2.16	0.44
7:I:663:THR:HG21	7:I:679:ILE:HD13	1.97	0.44
11:Q:115:ILE:CD1	11:R:105:ARG:HG3	2.46	0.44
11:R:38:LEU:HD23	11:R:42:ILE:HD11	1.98	0.44
8:J:20:LYS:O	8:J:21:LEU:HB3	2.16	0.44
10:O:650:ILE:HG22	10:O:651:GLN:N	2.32	0.44
7:I:647:GLU:OE1	7:I:648:LEU:N	2.50	0.44
12:S:139:ILE:HG22	12:S:140:LYS:N	2.33	0.44
1:A:696:ARG:O	2:B:346:SER:O	2.35	0.44
7:I:679:ILE:HD12	7:I:680:GLU:HB2	1.99	0.44
11:R:25:VAL:HG22	11:R:26:CYS:N	2.31	0.44
1:A:1126:GLU:O	1:A:1127:LEU:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:254:ASN:HA	3:C:271:LEU:O	2.18	0.44
7:I:130:ILE:HG22	7:I:131:LEU:N	2.33	0.44
9:L:37:LEU:HD23	10:O:791:ILE:HD13	1.99	0.44
1:A:24:ILE:HD12	1:A:35:THR:O	2.17	0.44
1:A:1013:THR:HG22	1:A:1014:ASP:OD1	2.18	0.44
11:Q:31:ILE:H	11:Q:31:ILE:HD12	1.83	0.44
1:A:991:VAL:HG11	1:A:1123:MET:HE1	2.00	0.43
3:C:119:GLU:OE1	3:C:119:GLU:N	2.48	0.43
4:E:107:SER:O	4:E:107:SER:OG	2.35	0.43
7:I:160:GLU:OE1	7:I:160:GLU:N	2.46	0.43
10:O:49:THR:HG23	10:O:219:ILE:HG23	1.99	0.43
2:B:231:VAL:HG22	2:B:232:ASN:N	2.34	0.43
7:I:113:ASP:OD1	7:I:117:ASN:ND2	2.52	0.43
11:R:23:ASP:OD1	11:R:23:ASP:C	2.61	0.43
12:S:139:ILE:CG2	12:S:140:LYS:N	2.81	0.43
1:A:1224:ALA:HB2	2:B:1136:VAL:HG13	2.00	0.43
10:O:619:THR:O	10:O:619:THR:CG2	2.65	0.43
1:A:596:VAL:O	1:A:599:ILE:HG22	2.19	0.43
2:B:287:ILE:O	2:B:291:VAL:HG23	2.18	0.43
7:I:564:LEU:HD12	7:I:564:LEU:H	1.82	0.43
3:C:80:LEU:HD23	3:C:80:LEU:C	2.43	0.43
10:O:302:GLY:HA2	10:O:315:ILE:HD12	2.01	0.43
10:O:328:LEU:HD22	10:O:352:TYR:CD1	2.53	0.43
12:S:117:PHE:CE2	12:S:121:LEU:HD12	2.54	0.43
14:Y:21:VAL:O	14:Y:21:VAL:CG2	2.67	0.43
14:Y:254:LYS:HB2	14:Y:478:ILE:HD11	2.00	0.43
1:A:1216:ASP:O	1:A:1217:ASN:HB2	2.19	0.43
3:C:115:ASP:OD1	3:C:115:ASP:N	2.44	0.43
11:R:25:VAL:CG1	11:R:30:LEU:HD21	2.48	0.43
1:A:978:ILE:N	1:A:978:ILE:HD12	2.33	0.43
5:F:61:HIS:ND1	5:F:61:HIS:N	2.67	0.43
2:B:440:ILE:HB	2:B:441:PRO:HD3	2.00	0.43
3:C:240:THR:O	3:C:240:THR:OG1	2.34	0.43
10:O:571:TYR:O	10:O:574:THR:HG22	2.18	0.43
14:Y:349:ASP:OD1	14:Y:350:ALA:N	2.49	0.43
7:I:661:HIS:C	7:I:663:THR:H	2.26	0.43
10:O:182:HIS:ND1	10:O:183:PRO:HD2	2.34	0.43
12:S:244:ILE:HD12	12:S:244:ILE:C	2.43	0.43
1:A:24:ILE:HB	1:A:66:VAL:HG22	2.00	0.42
1:A:804:ASP:OD1	1:A:805:GLU:N	2.52	0.42
2:B:152:VAL:O	2:B:153:ILE:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:132:ASP:OD2	4:E:132:ASP:C	2.62	0.42
6:G:38:ARG:HH11	6:G:38:ARG:HG2	1.84	0.42
14:Y:92:ASP:HB3	14:Y:93:PRO:HD3	2.00	0.42
8:J:35:VAL:HG12	8:J:36:LYS:N	2.33	0.42
7:I:718:GLU:HA	7:I:718:GLU:OE1	2.19	0.42
9:L:5:VAL:HA	9:L:8:ILE:HG22	2.00	0.42
14:Y:617:ASN:HB3	14:Y:618:PRO:HD3	2.01	0.42
2:B:481:GLN:OE1	2:B:481:GLN:HA	2.18	0.42
2:B:587:LEU:O	2:B:631:ASP:HA	2.20	0.42
4:E:74:VAL:CG1	4:E:75:ASP:N	2.81	0.42
10:O:298:VAL:HG21	10:O:317:LEU:HD11	2.01	0.42
12:S:136:ILE:HG22	12:S:137:ASP:N	2.35	0.42
1:A:66:VAL:HG12	1:A:67:SER:N	2.35	0.42
2:B:653:ASP:OD1	2:B:654:GLU:N	2.51	0.42
3:C:177:ILE:HG22	3:C:178:ASP:N	2.34	0.42
9:L:45:LEU:HG	9:L:253:TYR:HB3	2.01	0.42
3:C:134:LYS:H	3:C:134:LYS:HD3	1.84	0.42
6:G:137:VAL:HG12	6:G:138:THR:H	1.85	0.42
11:Q:88:PHE:CE1	11:Q:91:VAL:HG23	2.55	0.42
14:Y:24:MET:HE3	14:Y:24:MET:HB3	1.97	0.42
14:Y:429:GLU:O	14:Y:430:SER:OG	2.19	0.42
1:A:638:THR:HG23	1:A:677:MET:HE1	2.01	0.42
7:I:746:ASP:N	7:I:746:ASP:OD2	2.49	0.42
7:I:723:ASP:OD1	7:I:723:ASP:N	2.52	0.42
1:A:938:PHE:CD1	1:A:938:PHE:C	2.98	0.42
10:O:400:ASP:N	10:O:400:ASP:OD1	2.52	0.42
14:Y:190:SER:HA	14:Y:520:LYS:HZ3	1.84	0.42
10:O:66:PHE:CZ	10:O:99:ILE:HD11	2.55	0.42
11:Q:44:ILE:N	11:Q:44:ILE:HD13	2.35	0.42
11:R:49:PHE:CE2	11:R:51:LEU:HD11	2.55	0.42
1:A:582:ARG:O	1:A:583:PRO:C	2.63	0.41
1:A:1108:TYR:C	1:A:1109:THR:HG22	2.45	0.41
7:I:38:ASN:O	7:I:41:VAL:HG22	2.20	0.41
10:O:52:ASN:ND2	10:O:221:MET:SD	2.89	0.41
14:Y:328:ARG:HH12	14:Y:396:ILE:HG23	1.85	0.41
1:A:755:LEU:HD23	1:A:961:PHE:HE1	1.84	0.41
11:R:55:ASP:C	11:R:57:ASP:H	2.27	0.41
12:S:94:ILE:HG22	12:S:95:ALA:N	2.32	0.41
12:S:127:CYS:SG	12:S:132:VAL:HB	2.60	0.41
14:Y:85:VAL:O	14:Y:113:ASN:HA	2.20	0.41
1:A:386:ARG:NE	1:A:448:ASP:OD2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:VAL:O	12:S:144:TYR:OH	2.26	0.41
1:A:790:ILE:HG22	1:A:791:LEU:N	2.36	0.41
