Full wwPDB EM Validation Report ⓘ

Dec 4, 2024 – 05:15 am GMT

PDB ID	:	8S0F
EMDB ID	:	EMD-19624
Title	:	H. sapiens OC1M bound to double stranded DNA
Authors	:	Greiwe, J.F.; Weissmann, F.; Diffley, J.F.X.; Costa, A.
Deposited on	:	2024-02-13
Resolution	:	4.10 Å(reported)
Based on initial model	:	.

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:

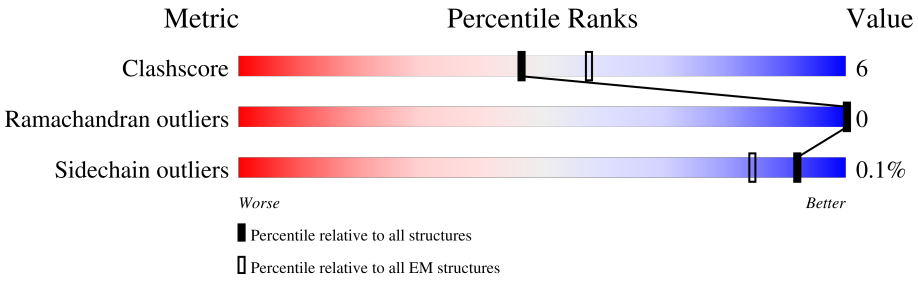
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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 <=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	B	577	28% 6% 66%
2	X	39	26% 74%
3	Y	39	23% 77%
4	5	734	31% 36% 62%
5	8	546	28% 39% 8% 53%
6	2	904	5% 51% 12% 37%
7	4	863	6% 48% 11% 41%
8	6	821	65% 12% 23%

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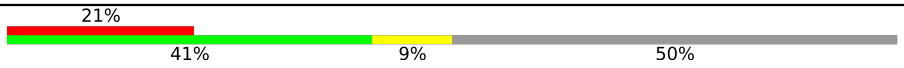
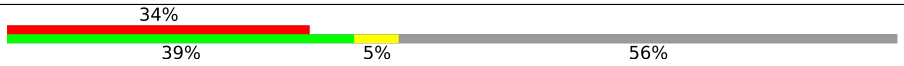
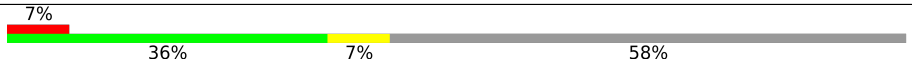
Mol	Chain	Length	Quality of chain
9	7	719	
10	C	711	
11	3	810	
12	A	861	
13	D	436	
14	E	435	

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 40819 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 Origin recognition complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	194	1600	1032	266	297	5	0	0

- Molecule 2 is a DNA chain called DNA (39-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	X	39	799	379	146	235	39	0	0

- Molecule 3 is a DNA chain called DNA (39-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	Y	39	800	379	149	233	39	0	0

- Molecule 4 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	279	2169	1364	383	408	14	0	0

- Molecule 5 is a protein called DNA replication factor Cdt1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	8	259	2097	1306	390	386	15	0	0

- Molecule 6 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	2	572	4513	2838	809	843	23	0	0

- Molecule 7 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	4	512	Total	C	N	O	S	0	0
			4110	2598	728	760	24		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	650	MET	LEU	variant	UNP P33991

- Molecule 8 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	6	629	Total	C	N	O	S	0	0
			5091	3223	888	955	25		

- Molecule 9 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	7	357	Total	C	N	O	S	0	0
			2841	1774	515	534	18		

- Molecule 10 is a protein called Origin recognition complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	574	Total	C	N	O	S	0	0
			4689	3027	781	854	27		

- Molecule 11 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	3	353	Total	C	N	O	S	0	0
			2748	1715	496	520	17		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-1	GLY	-	expression tag	UNP P25205
3	0	GLU	-	expression tag	UNP P25205

- Molecule 12 is a protein called Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	364	Total	C	N	O	S	0	0
			2889	1817	509	540	23		

- Molecule 13 is a protein called Origin recognition complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	406	Total	C	N	O	S	0	0
			3309	2113	575	601	20		

- Molecule 14 is a protein called Origin recognition complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	364	Total	C	N	O	S	0	0
			3003	1967	497	529	10		

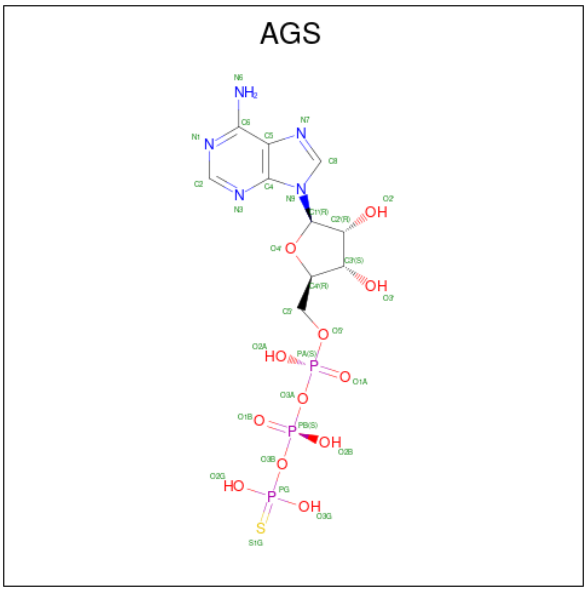
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
15	2	1	Total	Mg	0
			1	1	
15	6	1	Total	Mg	0
			1	1	
15	A	1	Total	Mg	0
			1	1	
15	D	1	Total	Mg	0
			1	1	
15	E	1	Total	Mg	0
			1	1	

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
16	4	1	Total	Zn	0
			1	1	

- Molecule 17 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



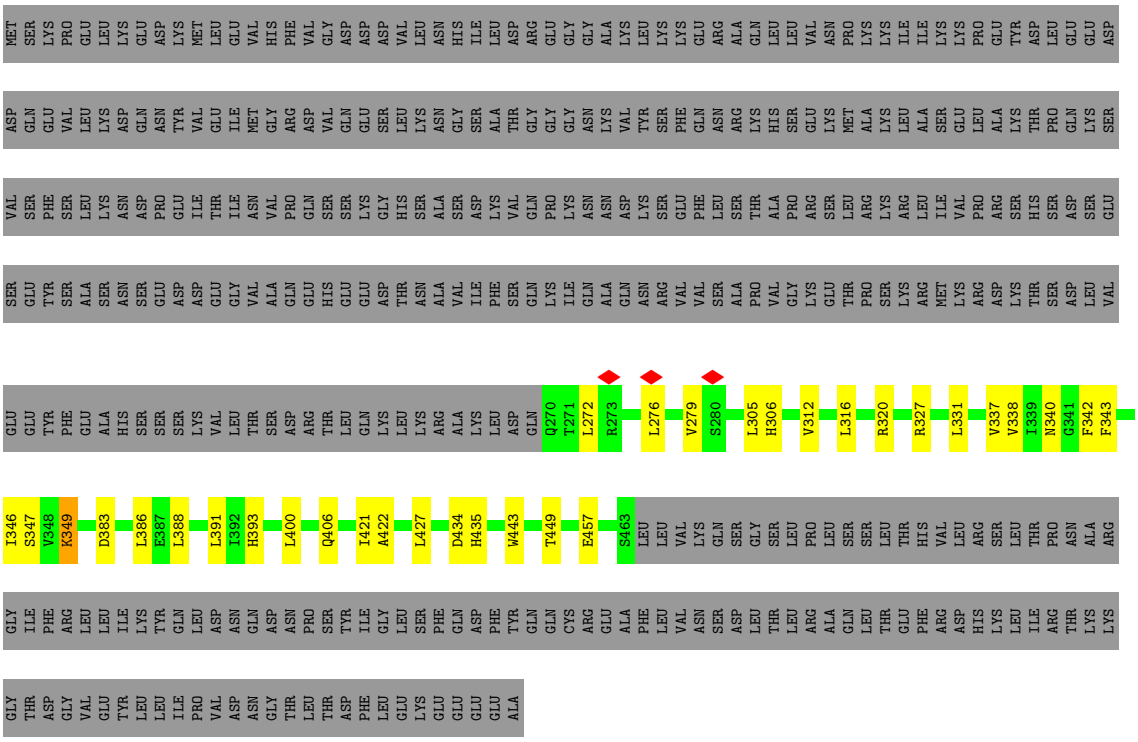
Mol	Chain	Residues	Atoms						AltConf
17	6	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	6	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

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.

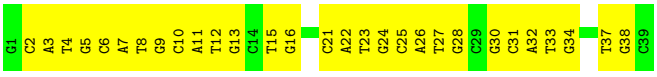
• Molecule 1: Origin recognition complex subunit 2

Chain B:



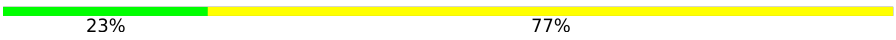
• Molecule 2: DNA (39-mer)

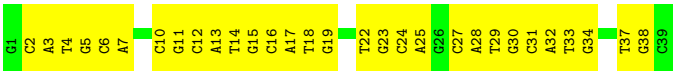
Chain X:



• Molecule 3: DNA (39-mer)

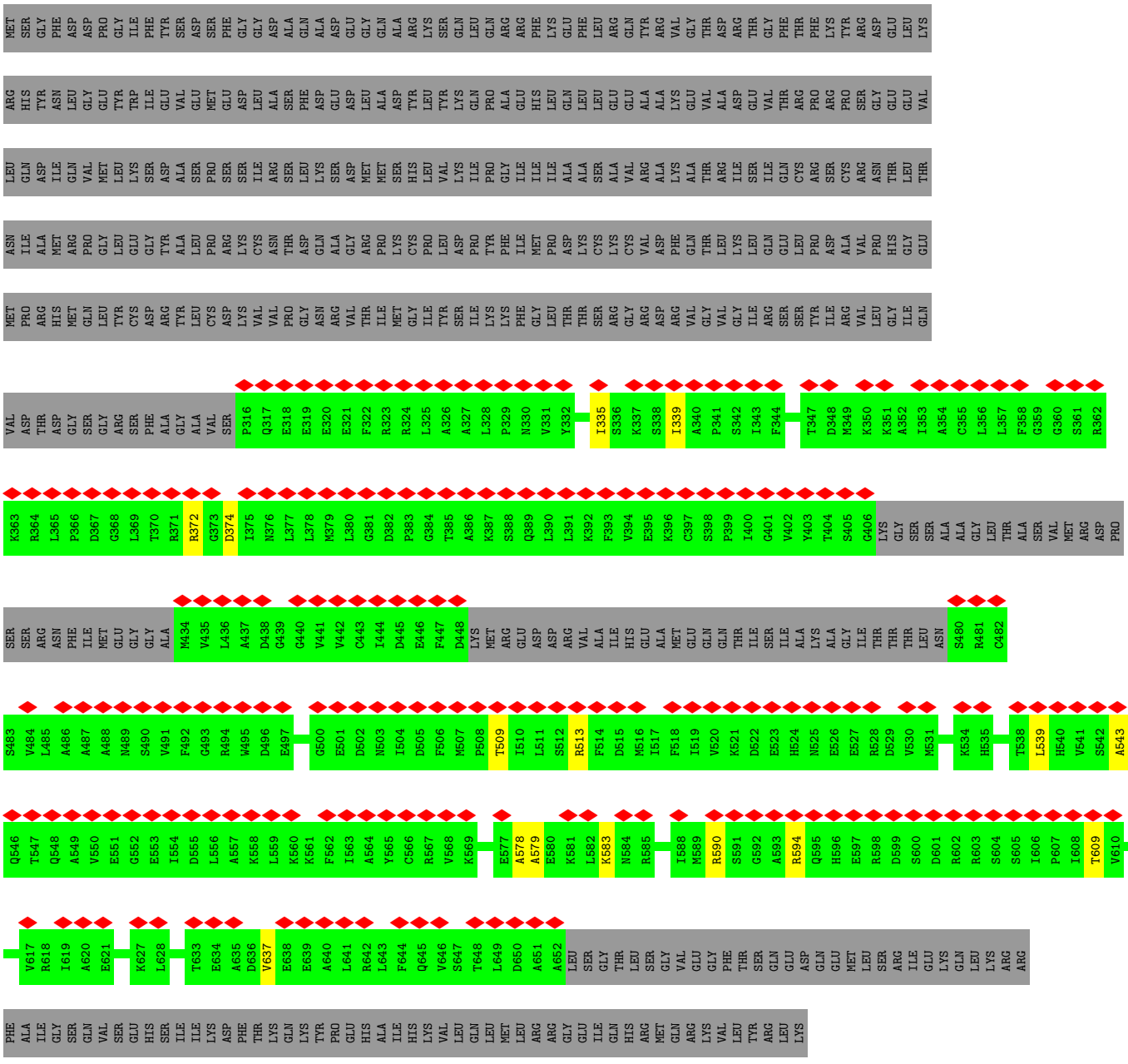
Chain Y:





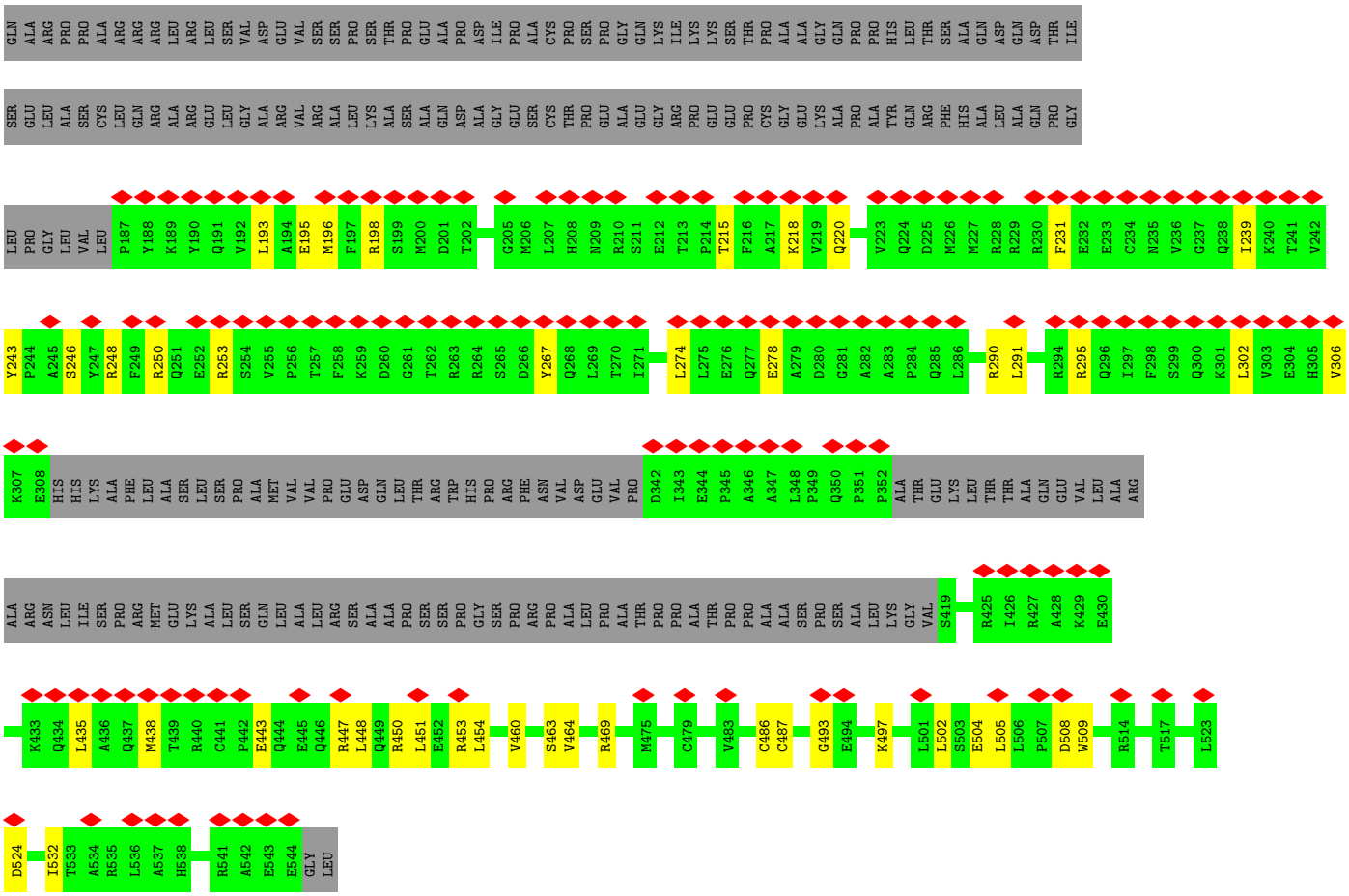
• Molecule 4: DNA replication licensing factor MCM5

Chain 5:



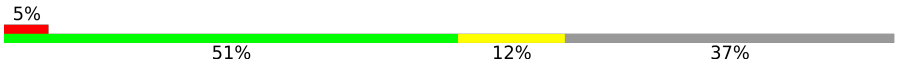
• Molecule 5: DNA replication factor Cdt1

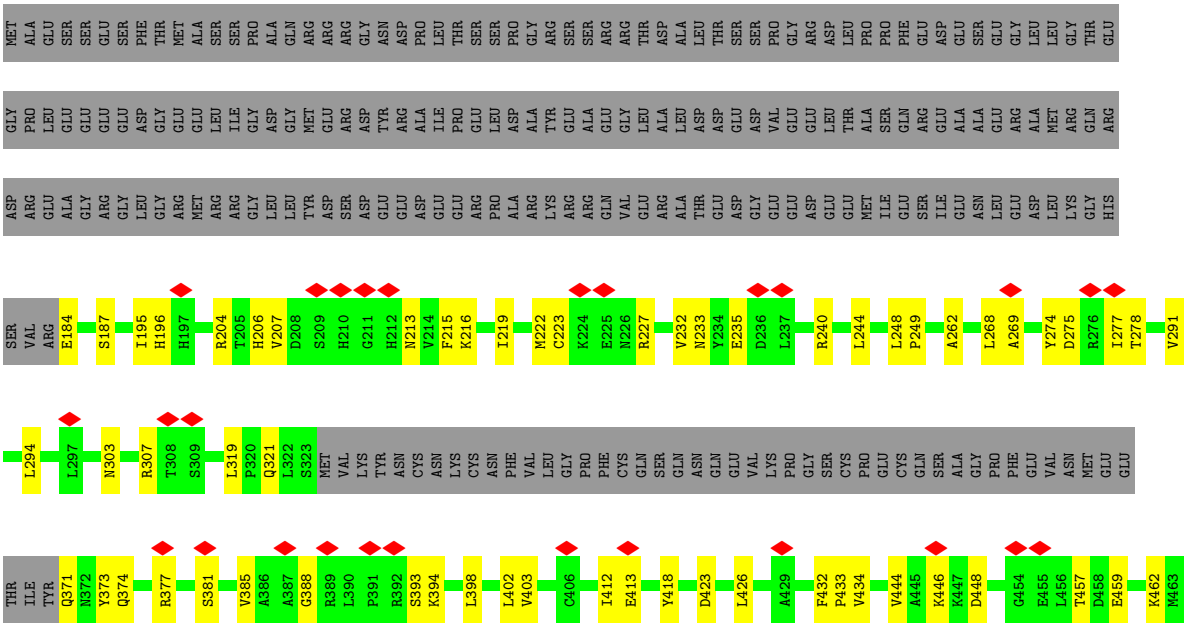
Chain 8:

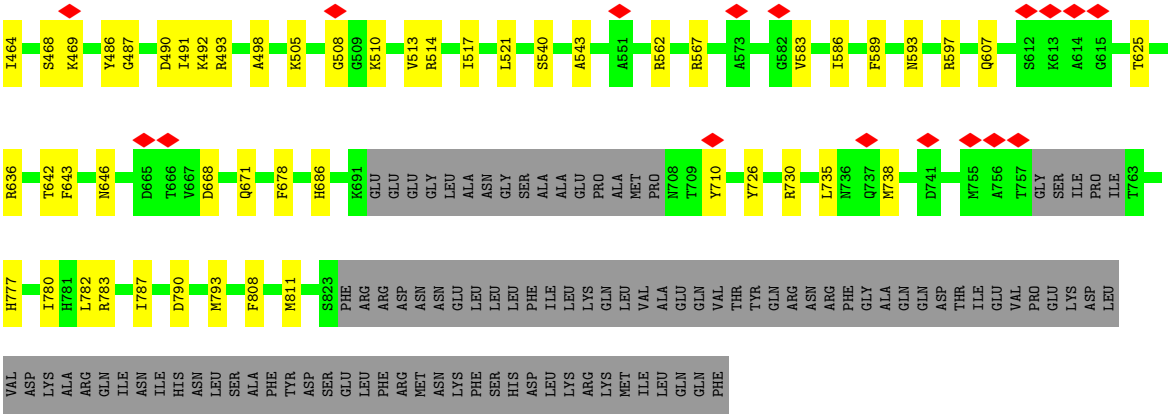


• Molecule 6: DNA replication licensing factor MCM2

Chain 2:

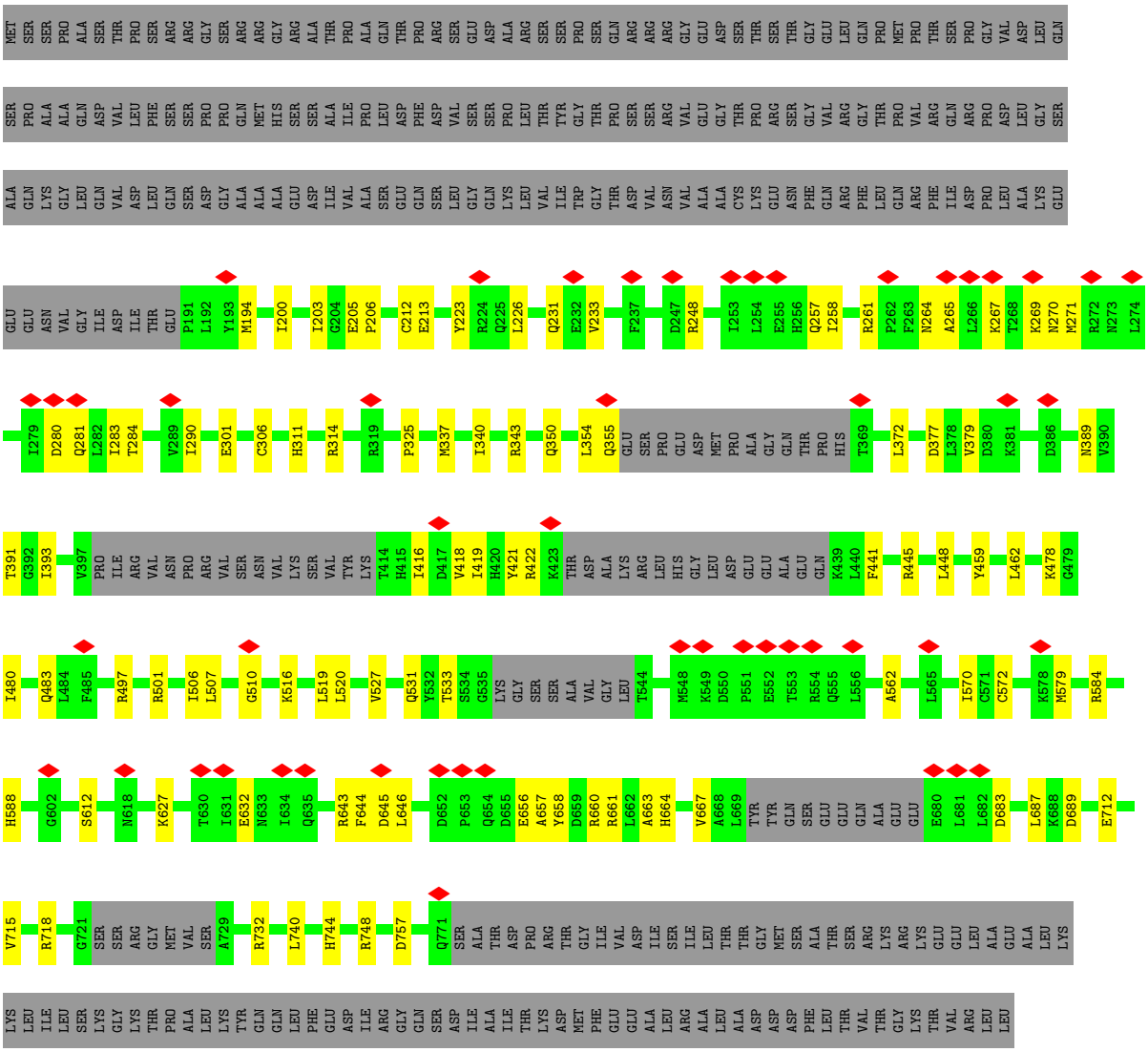






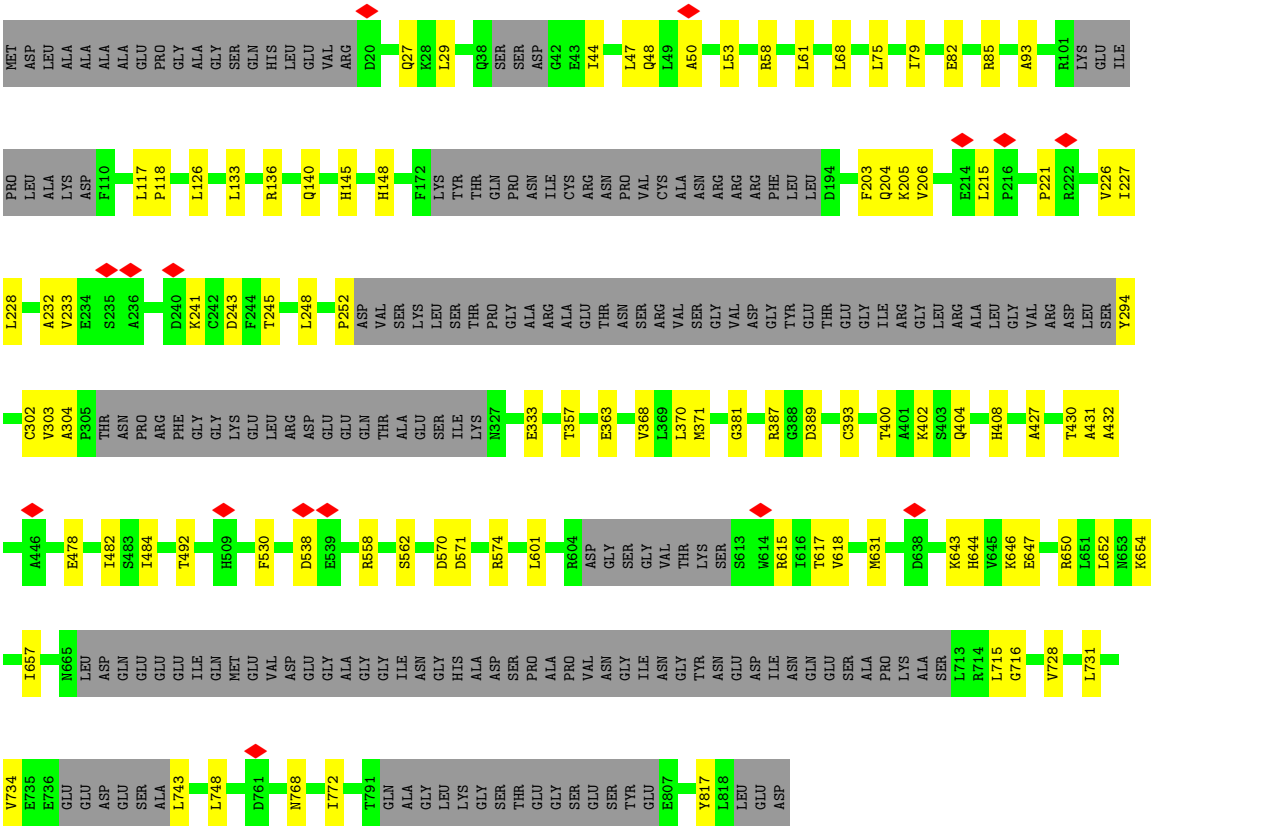
• Molecule 7: DNA replication licensing factor MCM4

Chain 4:



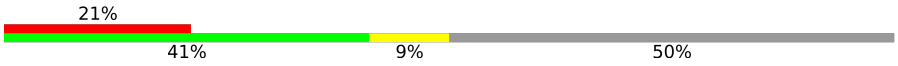
• Molecule 8: DNA replication licensing factor MCM6

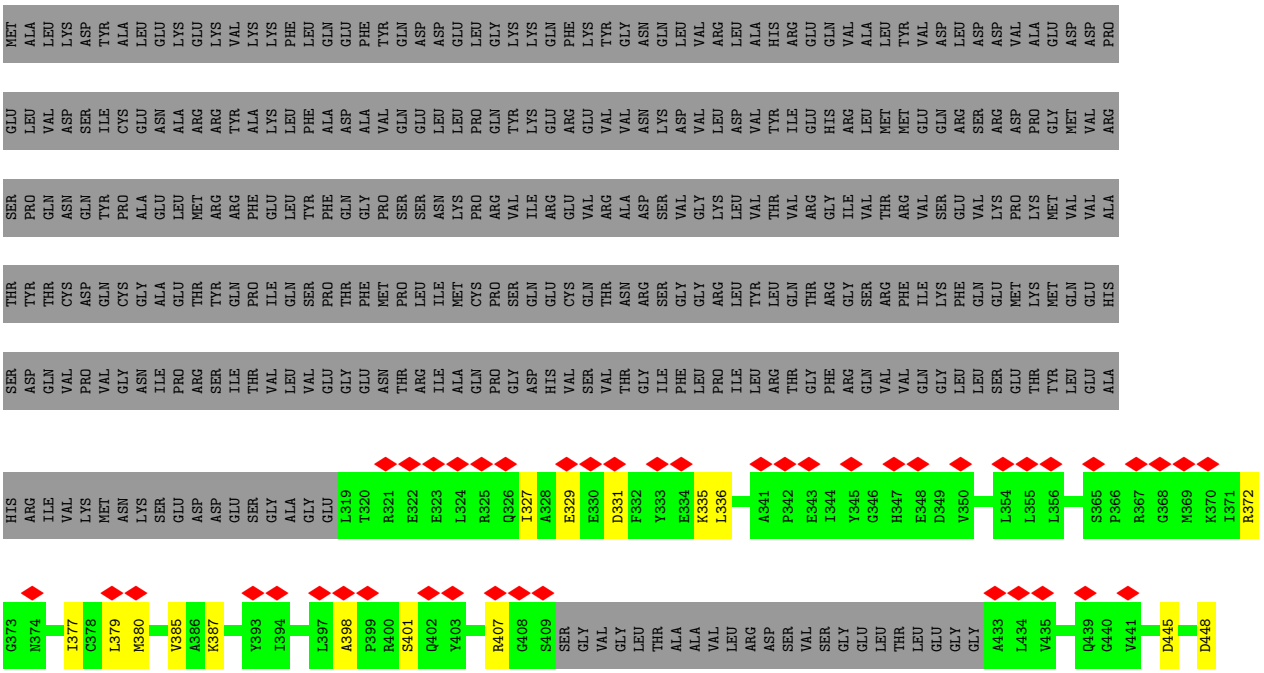
Chain 6:

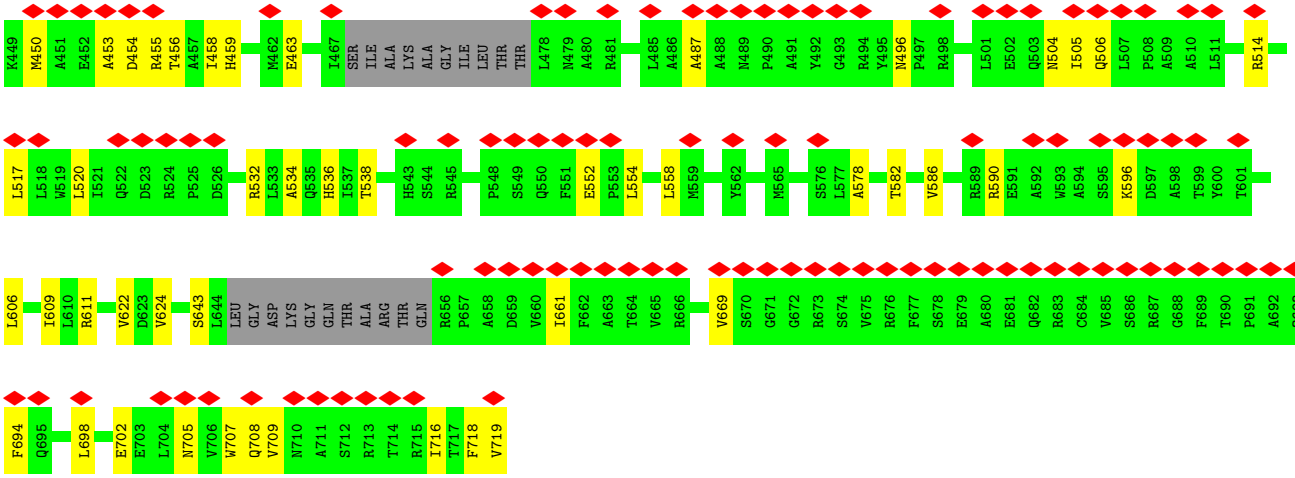


• Molecule 9: DNA replication licensing factor MCM7

Chain 7:

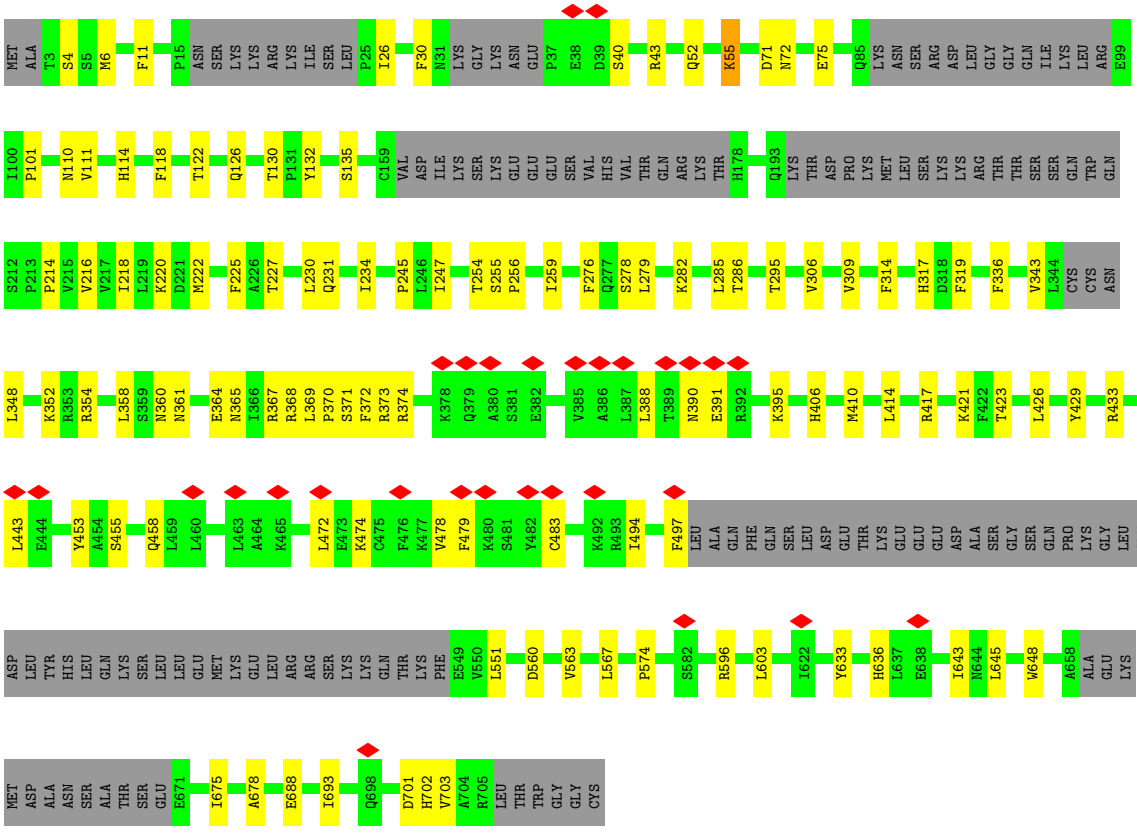






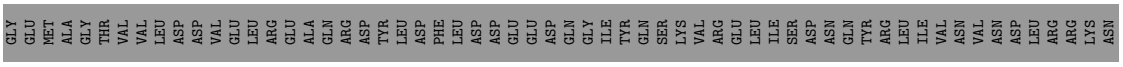
• Molecule 10: Origin recognition complex subunit 3

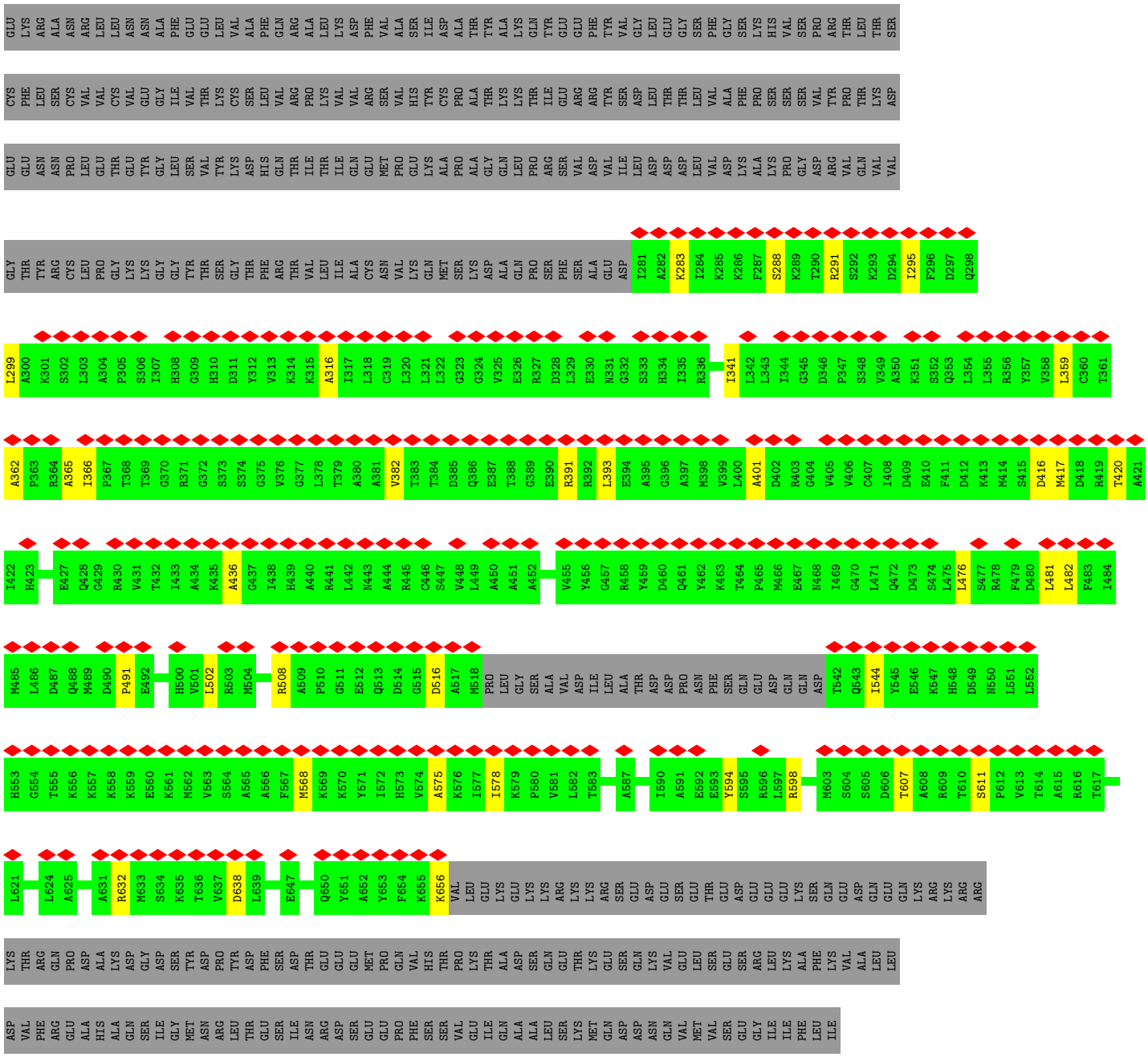
Chain C:



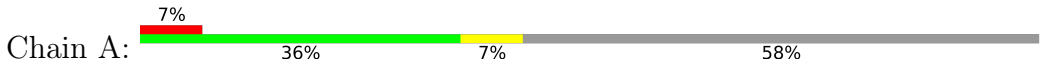
• Molecule 11: DNA replication licensing factor MCM3

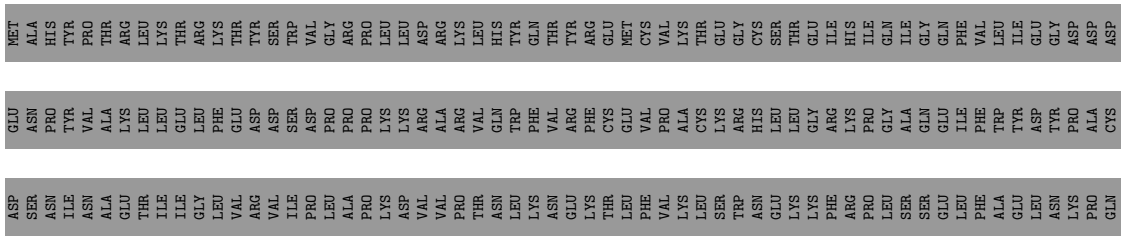
Chain 3:

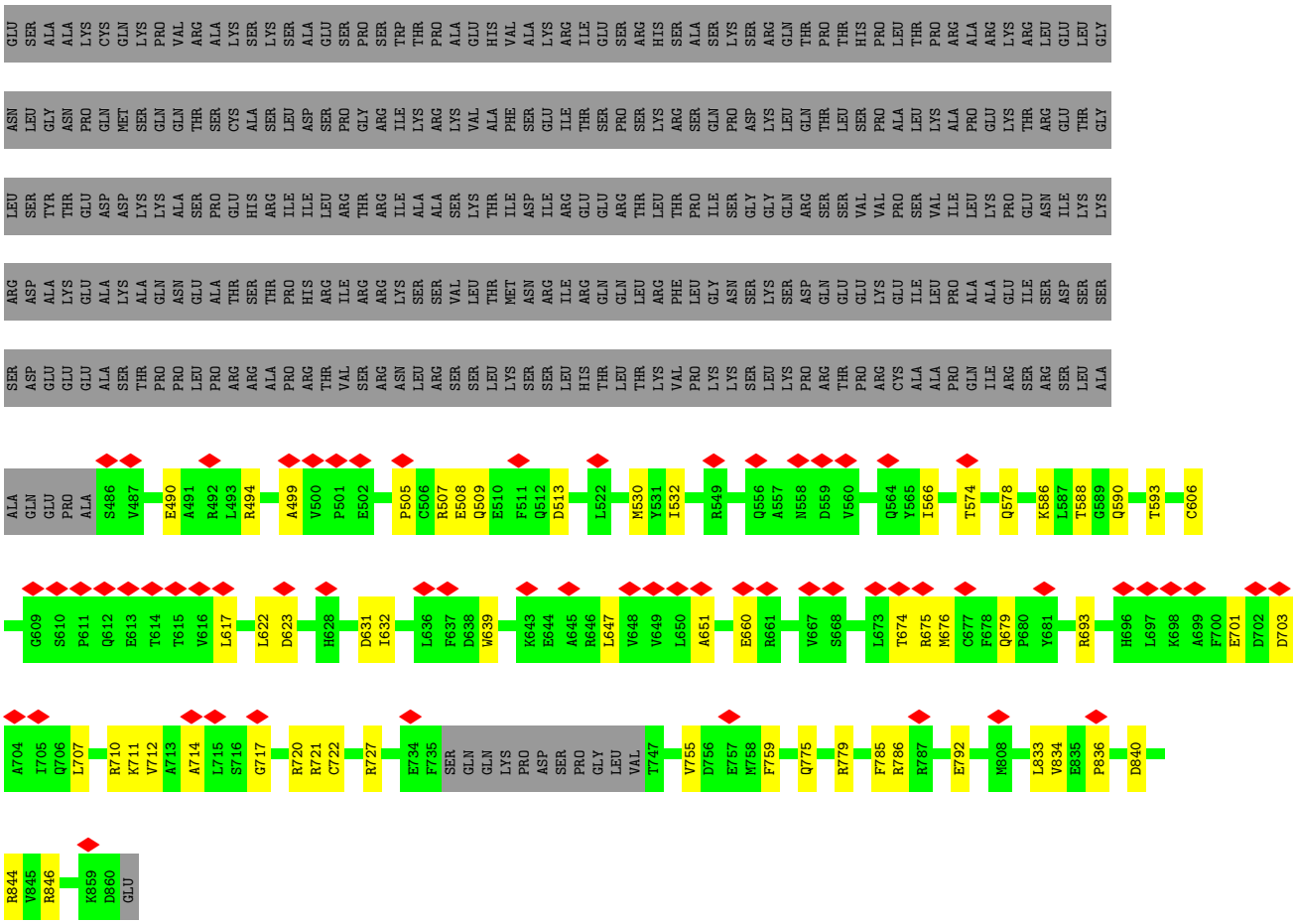




• Molecule 12: Origin recognition complex subunit 1

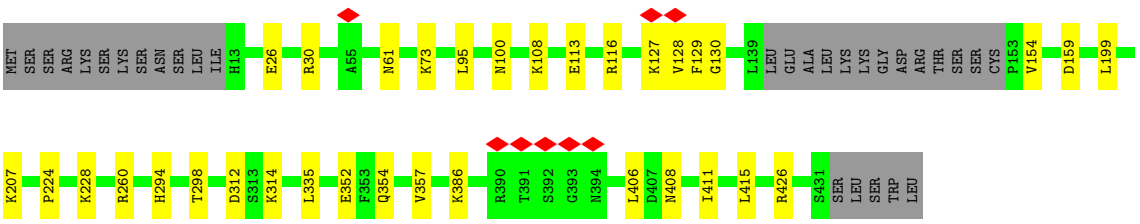






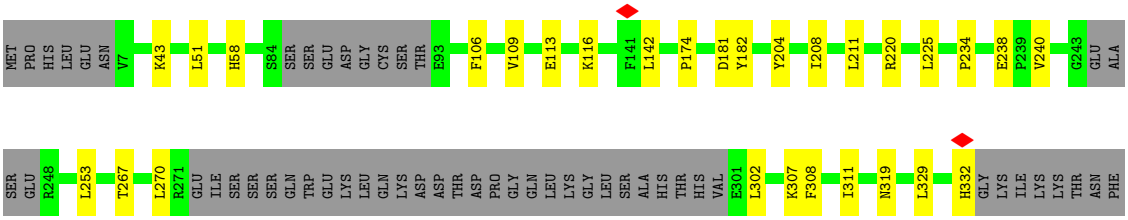
• Molecule 13: Origin recognition complex subunit 4