7:I:4:LYS:NZ	7:I:48:SER:O	2.51	0.41
11:R:38:LEU:CD2	11:R:42:ILE:HD11	2.50	0.41
14:Y:69:LEU:HD23	14:Y:72:LEU:HD11	2.02	0.41
1:A:613:VAL:HG13	1:A:620:PRO:HG3	2.02	0.41
6:G:37:HIS:O	6:G:150:SER:HA	2.19	0.41
7:I:172:LEU:HB2	7:I:173:PRO:HD3	2.01	0.41
10:O:33:GLU:OE1	10:O:33:GLU:HA	2.20	0.41
12:S:134:TYR:CD1	12:S:134:TYR:C	2.98	0.41
1:A:1180:GLN:N	1:A:1180:GLN:OE1	2.53	0.41
2:B:501:GLU:O	2:B:504:ASP:OD2	2.39	0.41
2:B:722:ILE:HD12	2:B:723:VAL:HG23	2.02	0.41
3:C:241:VAL:O	3:C:241:VAL:HG12	2.20	0.41
9:L:9:ARG:HG2	9:L:9:ARG:HH11	1.85	0.41
1:A:850:THR:O	1:A:850:THR:OG1	2.36	0.41
7:I:664:ASN:O	7:I:664:ASN:ND2	2.53	0.41
10:O:126:GLU:N	10:O:126:GLU:OE2	2.53	0.41
10:O:154:LYS:HD3	10:O:154:LYS:C	2.45	0.41
12:S:134:TYR:HD1	12:S:134:TYR:O	2.03	0.41
1:A:605:ALA:HB1	12:S:147:TYR:O	2.20	0.41
1:A:748:GLU:O	1:A:752:THR:HG23	2.20	0.41
4:E:82:ILE:C	4:E:83:ILE:HD12	2.46	0.41
1:A:1140:ASN:HA	4:E:106:ILE:HD11	2.02	0.41
11:Q:1:MET:HE3	11:Q:55:ASP:OD2	2.21	0.41
2:B:147:TYR:CG	2:B:148:LEU:N	2.88	0.41
2:B:507:LYS:NZ	2:B:511:GLU:OE2	2.48	0.41
2:B:603:VAL:O	2:B:603:VAL:HG23	2.21	0.41
3:C:124:LEU:HD21	8:J:22:ILE:HG21	2.03	0.41
7:I:457:GLU:OE1	7:I:457:GLU:N	2.52	0.41
7:I:462:LEU:HD21	7:I:555:VAL:HG11	2.03	0.41
9:L:43:TYR:CD1	10:O:575:LEU:HD22	2.55	0.41
12:S:127:CYS:O	12:S:131:GLY:N	2.53	0.41
12:S:240:ASP:OD1	12:S:240:ASP:C	2.63	0.41
1:A:91:ILE:O	1:A:91:ILE:CG2	2.67	0.41
1:A:304:PRO:HD2	1:A:307:ILE:HD12	2.03	0.41
6:G:137:VAL:HG12	6:G:138:THR:N	2.35	0.41
7:I:663:THR:HG21	7:I:679:ILE:CD1	2.51	0.41
1:A:807:MET:HE1	1:A:813:ILE:HG21	2.04	0.40
7:I:97:SER:OG	7:I:98:PHE:N	2.53	0.40
10:O:711:THR:OG1	10:O:712:MET:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Y:239:PHE:N	14:Y:239:PHE:CD2	2.89	0.40
1:A:37:LYS:O	1:A:37:LYS:HG2	2.20	0.40
7:I:753:ASN:O	7:I:753:ASN:CG	2.63	0.40
10:O:62:SER:OG	10:O:455:ASN:O	2.39	0.40
11:R:122:LYS:HB3	11:R:123:PHE:CD2	2.57	0.40
14:Y:172:ILE:HG13	14:Y:179:MET:HE2	2.03	0.40
7:I:303:LYS:NZ	7:I:304:LEU:O	2.53	0.40
10:O:80:ILE:C	10:O:80:ILE:CD1	2.94	0.40
10:O:512:ASN:O	10:O:515:VAL:HG22	2.22	0.40
2:B:400:HIS:CE1	7:I:538:THR:HG21	2.56	0.40
10:O:677:TRP:CD1	10:O:680:ALA:HB3	2.57	0.40
2:B:430:PRO:O	2:B:436:GLN:NE2	2.52	0.40
4:E:93:ASN:OD1	4:E:93:ASN:N	2.54	0.40
7:I:330:ILE:N	7:I:330:ILE:HD12	2.37	0.40
7:I:679:ILE:HD12	7:I:680:GLU:CB	2.52	0.40
10:O:257:ALA:CB	10:O:365:MET:HE1	2.52	0.40
10:O:552:GLU:OE1	10:O:552:GLU:N	2.55	0.40
11:R:25:VAL:HG22	11:R:26:CYS:H	1.87	0.40
12:S:12:ASN:OD1	12:S:12:ASN:N	2.53	0.40
12:S:109:GLY:O	12:S:110:THR:OG1	2.35	0.40
14:Y:92:ASP:CB	14:Y:93:PRO:HD3	2.52	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	1274/1286 (99%)	1193 (94%)	80 (6%)	1 (0%)	48 69
2	B	1123/1164 (96%)	1054 (94%)	69 (6%)	0	100 100
3	C	302/305 (99%)	278 (92%)	24 (8%)	0	100 100
4	E	182/185 (98%)	176 (97%)	6 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	107/164 (65%)	104 (97%)	3 (3%)	0	100	100
6	G	157/161 (98%)	144 (92%)	13 (8%)	0	100	100
7	I	765/795 (96%)	718 (94%)	47 (6%)	0	100	100
8	J	59/63 (94%)	53 (90%)	6 (10%)	0	100	100
9	L	280/287 (98%)	272 (97%)	8 (3%)	0	100	100
10	O	842/844 (100%)	818 (97%)	24 (3%)	0	100	100
11	Q	122/129 (95%)	115 (94%)	7 (6%)	0	100	100
11	R	128/129 (99%)	120 (94%)	8 (6%)	0	100	100
12	S	182/259 (70%)	163 (90%)	19 (10%)	0	100	100
14	Y	605/631 (96%)	568 (94%)	37 (6%)	0	100	100
All	All	6128/6402 (96%)	5776 (94%)	351 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	583	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1149/1157 (99%)	1137 (99%)	12 (1%)	73	88
2	B	1030/1064 (97%)	1017 (99%)	13 (1%)	65	85
3	C	286/287 (100%)	279 (98%)	7 (2%)	44	70
4	E	174/175 (99%)	174 (100%)	0	100	100
5	F	102/151 (68%)	102 (100%)	0	100	100
6	G	142/144 (99%)	142 (100%)	0	100	100
7	I	735/755 (97%)	725 (99%)	10 (1%)	62	83
8	J	60/62 (97%)	60 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	L	269/272 (99%)	268 (100%)	1 (0%)	89 96
10	O	774/774 (100%)	768 (99%)	6 (1%)	79 91
11	Q	117/121 (97%)	116 (99%)	1 (1%)	75 90
11	R	122/121 (101%)	121 (99%)	1 (1%)	79 91
12	S	171/237 (72%)	169 (99%)	2 (1%)	67 86
14	Y	554/573 (97%)	549 (99%)	5 (1%)	75 90
All	All	5685/5893 (96%)	5627 (99%)	58 (1%)	71 88