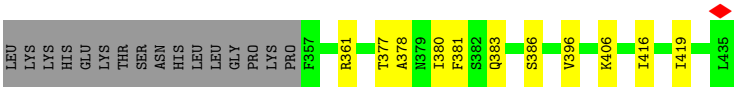
Chain D:



• Molecule 14: Origin recognition complex subunit 5

Chain E:




LEU
LYS
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GLU
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THR
SER
ASN
HIS
LEU
LEU
GLY
PRO
LYS
PRO
F357
R361
T377
A378
N379
I380
F381
S382
Q383
S386
V396
K406
I416
I419
L435

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49771	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	49.28	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.638	Depositor
Minimum map value	-0.227	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	432.00003, 432.00003, 432.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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	B	0.24	0/1638	0.44	0/2218
2	X	0.61	0/895	0.95	0/1379
3	Y	0.62	0/897	0.92	0/1382
4	5	0.24	0/2198	0.47	0/2954
5	8	0.24	0/2130	0.51	0/2866
6	2	0.24	0/4594	0.49	0/6207
7	4	0.24	0/4178	0.49	0/5636
8	6	0.24	0/5172	0.49	0/6973
9	7	0.25	0/2884	0.51	0/3893
10	C	0.24	0/4788	0.45	0/6476
11	3	0.23	0/2786	0.46	0/3749
12	A	0.24	0/2938	0.48	0/3975
13	D	0.24	0/3373	0.42	0/4548
14	E	0.25	0/3076	0.45	0/4172
All	All	0.27	0/41547	0.51	0/56428

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	B	1600	0	1584	23	0
2	X	799	0	439	18	0
3	Y	800	0	438	18	0
4	5	2169	0	2216	13	0
5	8	2097	0	2135	27	0
6	2	4513	0	4537	68	0
7	4	4110	0	4160	63	0
8	6	5091	0	5115	59	0
9	7	2841	0	2852	48	0
10	C	4689	0	4724	69	0
11	3	2748	0	2800	24	0
12	A	2889	0	2905	38	0
13	D	3309	0	3343	18	0
14	E	3003	0	3033	23	0
15	2	1	0	0	0	0
15	6	1	0	0	0	0
15	A	1	0	0	0	0
15	D	1	0	0	0	0
15	E	1	0	0	0	0
16	4	1	0	0	0	0
17	6	62	0	24	3	0
17	A	31	0	12	2	0
17	D	31	0	12	1	0
17	E	31	0	12	2	0
All	All	40819	0	40341	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 6.

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)
9:7:702:GLU:HG2	12:A:710:ARG:HH12	1.38	0.87
4:5:594:ARG:HH12	11:3:491:PRO:HD3	1.48	0.79
6:2:222:MET:HG2	6:2:227:ARG:HB2	1.66	0.78
1:B:340:ASN:HA	1:B:393:HIS:HB2	1.69	0.75
10:C:110:ASN:ND2	10:C:319:PHE:O	2.21	0.74
6:2:206:HIS:HE1	6:2:215:PHE:H	1.38	0.72
4:5:539:LEU:O	4:5:543:ALA:HB2	1.90	0.71
4:5:583:LYS:HD3	11:3:502:LEU:HD13	1.72	0.71
5:8:469:ARG:HH21	8:6:133:LEU:HD21	1.56	0.70
10:C:130:THR:HG22	10:C:132:TYR:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:6:204:GLN:HB2	8:6:233:VAL:HG13	1.74	0.70
10:C:101:PRO:HG2	10:C:247:ILE:HG22	1.74	0.70
11:3:476:LEU:HD22	11:3:482:LEU:HD11	1.71	0.70
5:8:453:ARG:NH2	8:6:333:GLU:OE2	2.25	0.70
7:4:527:VAL:HG11	7:4:570:ILE:HD12	1.73	0.69
4:5:544:LEU:HD23	6:2:508:GLY:H	1.57	0.69
7:4:445:ARG:HH12	7:4:448:LEU:HD13	1.58	0.69
10:C:254:THR:HG22	10:C:255:SER:H	1.58	0.68
8:6:643:LYS:HA	8:6:646:LYS:HD2	1.74	0.68
12:A:720:ARG:HE	17:A:901:AGS:H5'2	1.59	0.68
14:E:43:LYS:NZ	17:E:501:AGS:O2B	2.26	0.67
7:4:627:LYS:HD3	7:4:632:GLU:HB3	1.77	0.67
10:C:421:LYS:HG3	10:C:478:VAL:HG21	1.77	0.67
9:7:708:GLN:HG2	12:A:707:LEU:HD12	1.77	0.66
10:C:135:SER:HB2	10:C:220:LYS:HE3	1.78	0.66
10:C:688:GLU:HA	10:C:693:ILE:HB	1.78	0.66
6:2:402:LEU:HD22	6:2:444:VAL:HG23	1.78	0.65
9:7:398:ALA:HB3	9:7:401:SER:HB3	1.78	0.65
10:C:216:VAL:HG22	10:C:247:ILE:HD11	1.79	0.65
3:Y:29:DT:H2"	3:Y:30:DG:C8	2.32	0.64
6:2:562:ARG:HH21	6:2:567:ARG:HB3	1.63	0.63
5:8:220:GLN:HG3	5:8:231:PHE:HB3	1.81	0.63
4:5:578:ALA:HB1	4:5:637:VAL:HG21	1.81	0.63
10:C:222:MET:HA	10:C:225:PHE:HD2	1.62	0.63
7:4:325:PRO:HG2	7:4:337:MET:HG3	1.79	0.62
7:4:520:LEU:HD22	7:4:572:CYS:HB2	1.81	0.62
4:5:594:ARG:NH1	11:3:491:PRO:HD3	2.12	0.62
11:3:482:LEU:HD12	11:3:611:SER:HB2	1.79	0.62
2:X:2:DC:H2"	2:X:3:DA:C8	2.35	0.62
1:B:427:LEU:HD11	10:C:596:ARG:HG2	1.82	0.61
12:A:711:LYS:HG2	12:A:755:VAL:HG21	1.82	0.61
7:4:226:LEU:HA	7:4:233:VAL:HG21	1.82	0.61
7:4:588:HIS:HD2	7:4:643:ARG:HE	1.49	0.61
6:2:374:GLN:HG2	6:2:403:VAL:HG13	1.82	0.61
11:3:594:TYR:OH	11:3:598:ARG:NH2	2.34	0.61
7:4:506:ILE:HG12	7:4:646:LEU:HB2	1.82	0.61
14:E:181:ASP:OD2	14:E:220:ARG:NH2	2.34	0.60
14:E:396:VAL:HB	14:E:406:LYS:HB2	1.83	0.60
6:2:583:VAL:HG12	6:2:625:THR:HB	1.84	0.60
6:2:268:LEU:HD21	6:2:275:ASP:HB2	1.84	0.59
10:C:358:LEU:HB3	10:C:395:LYS:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:7:622:VAL:HG12	9:7:624:VAL:H	1.67	0.59
5:8:278:GLU:OE2	5:8:290:ARG:NH2	2.29	0.59
7:4:261:ARG:HH22	7:4:377:ASP:HB3	1.67	0.59
12:A:566:ILE:HG23	12:A:586:LYS:HG2	1.85	0.59
3:Y:4:DT:H2"	3:Y:5:DG:C8	2.37	0.59
3:Y:27:DC:H2"	3:Y:28:DA:C8	2.37	0.59
7:4:213:GLU:N	7:4:213:GLU:OE1	2.34	0.59
6:2:642:THR:O	6:2:646:ASN:ND2	2.36	0.59
8:6:427:ALA:HB1	8:6:432:ALA:HB2	1.85	0.59
7:4:267:LYS:NZ	7:4:281:GLN:OE1	2.36	0.58
10:C:371:SER:HB2	10:C:574:PRO:HA	1.84	0.58
13:D:127:LYS:HE3	13:D:129:PHE:HB3	1.85	0.58
8:6:558:ARG:HD2	8:6:562:SER:HB3	1.85	0.58
3:Y:31:DC:H2"	3:Y:32:DA:C8	2.37	0.58
8:6:404:GLN:O	8:6:408:HIS:ND1	2.32	0.58
11:3:362:ALA:HB3	11:3:365:ALA:HB2	1.85	0.58
12:A:507:ARG:NH2	12:A:679:GLN:O	2.26	0.58
6:2:206:HIS:CE1	6:2:215:PHE:H	2.20	0.58
6:2:412:ILE:HG22	6:2:446:LYS:HA	1.86	0.58
6:2:446:LYS:NZ	6:2:448:ASP:OD1	2.29	0.58
6:2:468:SER:HB2	6:2:782:LEU:HD12	1.86	0.58
10:C:343:VAL:O	10:C:354:ARG:NH1	2.36	0.58
5:8:509:TRP:NE1	5:8:524:ASP:O	2.32	0.58
9:7:606:LEU:HD12	9:7:609:ILE:HD11	1.85	0.57
11:3:366:ILE:HD12	11:3:401:ALA:HB2	1.85	0.57
3:Y:14:DT:H2"	3:Y:15:DG:C8	2.39	0.57
9:7:698:LEU:O	9:7:702:GLU:HB2	2.05	0.57
6:2:777:HIS:ND1	6:2:790:ASP:OD1	2.34	0.57
11:3:341:ILE:HG12	11:3:481:LEU:HB2	1.86	0.57
2:X:15:DT:H2"	2:X:16:DG:C8	2.39	0.57
7:4:656:GLU:OE2	9:7:590:ARG:NH2	2.37	0.57
8:6:243:ASP:HB2	8:6:304:ALA:HB3	1.86	0.57
10:C:479:PHE:HA	10:C:483:CYS:HB2	1.85	0.57
2:X:27:DT:H2"	2:X:28:DG:C8	2.40	0.57
2:X:37:DT:H2"	2:X:38:DG:C8	2.40	0.57
4:5:590:ARG:HH21	4:5:609:THR:HA	1.70	0.57
9:7:707:TRP:HA	9:7:719:VAL:H	1.70	0.57
14:E:302:LEU:O	14:E:307:LYS:NZ	2.32	0.57
6:2:540:SER:HB3	6:2:543:ALA:HB2	1.86	0.56
9:7:554:LEU:HB3	9:7:558:LEU:HD23	1.86	0.56
8:6:27:GLN:HG3	8:6:93:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:294:HIS:NE2	13:D:298:THR:OG1	2.35	0.56
13:D:415:LEU:HD21	13:D:426:ARG:HG2	1.87	0.56
7:4:301:GLU:OE1	7:4:314:ARG:NH1	2.38	0.56
7:4:744:HIS:ND1	7:4:757:ASP:OD1	2.37	0.56
8:6:29:LEU:HB3	8:6:75:LEU:HD22	1.87	0.56
3:Y:12:DC:H2"	3:Y:13:DA:C8	2.41	0.56
8:6:126:LEU:HD22	8:6:248:LEU:HD22	1.88	0.56
12:A:712:VAL:O	12:A:717:GLY:N	2.30	0.56
2:X:23:DT:H2"	2:X:24:DG:C8	2.41	0.55
5:8:193:LEU:HD23	5:8:302:LEU:HD21	1.88	0.55
9:7:698:LEU:HD21	9:7:709:VAL:HG21	1.88	0.55
10:C:135:SER:HA	10:C:218:ILE:HB	1.88	0.55
12:A:720:ARG:NH2	17:A:901:AGS:O2A	2.40	0.55
7:4:306:CYS:HB3	7:4:311:HIS:H	1.71	0.55
9:7:661:ILE:HD13	9:7:694:PHE:HA	1.87	0.55
6:2:321:GLN:NE2	6:2:371:GLN:O	2.39	0.55
11:3:391:ARG:NH1	11:3:436:ALA:O	2.40	0.55
6:2:207:VAL:H	6:2:240:ARG:NH2	2.05	0.55
7:4:480:ILE:HD11	7:4:519:LEU:HD21	1.88	0.55
7:4:418:VAL:HG11	7:4:421:TYR:CZ	2.41	0.55
5:8:448:LEU:HD23	5:8:451:LEU:HD12	1.88	0.55
8:6:368:VAL:HA	8:6:371:MET:HG2	1.88	0.55
10:C:406:HIS:O	10:C:410:MET:HG2	2.07	0.55
14:E:267:THR:HB	14:E:270:LEU:HB2	1.88	0.55
5:8:435:LEU:HA	5:8:438:MET:HG2	1.89	0.54
2:X:21:DC:H2"	2:X:22:DA:C8	2.43	0.54
6:2:303:ASN:N	6:2:418:TYR:O	2.37	0.54
6:2:514:ARG:HD2	6:2:607:GLN:HE22	1.72	0.54
12:A:494:ARG:O	12:A:693:ARG:NH1	2.41	0.54
7:4:660:ARG:O	7:4:664:HIS:ND1	2.26	0.54
6:2:294:LEU:HD22	6:2:394:LYS:HG3	1.88	0.54
6:2:457:THR:HG22	6:2:459:GLU:H	1.73	0.54
7:4:510:GLY:O	7:4:516:LYS:NZ	2.37	0.54
8:6:363:GLU:HG3	8:6:657:ILE:HD13	1.90	0.53
9:7:702:GLU:HG2	12:A:710:ARG:NH1	2.16	0.53
1:B:434:ASP:OD1	1:B:435:HIS:N	2.38	0.53
1:B:276:LEU:HD22	10:C:678:ALA:HB2	1.90	0.53
8:6:252:PRO:HA	8:6:294:TYR:HD1	1.72	0.53
1:B:312:VAL:HG22	1:B:422:ALA:HB3	1.91	0.53
8:6:647:GLU:OE1	8:6:650:ARG:NH1	2.42	0.53
10:C:693:ILE:HG23	10:C:703:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:7:380:MET:SD	9:7:505:ILE:HG12	2.48	0.53
7:4:658:TYR:HA	7:4:661:ARG:HE	1.73	0.53
8:6:50:ALA:HA	8:6:53:LEU:HD12	1.91	0.53
7:4:284:THR:HG22	7:4:391:THR:HG22	1.91	0.53
8:6:601:LEU:HD21	8:6:652:LEU:HD22	1.91	0.53
5:8:291:LEU:O	5:8:295:ARG:HG2	2.08	0.53
7:4:269:LYS:HB2	7:4:283:ILE:HD11	1.91	0.53
8:6:400:THR:O	17:6:902:AGS:O2B	2.27	0.53
12:A:574:THR:OG1	12:A:578:GLN:OE1	2.27	0.53
14:E:377:THR:O	14:E:380:ILE:HG22	2.09	0.53
14:E:113:GLU:HA	14:E:116:LYS:HE2	1.89	0.53
8:6:734:VAL:HG21	8:6:743:LEU:HD11	1.91	0.52
7:4:340:ILE:HG22	7:4:343:ARG:H	1.75	0.52
5:8:454:LEU:HD22	5:8:502:LEU:HD21	1.92	0.52
6:2:377:ARG:NH2	6:2:393:SER:OG	2.42	0.52
11:3:316:ALA:HB1	11:3:341:ILE:HD13	1.91	0.52
5:8:195:GLU:OE2	5:8:198:ARG:NH2	2.43	0.52
2:X:31:DC:H2"	2:X:32:DA:C8	2.44	0.52
1:B:272:LEU:O	1:B:276:LEU:HG	2.10	0.52
2:X:10:DC:H2"	2:X:11:DA:C8	2.44	0.52
2:X:32:DA:H2'	2:X:33:DT:H71	1.92	0.52
3:Y:24:DC:H2"	3:Y:25:DA:C8	2.45	0.52
10:C:370:PRO:HB2	10:C:374:ARG:HH22	1.75	0.52
14:E:234:PRO:O	14:E:238:GLU:HG3	2.10	0.52
7:4:194:MET:HB2	7:4:248:ARG:HH12	1.74	0.51
10:C:43:ARG:NH1	10:C:336:PHE:O	2.43	0.51
10:C:254:THR:HG22	10:C:255:SER:N	2.25	0.51
5:8:248:ARG:HE	5:8:250:ARG:HE	1.57	0.51
11:3:288:SER:HA	11:3:295:ILE:HD11	1.90	0.51
7:4:203:ILE:HG23	7:4:205:GLU:H	1.75	0.51
13:D:95:LEU:HB2	13:D:154:VAL:HG22	1.92	0.51
1:B:337:VAL:HG23	1:B:388:LEU:HD11	1.93	0.51
3:Y:16:DC:H2"	3:Y:17:DA:C8	2.46	0.51
6:2:222:MET:SD	6:2:274:TYR:OH	2.58	0.51
9:7:377:ILE:HG12	9:7:517:LEU:HB2	1.92	0.51
9:7:385:VAL:HG23	9:7:387:LYS:HG2	1.92	0.51
7:4:497:ARG:NH2	8:6:357:THR:O	2.44	0.51
10:C:369:LEU:HB2	10:C:372:PHE:HB3	1.92	0.51