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	36	VAL
1	A	77	GLU
1	A	90	CYS
1	A	136	MET
1	A	366	VAL
1	A	555	ILE
1	A	683	TYR
1	A	746	VAL
1	A	1062	ASP
1	A	1107	ASP
1	A	1142	ASN
2	B	52	VAL
2	B	100	VAL
2	B	189	THR
2	B	215	SER
2	B	229	ILE
2	B	237	SER
2	B	243	VAL
2	B	275	THR
2	B	325	GLN
2	B	728	LEU
2	B	863	ASP
2	B	1061	LEU
2	B	1083	ASP
3	C	61	THR
3	C	135	SER
3	C	161	LEU
3	C	211	CYS

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Mol	Chain	Res	Type
3	C	240	THR
3	C	296	LYS
3	C	300	SER
7	I	24	ILE
7	I	63	GLU
7	I	185	SER
7	I	197	HIS
7	I	220	LEU
7	I	462	LEU
7	I	538	THR
7	I	647	GLU
7	I	703	ASN
7	I	746	ASP
9	L	7	ASN
10	O	1	MET
10	O	124	SER
10	O	229	LEU
10	O	362	VAL
10	O	567	ILE
10	O	604	ASP
11	Q	17	PHE
11	R	117	VAL
12	S	12	ASN
12	S	55	ASN
14	Y	17	THR
14	Y	50	SER
14	Y	78	ASN
14	Y	92	ASP
14	Y	510	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	72	HIS
1	A	183	HIS
1	A	327	GLN
1	A	413	ASN
1	A	427	GLN
1	A	428	ASN
1	A	481	ASN
1	A	685	GLN

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Mol	Chain	Res	Type
1	A	686	GLN
2	B	357	HIS
2	B	389	HIS
2	B	620	GLN
2	B	714	HIS
2	B	789	ASN
2	B	1122	HIS
2	B	1132	ASN
3	C	27	ASN
3	C	229	ASN
3	C	230	HIS
4	E	65	ASN
4	E	125	ASN
5	F	115	HIS
6	G	63	ASN
6	G	64	ASN
6	G	129	ASN
7	I	46	ASN
7	I	252	HIS
7	I	253	ASN
7	I	254	ASN
7	I	284	HIS
7	I	674	HIS
7	I	703	ASN
7	I	792	ASN
7	I	794	ASN
8	J	57	GLN
10	O	129	HIS
10	O	178	HIS
10	O	234	ASN
10	O	281	HIS
10	O	401	GLN
10	O	486	ASN
10	O	511	HIS
10	O	558	ASN
10	O	696	ASN
11	Q	112	HIS
11	R	32	ASN
11	R	120	ASN
11	R	121	HIS
12	S	213	HIS
12	S	226	ASN

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Mol	Chain	Res	Type
14	Y	55	HIS
14	Y	71	HIS
14	Y	208	HIS
14	Y	262	ASN
14	Y	408	ASN
14	Y	481	ASN
14	Y	573	ASN
14	Y	587	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	U	68/72 (94%)	11 (16%)	0

All (11) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	U	4	C
13	U	16	U
13	U	17	G
13	U	34	5MU
13	U	35	U
13	U	37	A
13	U	41	C
13	U	46	A
13	U	48	C
13	U	60	C
13	U	72	U

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	SEP	S	228	12	8,9,10	1.51	1 (12%)	8,12,14	1.43	2 (25%)
12	SEP	S	237	12	8,9,10	1.52	1 (12%)	8,12,14	1.58	2 (25%)
13	OMC	U	32	13	19,22,23	0.55	0	26,31,34	0.61	0
12	SEP	S	232	12	8,9,10	1.53	1 (12%)	8,12,14	1.61	2 (25%)
13	1MA	U	57	13	16,25,26	0.88	2 (12%)	18,37,40	1.04	2 (11%)
13	5MU	U	34	13	19,22,23	0.40	0	28,32,35	0.61	0

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
12	SEP	S	228	12	-	3/5/8/10	-
12	SEP	S	237	12	-	0/5/8/10	-
13	OMC	U	32	13	-	0/9/27/28	0/2/2/2
12	SEP	S	232	12	-	0/5/8/10	-
13	1MA	U	57	13	-	0/3/25/26	0/3/3/3
13	5MU	U	34	13	-	1/7/25/26	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	S	232	SEP	P-O1P	3.34	1.61	1.50
12	S	237	SEP	P-O1P	3.32	1.61	1.50
12	S	228	SEP	P-O1P	3.29	1.61	1.50
13	U	57	1MA	C8-N7	-2.23	1.31	1.35
13	U	57	1MA	C5-C4	-2.17	1.37	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	S	232	SEP	P-OG-CB	-3.08	109.82	118.30
12	S	237	SEP	OG-CB-CA	2.89	110.95	108.14
12	S	232	SEP	OG-CB-CA	2.81	110.88	108.14
12	S	228	SEP	OG-CB-CA	2.76	110.83	108.14
12	S	237	SEP	P-OG-CB	-2.70	110.86	118.30
13	U	57	1MA	N1-C6-N6	2.18	125.31	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	U	57	1MA	C5-C6-N1	-2.07	110.81	113.90
12	S	228	SEP	P-OG-CB	-2.05	112.64	118.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	S	228	SEP	CB-OG-P-O1P
12	S	228	SEP	CB-OG-P-O3P
13	U	34	5MU	O4'-C4'-C5'-O5'
12	S	228	SEP	CB-OG-P-O2P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	U	57	1MA	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

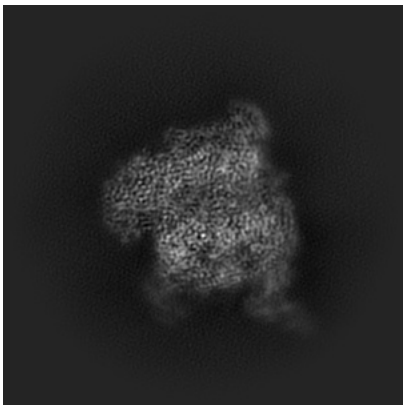
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50644. These allow visual inspection of the internal detail of the map and identification of artifacts.

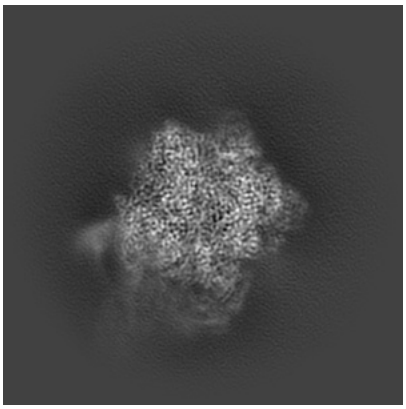
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

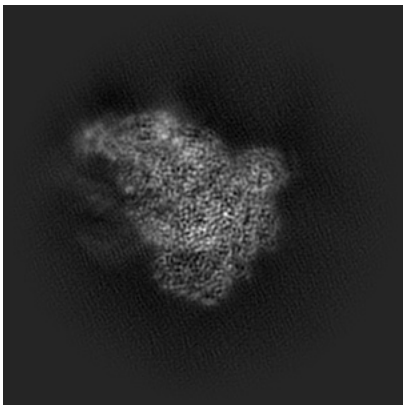
6.1.1 Primary map



X

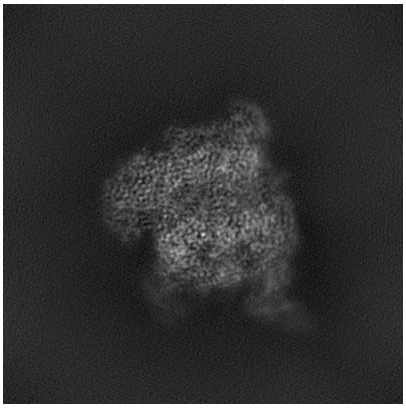


Y

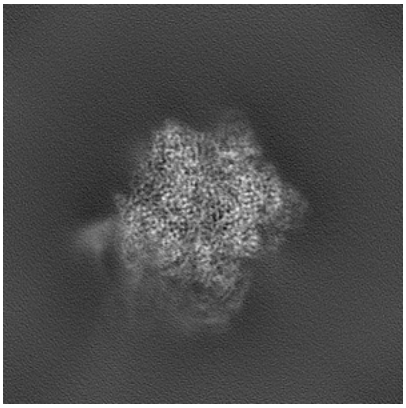


Z

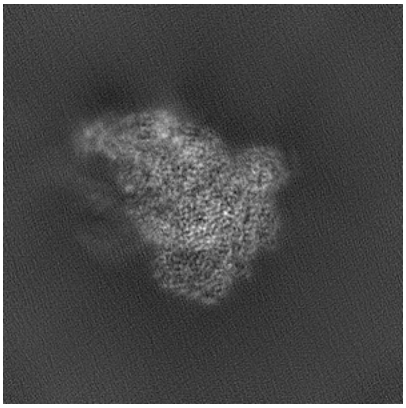
6.1.2 Raw map



X



Y

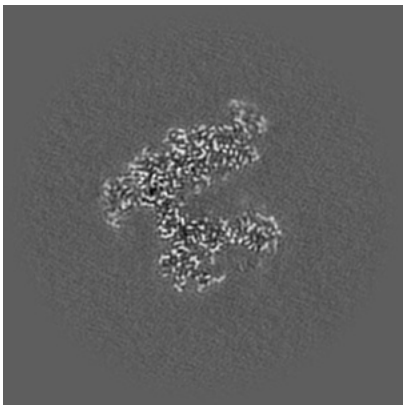


Z

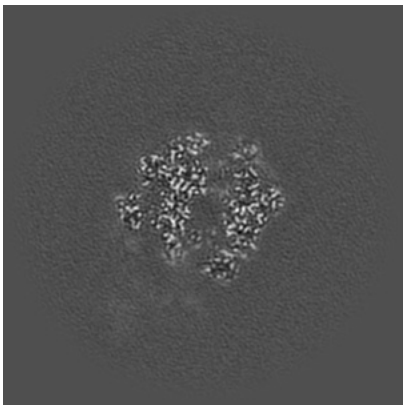
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

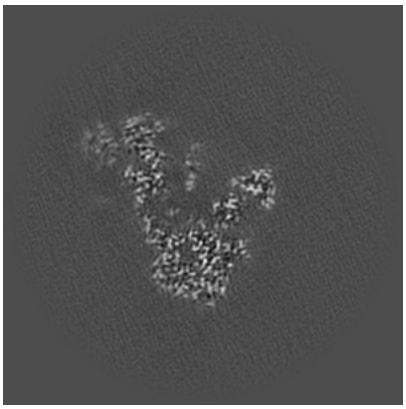
6.2.1 Primary map



X Index: 160

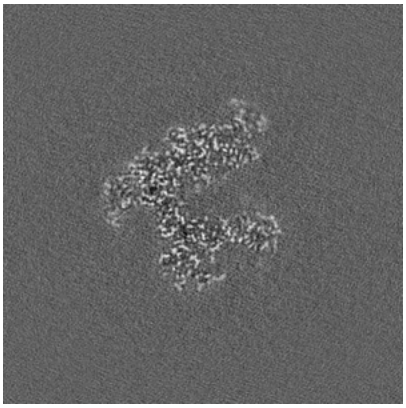


Y Index: 160

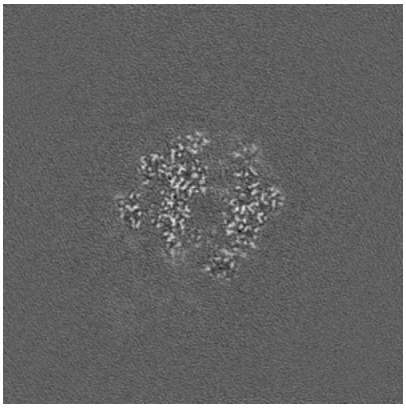


Z Index: 160

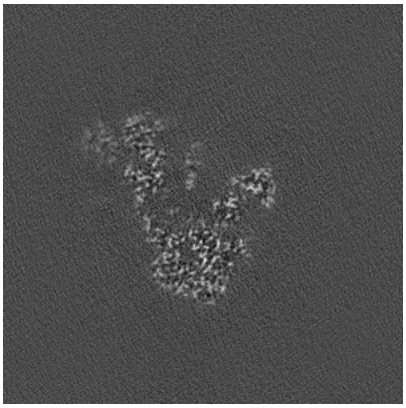
6.2.2 Raw map



X Index: 160



Y Index: 160

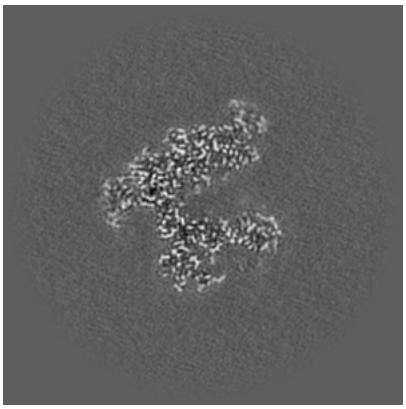


Z Index: 160

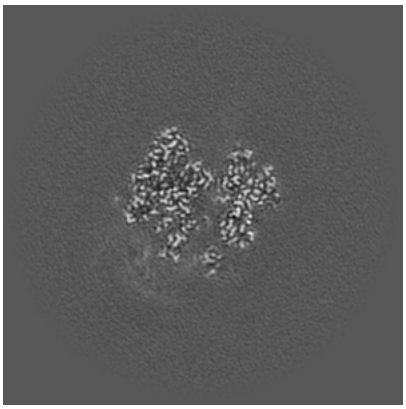
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