14:E:378:ALA:HA	14:E:381:PHE:HD2	1.76	0.51
13:D:312:ASP:OD1	13:D:312:ASP:N	2.43	0.51
10:C:317:HIS:HA	14:E:383:GLN:HE21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:199:LEU:O	13:D:207:LYS:NZ	2.33	0.51
8:6:117:LEU:HB2	8:6:136:ARG:HD2	1.92	0.50
9:7:454:ASP:O	9:7:458:ILE:HG13	2.11	0.50
10:C:118:PHE:CE2	10:C:220:LYS:HG2	2.46	0.50
11:3:359:LEU:HD23	11:3:365:ALA:HB1	1.92	0.50
6:2:388:GLY:HA2	8:6:492:THR:O	2.11	0.50
8:6:302:CYS:SG	8:6:303:VAL:N	2.85	0.50
11:3:607:THR:HG22	11:3:656:LYS:HG2	1.94	0.50
12:A:834:VAL:HG13	12:A:836:PRO:HD3	1.94	0.50
6:2:204:ARG:HH22	6:2:269:ALA:HB3	1.76	0.49
6:2:636:ARG:HH22	8:6:615:ARG:HG3	1.77	0.49
12:A:617:LEU:HB2	12:A:647:LEU:HD11	1.93	0.49
1:B:320:ARG:NH2	10:C:4:SER:O	2.42	0.49
6:2:291:VAL:HG22	6:2:307:ARG:HD3	1.94	0.49
6:2:432:PHE:HB2	6:2:433:PRO:HD2	1.93	0.49
12:A:622:LEU:HD22	12:A:651:ALA:HB1	1.94	0.49
2:X:22:DA:H2'	2:X:23:DT:H71	1.95	0.49
1:B:316:LEU:H	1:B:449:THR:HG22	1.76	0.49
6:2:233:ASN:HD21	6:2:235:GLU:HB2	1.77	0.49
8:6:570:ASP:O	8:6:574:ARG:HG3	2.13	0.49
4:5:583:LYS:HE2	11:3:502:LEU:HD22	1.95	0.49
6:2:808:PHE:HA	6:2:811:MET:HG2	1.95	0.49
5:8:248:ARG:HB2	5:8:274:LEU:HD21	1.94	0.49
2:X:25:DC:H2"	2:X:26:DA:C8	2.47	0.49
2:X:33:DT:H2"	2:X:34:DG:C8	2.48	0.49
10:C:472:LEU:HD22	10:C:494:ILE:HG12	1.95	0.49
13:D:224:PRO:O	13:D:228:LYS:HG2	2.13	0.49
14:E:106:PHE:HA	14:E:109:VAL:HG12	1.95	0.49
7:4:718:ARG:NH2	8:6:538:ASP:OD2	2.32	0.48
8:6:206:VAL:HB	8:6:226:VAL:HB	1.95	0.48
10:C:365:ASN:OD1	10:C:368:ARG:NH2	2.42	0.48
14:E:182:TYR:OH	17:E:501:AGS:N6	2.45	0.48
5:8:196:MET:SD	5:8:239:ILE:HD11	2.53	0.48
6:2:486:TYR:HB2	6:2:678:PHE:CD2	2.48	0.48
9:7:327:ILE:HG23	9:7:336:LEU:HD21	1.95	0.48
10:C:118:PHE:HE2	10:C:220:LYS:HG2	1.78	0.48
11:3:632:ARG:NH2	11:3:638:ASP:OD2	2.39	0.48
2:X:8:DT:H2"	2:X:9:DG:C8	2.49	0.48
8:6:650:ARG:O	8:6:654:LYS:HG3	2.14	0.48
7:4:231:GLN:HG3	7:4:393:ILE:HD13	1.94	0.48
8:6:431:ALA:HB3	8:6:484:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:71:ASP:OD1	10:C:72:ASN:N	2.46	0.48
6:2:319:LEU:HB2	6:2:373:TYR:HB3	1.94	0.48
9:7:505:ILE:O	9:7:506:GLN:HG3	2.13	0.48
6:2:374:GLN:HB2	6:2:398:LEU:HB2	1.95	0.48
9:7:331:ASP:O	9:7:335:LYS:HG2	2.13	0.48
12:A:532:ILE:HG12	12:A:676:MET:HB2	1.95	0.48
12:A:660:GLU:OE2	12:A:675:ARG:NH1	2.46	0.48
10:C:563:VAL:HG13	10:C:567:LEU:HD12	1.95	0.48
2:X:12:DT:H2"	2:X:13:DG:C8	2.49	0.48
3:Y:22:DT:H2"	3:Y:23:DG:C8	2.49	0.48
7:4:265:ALA:H	7:4:284:THR:HG21	1.79	0.48
7:4:483:GLN:HE21	7:4:612:SER:HB2	1.78	0.48
8:6:393:CYS:HB2	8:6:530:PHE:CD2	2.49	0.48
12:A:833:LEU:HD12	12:A:846:ARG:HB2	1.95	0.48
7:4:588:HIS:CD2	7:4:643:ARG:HE	2.31	0.48
5:8:243:TYR:HD2	5:8:246:SER:HB3	1.79	0.47
7:4:212:CYS:HB3	7:4:223:TYR:HE1	1.78	0.47
8:6:387:ARG:HG2	8:6:389:ASP:H	1.78	0.47
10:C:72:ASN:HB3	10:C:276:PHE:CE2	2.49	0.47
6:2:498:ALA:HA	6:2:517:ILE:HD12	1.96	0.47
8:6:53:LEU:HD23	8:6:58:ARG:HG3	1.95	0.47
8:6:571:ASP:OD1	8:6:574:ARG:NH2	2.39	0.47
10:C:227:THR:HB	10:C:231:GLN:HE22	1.80	0.47
7:4:389:ASN:HB2	7:4:422:ARG:HB3	1.97	0.47
1:B:342:PHE:CD2	1:B:457:GLU:HA	2.48	0.47
10:C:367:ARG:HE	10:C:388:LEU:HD22	1.80	0.47
9:7:669:VAL:HG22	9:7:718:PHE:HE2	1.78	0.47
13:D:26:GLU:HG2	13:D:30:ARG:HH12	1.78	0.47
5:8:443:GLU:O	5:8:447:ARG:HG2	2.14	0.47
7:4:350:GLN:HB2	7:4:379:VAL:HG13	1.97	0.47
8:6:68:LEU:HD21	8:6:79:ILE:HD12	1.97	0.47
1:B:312:VAL:HG23	1:B:443:TRP:CZ3	2.50	0.47
1:B:338:VAL:HG22	1:B:391:LEU:HD12	1.97	0.47
2:X:31:DC:H2"	2:X:32:DA:H8	1.80	0.47
2:X:6:DC:H2"	2:X:7:DA:C8	2.50	0.47
6:2:248:LEU:HB3	6:2:249:PRO:HD3	1.97	0.47
7:4:206:PRO:HB2	7:4:258:ILE:HA	1.97	0.47
3:Y:6:DC:H2"	3:Y:7:DA:C8	2.50	0.47
8:6:203:PHE:CZ	8:6:205:LYS:HB2	2.50	0.47
9:7:450:MET:O	9:7:455:ARG:NH2	2.48	0.47
10:C:72:ASN:O	10:C:75:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:3:299:LEU:HD22	11:3:568:MET:HG3	1.96	0.47
5:8:302:LEU:O	5:8:306:VAL:HG23	2.15	0.46
6:2:505:LYS:O	6:2:513:VAL:N	2.41	0.46
1:B:306:HIS:NE2	10:C:26:ILE:HG12	2.30	0.46
8:6:136:ARG:HB3	8:6:245:THR:HG22	1.96	0.46
3:Y:2:DC:H2"	3:Y:3:DA:C8	2.49	0.46
6:2:184:GLU:O	6:2:187:SER:OG	2.27	0.46
8:6:228:LEU:HD22	8:6:232:ALA:HB1	1.97	0.46
9:7:372:ARG:O	9:7:611:ARG:NE	2.48	0.46
10:C:643:ILE:O	10:C:702:HIS:HA	2.15	0.46
4:5:579:ALA:O	4:5:583:LYS:HG3	2.16	0.46
14:E:416:ILE:HA	14:E:419:ILE:HG22	1.98	0.46
8:6:82:GLU:HB3	8:6:85:ARG:HB3	1.96	0.46
5:8:508:ASP:N	5:8:508:ASP:OD1	2.49	0.46
6:2:586:ILE:HG21	6:2:589:PHE:HD1	1.80	0.46
8:6:44:ILE:HD12	8:6:47:LEU:HD11	1.97	0.46
9:7:520:LEU:O	9:7:643:SER:OG	2.34	0.46
4:5:509:THR:O	4:5:513:ARG:NH1	2.47	0.46
10:C:285:LEU:HD22	10:C:314:PHE:CE2	2.51	0.46
6:2:686:HIS:CE1	8:6:381:GLY:H	2.34	0.45
7:4:459:TYR:CE2	7:4:478:LYS:HE3	2.50	0.45
12:A:509:GLN:NE2	12:A:513:ASP:OD2	2.49	0.45
3:Y:18:DT:H2"	3:Y:19:DG:C8	2.52	0.45
6:2:491:ILE:HD11	6:2:521:LEU:HD13	1.99	0.45
6:2:508:GLY:O	6:2:510:LYS:NZ	2.31	0.45
10:C:230:LEU:O	10:C:234:ILE:HG12	2.16	0.45
8:6:402:LYS:N	17:6:902:AGS:O1A	2.49	0.45
9:7:532:ARG:O	9:7:536:HIS:ND1	2.49	0.45
9:7:705:ASN:HD22	12:A:714:ALA:HB2	1.81	0.45
12:A:775:GLN:OE1	12:A:779:ARG:NH2	2.49	0.45
8:6:631:MET:HB3	8:6:644:HIS:HB3	1.97	0.45
10:C:439:TYR:CZ	10:C:443:LEU:HD11	2.52	0.45
5:8:493:GLY:O	5:8:497:LYS:HG3	2.16	0.45
10:C:306:VAL:HA	10:C:309:VAL:HG12	1.99	0.45
14:E:319:ASN:O	14:E:361:ARG:NH2	2.47	0.45
6:2:307:ARG:HH21	6:2:413:GLU:HG3	1.80	0.45
11:3:575:ALA:HA	11:3:578:ILE:HD12	1.98	0.45
8:6:48:GLN:H	8:6:48:GLN:CD	2.20	0.45
10:C:636:HIS:HB2	10:C:648:TRP:CZ2	2.52	0.45
12:A:530:MET:HG3	12:A:674:THR:HG22	1.99	0.45
9:7:379:LEU:HB3	9:7:387:LYS:HZ1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:7:463:GLU:HB2	9:7:514:ARG:NH1	2.32	0.45
9:7:578:ALA:O	9:7:582:THR:HG23	2.16	0.45
10:C:6:MET:HB2	10:C:11:PHE:HZ	1.82	0.45
3:Y:17:DA:H2'	3:Y:18:DT:H71	1.98	0.45
4:5:372:ARG:HG2	4:5:374:ASP:H	1.81	0.45
6:2:423:ASP:HB3	6:2:426:LEU:HD12	1.99	0.45
7:4:570:ILE:HG12	7:4:612:SER:OG	2.17	0.45
9:7:453:ALA:O	9:7:456:THR:OG1	2.31	0.45
9:7:707:TRP:CB	9:7:718:PHE:HA	2.47	0.45
8:6:731:LEU:HD21	8:6:748:LEU:HD22	1.99	0.44
7:4:663:ALA:HB1	9:7:582:THR:HG22	1.99	0.44
10:C:429:TYR:CD1	10:C:433:ARG:HG2	2.52	0.44
6:2:487:GLY:O	6:2:492:LYS:NZ	2.44	0.44
6:2:493:ARG:NH2	6:2:710:TYR:OH	2.50	0.44
6:2:777:HIS:HA	6:2:780:ILE:HD12	1.99	0.44
9:7:705:ASN:ND2	12:A:710:ARG:O	2.50	0.44
1:B:435:HIS:ND1	14:E:386:SER:OG	2.45	0.44
6:2:216:LYS:HA	6:2:219:ILE:HG22	1.99	0.44
9:7:709:VAL:HG13	9:7:716:ILE:HG12	1.99	0.44
13:D:408:ASN:HA	13:D:411:ILE:HD12	2.00	0.44
7:4:290:ILE:HD11	7:4:355:GLN:HB2	1.99	0.44
9:7:445:ASP:HA	9:7:487:ALA:HB3	1.99	0.44
12:A:505:PRO:HA	12:A:508:GLU:HB2	1.98	0.44
8:6:430:THR:HB	8:6:482:ILE:HG12	2.00	0.44
9:7:379:LEU:HB3	9:7:387:LYS:NZ	2.32	0.44
10:C:603:LEU:HB3	10:C:633:TYR:CD2	2.52	0.44
1:B:400:LEU:O	1:B:406:GLN:NE2	2.50	0.44
5:8:215:THR:HG23	5:8:218:LYS:H	1.82	0.44
12:A:840:ASP:OD1	12:A:840:ASP:N	2.51	0.44
6:2:213:ASN:HB3	6:2:216:LYS:HD3	2.00	0.44
6:2:432:PHE:HZ	8:6:203:PHE:CE2	2.36	0.44
12:A:490:GLU:O	12:A:494:ARG:HG2	2.18	0.44
13:D:73:LYS:N	17:D:901:AGS:O2B	2.51	0.44
10:C:370:PRO:HA	10:C:373:ARG:HG2	2.00	0.44
13:D:335:LEU:HD21	13:D:352:GLU:OE1	2.17	0.44
7:4:462:LEU:HD22	7:4:687:LEU:HD22	2.00	0.43
10:C:317:HIS:HA	14:E:383:GLN:NE2	2.33	0.43
13:D:128:VAL:HG12	13:D:128:VAL:O	2.18	0.43
1:B:279:VAL:HG22	10:C:675:ILE:HG23	2.01	0.43
7:4:748:ARG:NH1	7:4:757:ASP:OD1	2.51	0.43
3:Y:10:DC:H2"	3:Y:11:DG:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:4:231:GLN:HE22	7:4:280:ASP:HB3	1.83	0.43
7:4:393:ILE:HG13	7:4:419:ILE:HD11	2.01	0.43
7:4:712:GLU:HA	7:4:715:VAL:HG12	2.01	0.43
6:2:223:CYS:HA	6:2:274:TYR:CE1	2.54	0.43
7:4:354:LEU:HD22	7:4:372:LEU:HD11	2.01	0.43