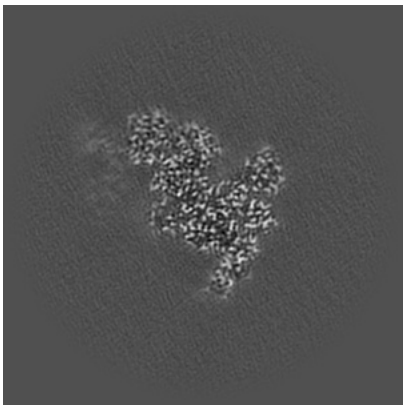
6.3.1 Primary map



X Index: 160

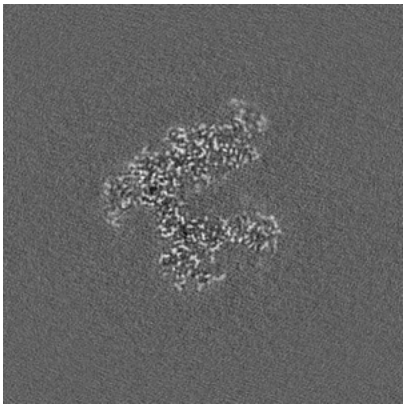


Y Index: 149

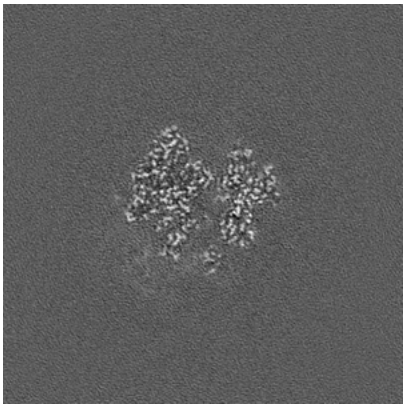


Z Index: 141

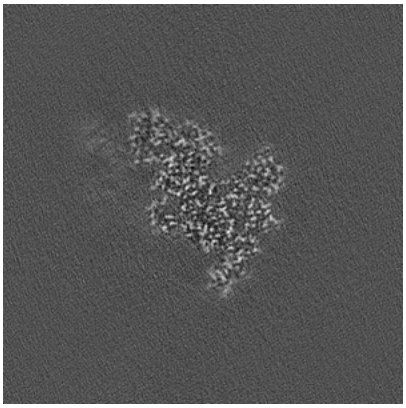
6.3.2 Raw map



X Index: 160



Y Index: 149

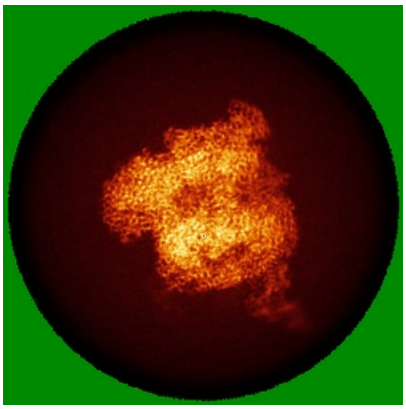


Z Index: 140

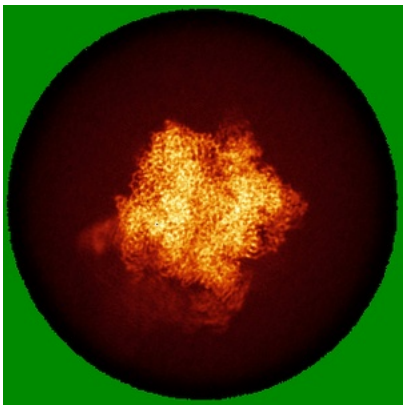
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

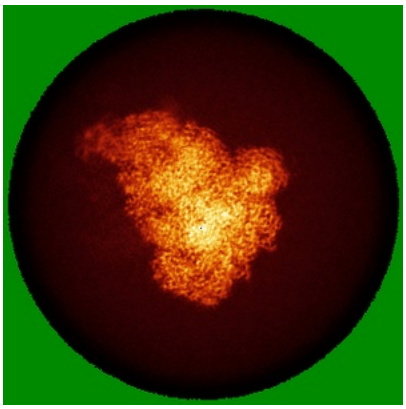
6.4.1 Primary map



X

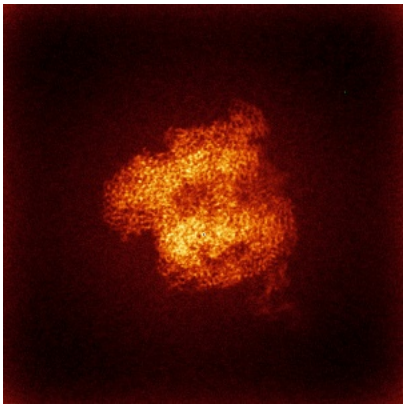


Y

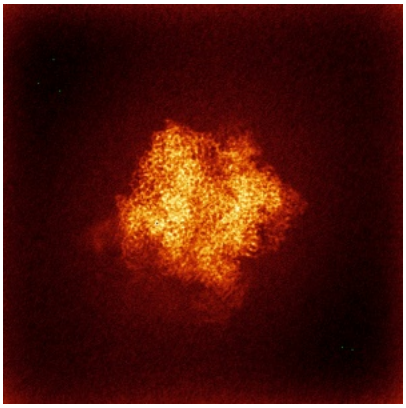


Z

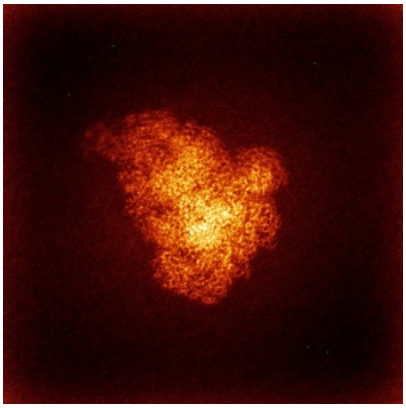
6.4.2 Raw map



X



Y

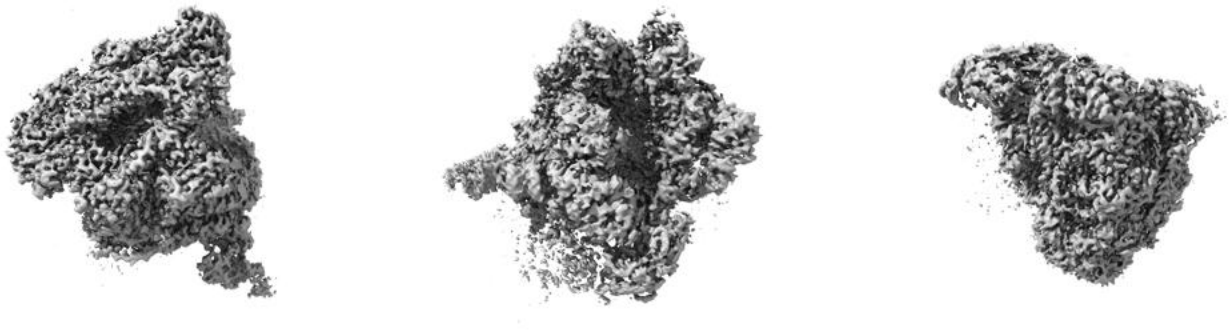


Z

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)

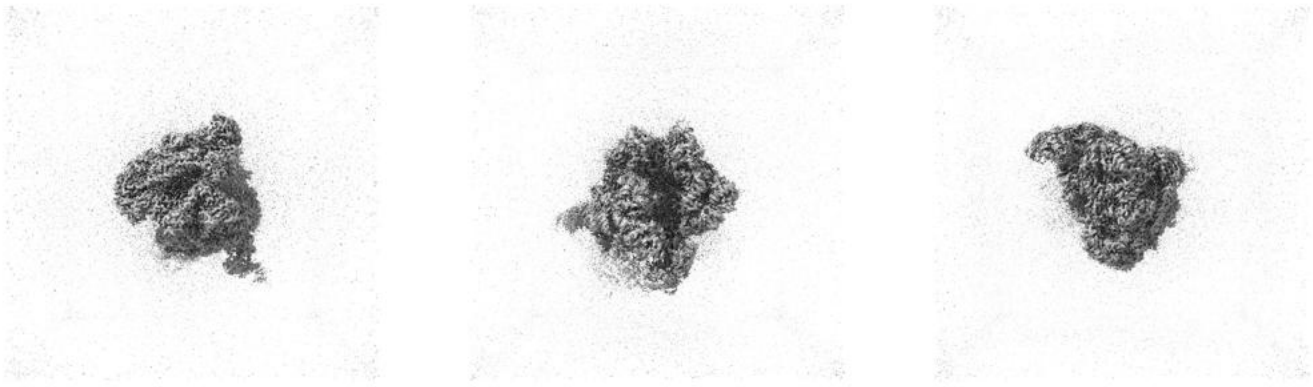
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

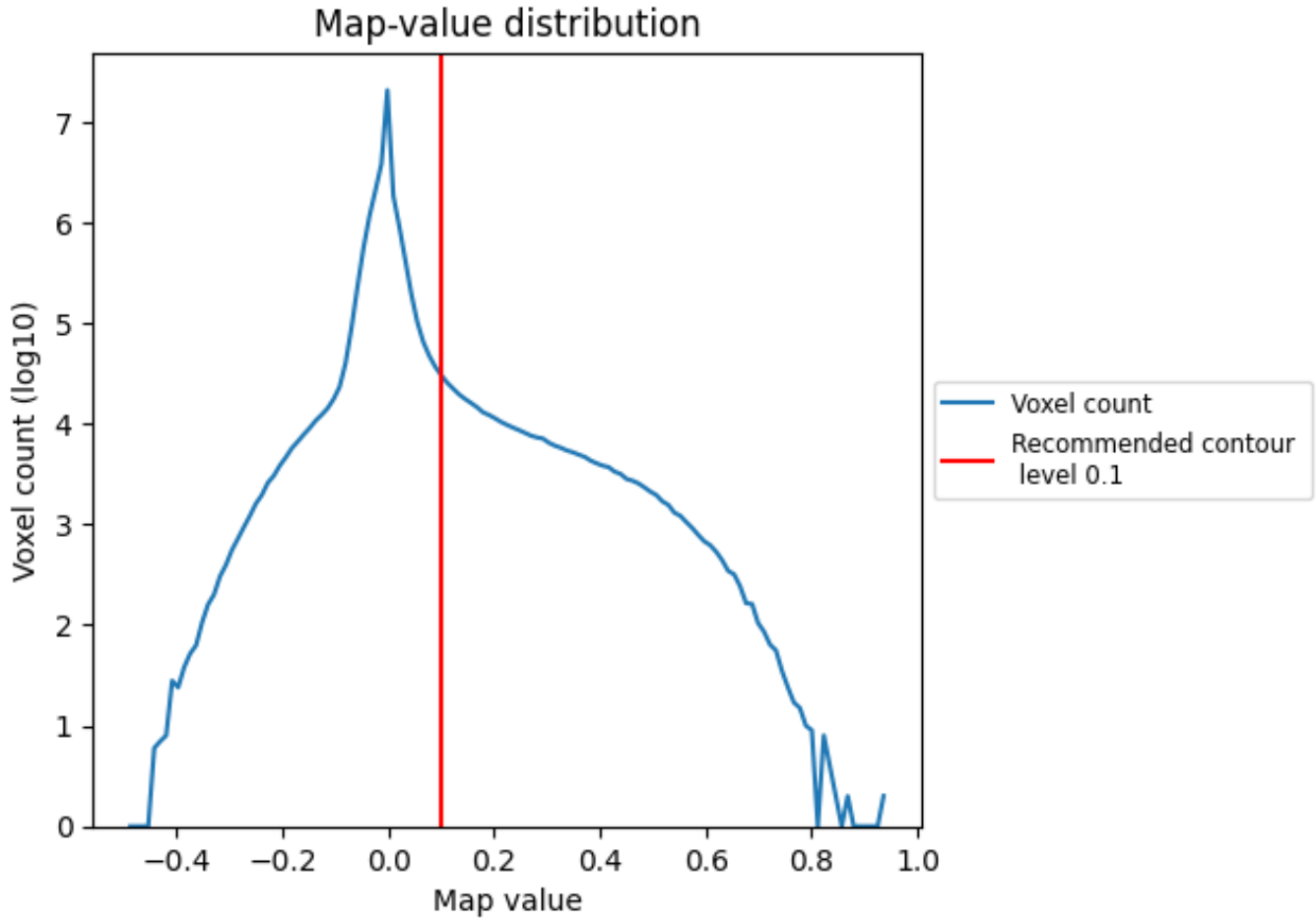
6.6 Mask visualisation (i)

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

7 Map analysis

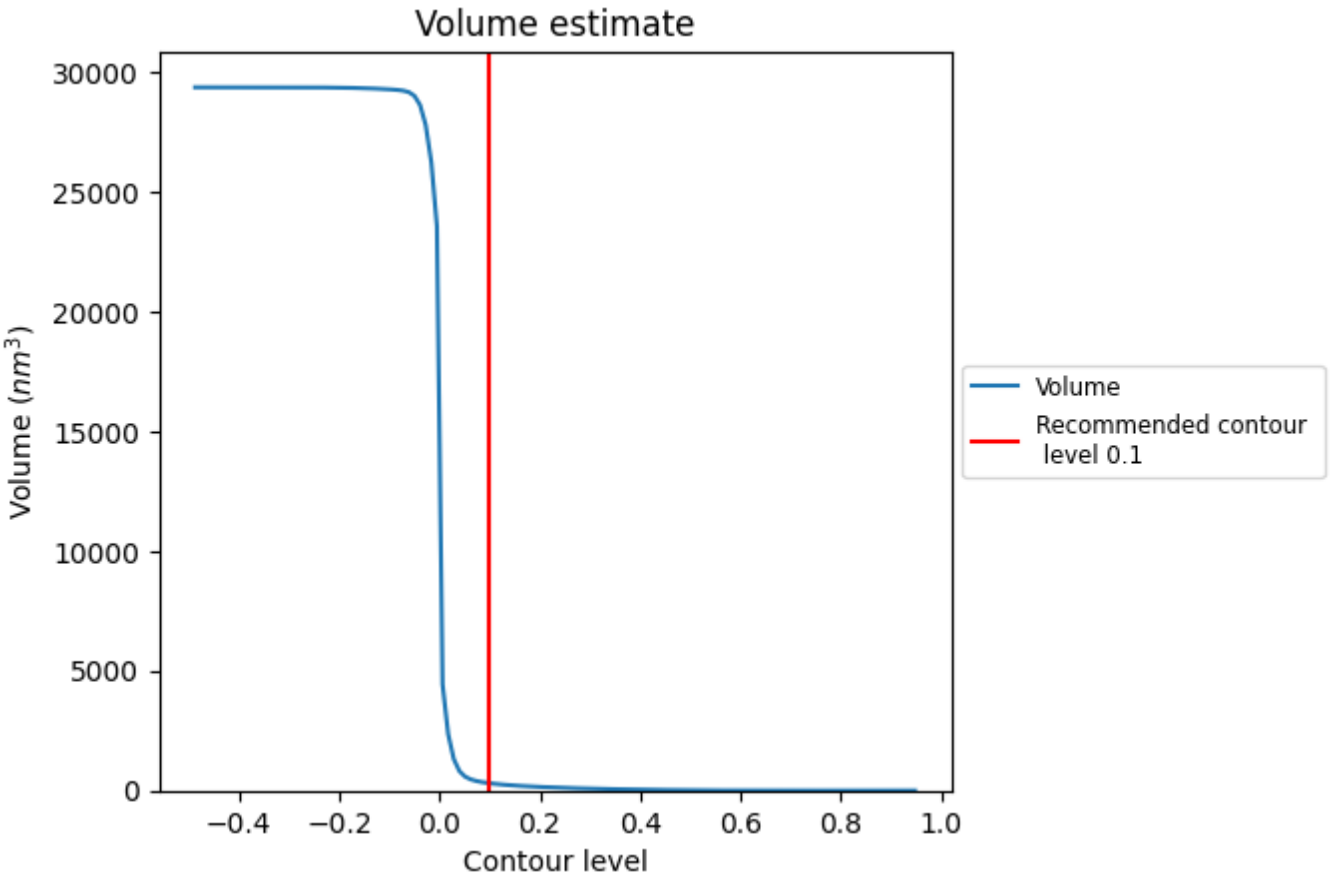
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

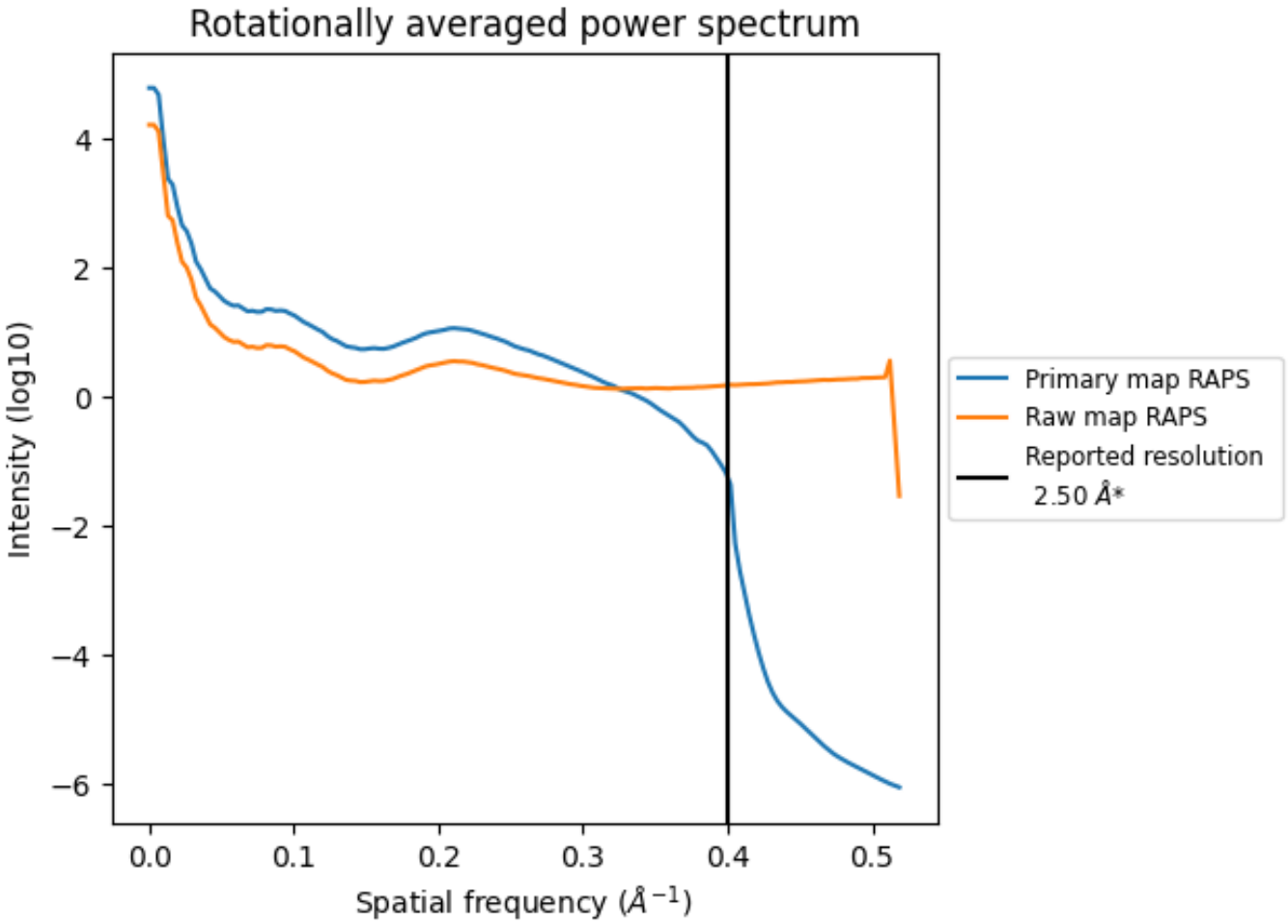
7.2 Volume estimate



The volume at the recommended contour level is 306 nm^3; this corresponds to an approximate mass of 276 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)

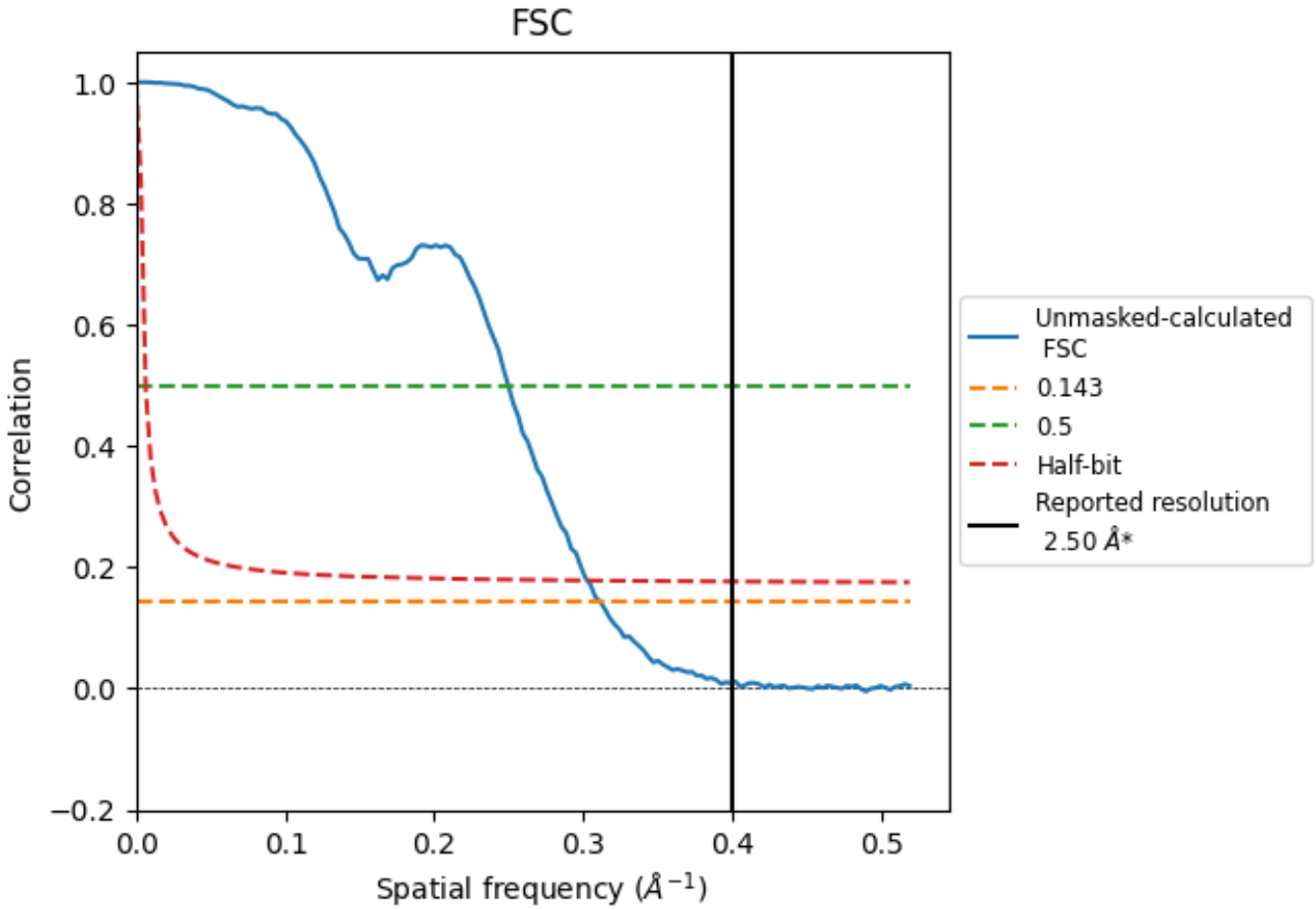


*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8.2 Resolution estimates (i)

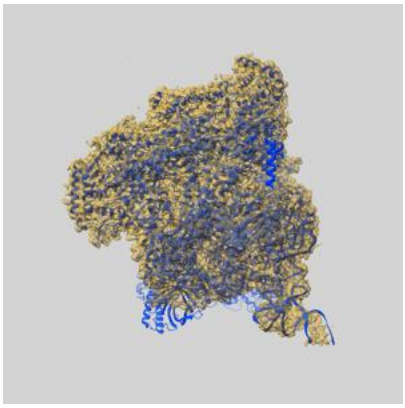
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.21	4.01	3.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.21 differs from the reported value 2.5 by more than 10 %

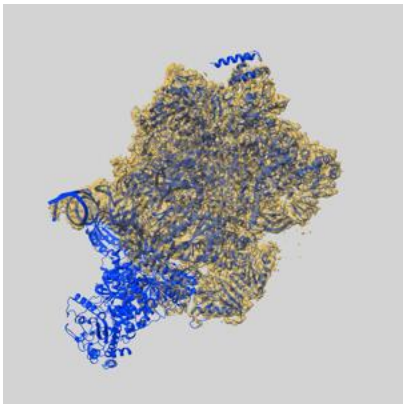
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50644 and PDB model 9FQ6. Per-residue inclusion information can be found in section 3 on page 8.

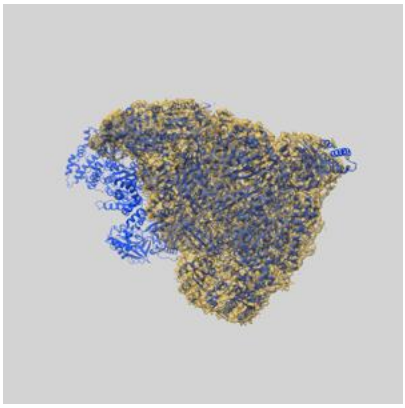
9.1 Map-model overlay



X



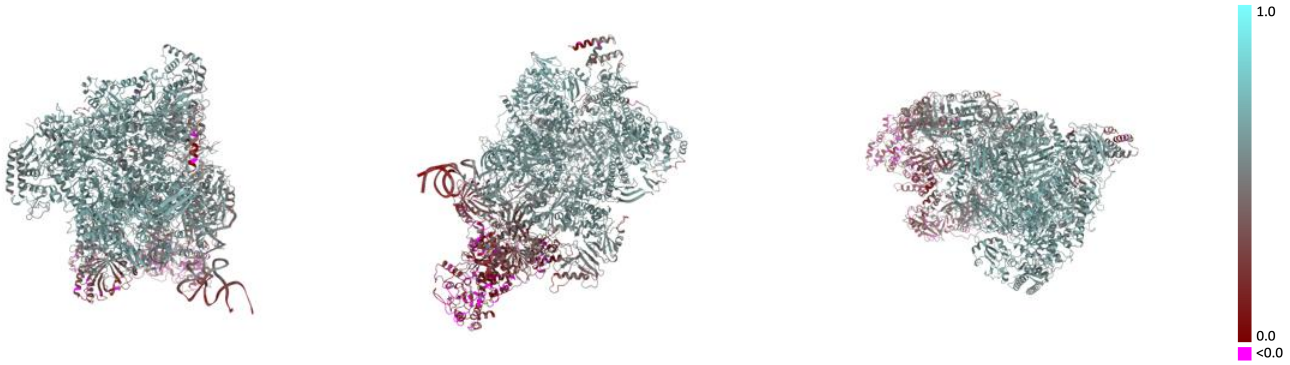
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

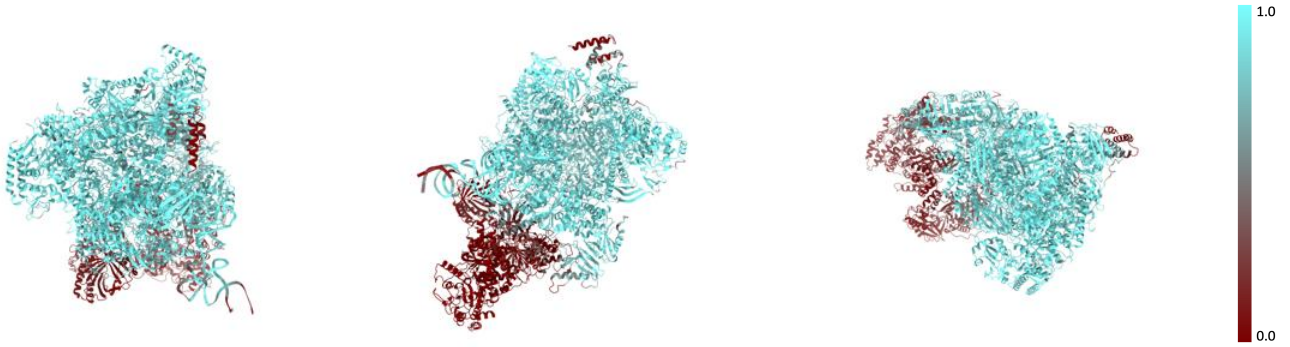
9.2 Q-score mapped to coordinate model



X Y Z

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

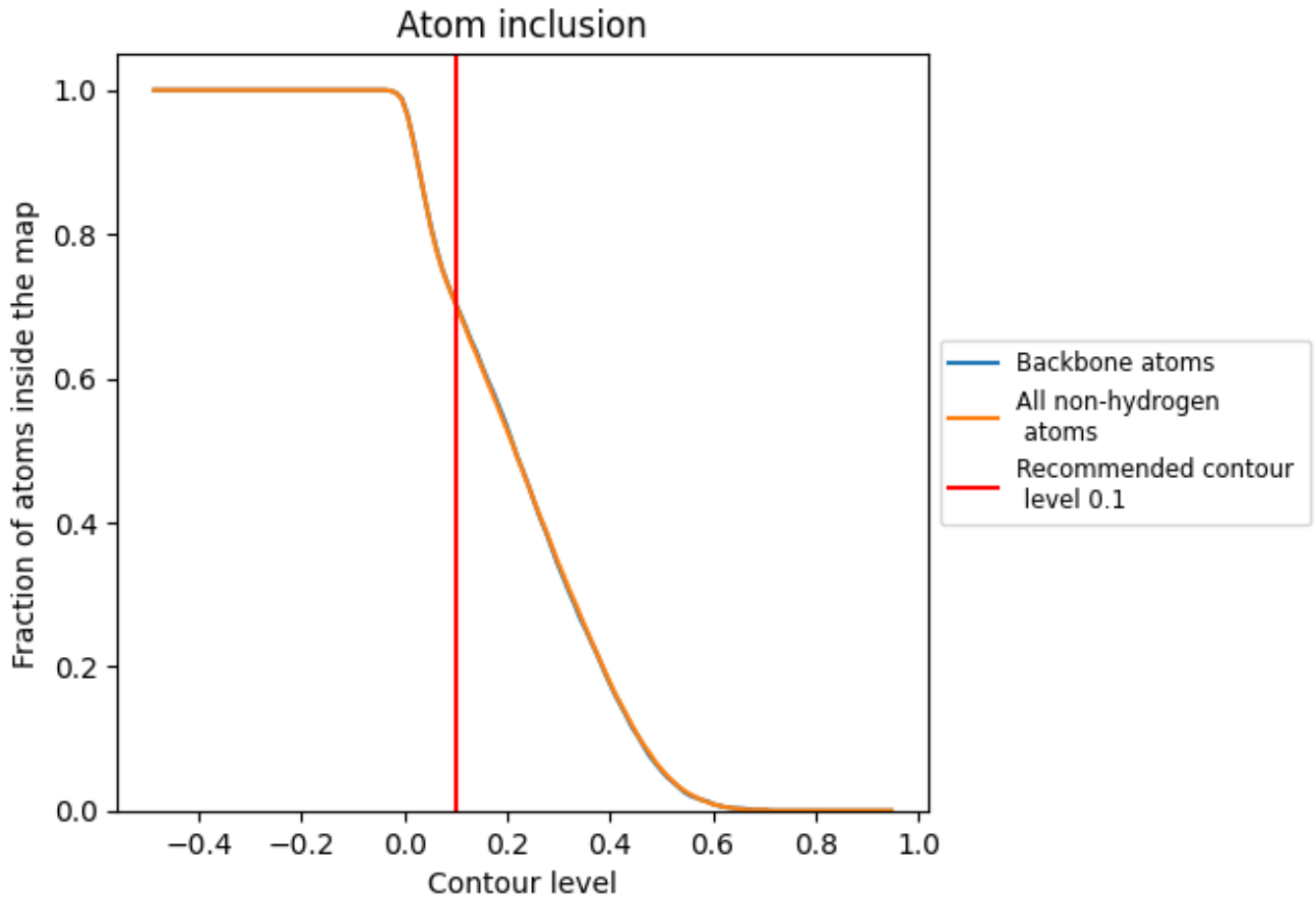
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 70% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7020	0.4920
A	0.9450	0.6000
B	0.9640	0.6150
C	0.9460	0.5690
E	0.9710	0.6130
F	0.9630	0.6260
G	0.9300	0.5770
I	0.7960	0.5210
J	0.9520	0.5830
L	0.0000	0.1380
O	0.0450	0.2590
Q	0.6390	0.4220
R	0.8420	0.5050
S	0.6020	0.4800
U	0.7630	0.3830
Y	0.4820	0.4090