8:6:53:LEU:HD11	8:6:61:LEU:HB2	2.00	0.43
7:4:683:ASP:O	7:4:687:LEU:HB2	2.19	0.43
8:6:140:GLN:HA	8:6:241:LYS:HA	2.00	0.43
8:6:728:VAL:HG11	8:6:817:TYR:CD2	2.53	0.43
12:A:623:ASP:OD1	12:A:623:ASP:N	2.52	0.43
6:2:195:ILE:HG23	6:2:244:LEU:HD21	2.01	0.43
6:2:777:HIS:NE2	6:2:793:MET:SD	2.92	0.43
7:4:372:LEU:HD23	7:4:416:ILE:HB	2.01	0.43
9:7:669:VAL:HG12	9:7:669:VAL:O	2.19	0.43
10:C:256:PRO:O	10:C:259:ILE:HG22	2.19	0.43
10:C:295:THR:HG22	10:C:417:ARG:HH22	1.84	0.43
10:C:370:PRO:O	10:C:373:ARG:HG2	2.19	0.43
10:C:390:ASN:OD1	10:C:391:GLU:N	2.52	0.43
12:A:701:GLU:OE2	12:A:703:ASP:HB2	2.19	0.43
1:B:305:LEU:HD11	1:B:421:ILE:HD11	2.01	0.43
2:X:4:DT:H2"	2:X:5:DG:C8	2.54	0.43
9:7:552:GLU:OE1	9:7:552:GLU:N	2.52	0.43
9:7:596:LYS:HD3	9:7:596:LYS:N	2.34	0.43
12:A:727:ARG:NH2	13:D:61:ASN:HD21	2.17	0.43
13:D:100:ASN:HA	13:D:159:ASP:HB2	2.00	0.43
6:2:321:GLN:NE2	6:2:373:TYR:HB2	2.34	0.42
6:2:434:VAL:HG13	8:6:148:HIS:HB3	2.01	0.42
6:2:730:ARG:NH2	6:2:782:LEU:HB3	2.34	0.42
7:4:270:ASN:OD1	7:4:271:MET:N	2.52	0.42
7:4:441:PHE:HE2	7:4:689:ASP:HB3	1.84	0.42
7:4:660:ARG:NH1	9:7:586:VAL:HG11	2.34	0.42
14:E:204:TYR:O	14:E:208:ILE:HG12	2.19	0.42
1:B:343:PHE:HD2	1:B:346:ILE:HG13	1.84	0.42
7:4:657:ALA:O	7:4:661:ARG:HG3	2.19	0.42
10:C:453:TYR:OH	10:C:560:ASP:OD1	2.24	0.42
11:3:416:ASP:O	11:3:420:THR:HG23	2.19	0.42
1:B:327:ARG:HA	1:B:331:LEU:HB2	2.01	0.42
9:7:329:GLU:N	9:7:329:GLU:OE1	2.53	0.42
10:C:30:PHE:HD2	10:C:40:SER:HB3	1.84	0.42
10:C:364:GLU:OE1	10:C:368:ARG:NH2	2.52	0.42
7:4:501:ARG:NH2	7:4:645:ASP:OD2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:7:586:VAL:HG12	9:7:590:ARG:HH12	1.84	0.42
10:C:423:THR:HG23	10:C:426:LEU:HD12	2.00	0.42
11:3:291:ARG:HA	11:3:291:ARG:HD3	1.90	0.42
7:4:579:MET:O	7:4:584:ARG:NH2	2.41	0.42
9:7:496:ASN:O	9:7:504:ASN:ND2	2.43	0.42
11:3:508:ARG:NH2	11:3:516:ASP:O	2.52	0.42
12:A:631:ASP:OD1	12:A:632:ILE:N	2.52	0.42
12:A:785:PHE:HB3	12:A:786:ARG:HH21	1.84	0.42
3:Y:4:DT:OP1	12:A:593:THR:HG22	2.19	0.42
7:4:264:ASN:H	7:4:391:THR:HG21	1.85	0.42
8:6:715:LEU:HD23	8:6:716:GLY:O	2.19	0.42
7:4:531:GLN:HG2	7:4:562:ALA:HB1	2.02	0.42
7:4:660:ARG:HH12	9:7:586:VAL:HG11	1.85	0.42
8:6:203:PHE:CE1	8:6:227:ILE:HG23	2.55	0.42
9:7:407:ARG:NH1	11:3:417:MET:O	2.53	0.42
6:2:459:GLU:HA	6:2:462:LYS:HG2	2.01	0.42
10:C:360:ASN:OD1	10:C:361:ASN:N	2.53	0.42
12:A:712:VAL:HG12	12:A:717:GLY:HA2	2.02	0.42
3:Y:30:DG:H2"	3:Y:31:DC:C6	2.55	0.42
5:8:460:VAL:O	5:8:464:VAL:HG23	2.20	0.42
6:2:643:PHE:HA	6:2:646:ASN:HD22	1.83	0.42
5:8:463:SER:OG	8:6:118:PRO:HG2	2.20	0.42
10:C:348:LEU:O	10:C:352:LYS:HG2	2.20	0.42
9:7:448:ASP:HB2	9:7:506:GLN:HE21	1.85	0.41
11:3:283:LYS:HB3	11:3:544:ILE:HD11	2.02	0.41
12:A:499:ALA:HB3	12:A:693:ARG:HH12	1.83	0.41
7:4:740:LEU:HD23	7:4:740:LEU:HA	1.90	0.41
8:6:387:ARG:HH12	8:6:478:GLU:HA	1.85	0.41
8:6:617:THR:OG1	8:6:618:VAL:N	2.53	0.41
10:C:429:TYR:CG	10:C:433:ARG:HG2	2.55	0.41
14:E:240:VAL:HG13	14:E:253:LEU:HD21	2.02	0.41
1:B:347:SER:OG	1:B:349:LYS:HG3	2.20	0.41
3:Y:37:DT:H2"	3:Y:38:DG:C8	2.55	0.41
10:C:278:SER:OG	10:C:279:LEU:N	2.53	0.41
10:C:282:LYS:O	10:C:286:THR:HG23	2.20	0.41
10:C:455:SER:O	10:C:458:GLN:HG3	2.19	0.41
12:A:792:GLU:OE1	12:A:844:ARG:NH2	2.52	0.41
13:D:314:LYS:HD2	13:D:406:LEU:HD21	2.01	0.41
4:5:543:ALA:HB1	6:2:508:GLY:HA3	2.01	0.41
12:A:588:THR:HG23	12:A:590:GLN:H	1.86	0.41
3:Y:33:DT:H2"	3:Y:34:DG:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:6:768:ASN:O	8:6:772:ILE:HG12	2.20	0.41
9:7:534:ALA:O	9:7:538:THR:HG23	2.20	0.41
13:D:113:GLU:OE2	13:D:116:ARG:NH2	2.41	0.41
6:2:196:HIS:CD2	6:2:262:ALA:HB2	2.55	0.41
6:2:668:ASP:HB2	6:2:671:GLN:HB2	2.01	0.41
2:X:30:DG:H2"	2:X:31:DC:C6	2.55	0.41
8:6:215:LEU:HD12	8:6:221:PRO:HB3	2.02	0.41
10:C:52:GLN:OE1	10:C:55:LYS:HE3	2.20	0.41
11:3:382:VAL:HG22	11:3:393:LEU:HD23	2.02	0.41
1:B:383:ASP:HB3	1:B:386:LEU:HD23	2.03	0.41
6:2:381:SER:O	6:2:385:VAL:HG23	2.21	0.41
9:7:459:HIS:O	9:7:514:ARG:NH1	2.53	0.41
10:C:214:PRO:HA	10:C:245:PRO:HG2	2.02	0.41
10:C:645:LEU:HB2	10:C:701:ASP:HB3	2.02	0.41
5:8:450:ARG:O	5:8:454:LEU:HG	2.21	0.41
6:2:215:PHE:CZ	6:2:232:VAL:HG23	2.55	0.41
6:2:277:ILE:HG23	6:2:278:THR:HG23	2.03	0.41
6:2:464:ILE:HG21	6:2:726:TYR:HD2	1.85	0.41
7:4:732:ARG:NH2	17:6:902:AGS:O2A	2.53	0.41
9:7:606:LEU:HA	9:7:609:ILE:HG12	2.02	0.41
13:D:108:LYS:NZ	13:D:130:GLY:HA2	2.36	0.41
10:C:474:LYS:HA	10:C:474:LYS:HD3	1.86	0.41
12:A:712:VAL:HG21	12:A:722:CYS:HB2	2.03	0.41
14:E:51:LEU:HD12	14:E:58:HIS:HB3	2.02	0.41
14:E:329:LEU:HB3	14:E:332:HIS:CE1	2.55	0.41
7:4:507:LEU:HD22	7:4:644:PHE:CE2	2.56	0.40
7:4:664:HIS:HA	7:4:667:VAL:HG22	2.02	0.40
10:C:122:THR:O	10:C:126:GLN:HG2	2.21	0.40
14:E:142:LEU:HD22	14:E:174:PRO:HG3	2.03	0.40
1:B:340:ASN:HB2	1:B:342:PHE:CE1	2.56	0.40
5:8:253:ARG:NH2	5:8:267:TYR:OH	2.54	0.40
5:8:486:CYS:SG	5:8:487:CYS:N	2.93	0.40
6:2:490:ASP:OD1	6:2:491:ILE:N	2.54	0.40
6:2:783:ARG:NH1	6:2:787:ILE:HD12	2.35	0.40
7:4:257:GLN:OE1	7:4:257:GLN:N	2.52	0.40
8:6:145:HIS:HB2	8:6:205:LYS:HB3	2.03	0.40
12:A:721:ARG:HD2	12:A:759:PHE:CZ	2.57	0.40
1:B:340:ASN:HB2	1:B:342:PHE:HE1	1.87	0.40
6:2:593:ASN:O	6:2:597:ARG:HG3	2.22	0.40
10:C:111:VAL:HA	10:C:114:HIS:ND1	2.37	0.40
10:C:497:PHE:CD1	10:C:551:LEU:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:354:GLN:HA	13:D:357:VAL:HG22	2.04	0.40
4:5:335:ILE:O	4:5:339:ILE:HG12	2.22	0.40
5:8:504:GLU:OE1	5:8:505:LEU:HD23	2.21	0.40
6:2:735:LEU:HB3	6:2:738:MET:SD	2.62	0.40
7:4:200:ILE:HA	7:4:203:ILE:HG22	2.03	0.40
10:C:414:LEU:HD12	10:C:483:CYS:SG	2.62	0.40
12:A:606:CYS:HB3	12:A:639:TRP:CH2	2.55	0.40
14:E:211:LEU:HG	14:E:225:LEU:HD11	2.01	0.40
5:8:509:TRP:CZ3	5:8:532:ILE:HG21	2.56	0.40
7:4:531:GLN:HE21	7:4:533:THR:HG23	1.86	0.40
8:6:370:LEU:HD21	8:6:631:MET:CE	2.52	0.40
14:E:308:PHE:HA	14:E:311:ILE:HG12	2.03	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	B	192/577 (33%)	187 (97%)	5 (3%)	0	100	100
4	5	273/734 (37%)	269 (98%)	4 (2%)	0	100	100
5	8	253/546 (46%)	250 (99%)	3 (1%)	0	100	100
6	2	564/904 (62%)	559 (99%)	5 (1%)	0	100	100
7	4	498/863 (58%)	483 (97%)	15 (3%)	0	100	100
8	6	609/821 (74%)	601 (99%)	8 (1%)	0	100	100
9	7	349/719 (48%)	343 (98%)	6 (2%)	0	100	100
10	C	556/711 (78%)	547 (98%)	9 (2%)	0	100	100
11	3	349/810 (43%)	344 (99%)	5 (1%)	0	100	100
12	A	360/861 (42%)	348 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	D	402/436 (92%)	391 (97%)	11 (3%)	0	100	100
14	E	354/435 (81%)	347 (98%)	7 (2%)	0	100	100
All	All	4759/8417 (56%)	4669 (98%)	90 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	B	182/529 (34%)	181 (100%)	1 (0%)	86	90
4	5	235/625 (38%)	235 (100%)	0	100	100
5	8	230/456 (50%)	230 (100%)	0	100	100
6	2	496/781 (64%)	495 (100%)	1 (0%)	92	94
7	4	456/753 (61%)	456 (100%)	0	100	100
8	6	571/724 (79%)	571 (100%)	0	100	100
9	7	304/619 (49%)	304 (100%)	0	100	100
10	C	535/659 (81%)	534 (100%)	1 (0%)	92	94
11	3	295/708 (42%)	295 (100%)	0	100	100
12	A	321/766 (42%)	321 (100%)	0	100	100
13	D	375/403 (93%)	373 (100%)	2 (0%)	86	90
14	E	335/399 (84%)	335 (100%)	0	100	100
All	All	4335/7422 (58%)	4330 (100%)	5 (0%)	92	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	349	LYS
6	2	469	LYS
10	C	55	LYS
13	D	260	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	D	386	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
6	2	206	HIS
6	2	321	GLN
6	2	646	ASN
7	4	531	GLN
9	7	705	ASN
10	C	85	GLN
10	C	317	HIS
14	E	186	ASN
14	E	383	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 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	$\#\|Z\|>2$
17	AGS	6	902	15	26,33,33	0.72	1 (3%)	26,52,52	1.00	2 (7%)
17	AGS	D	901	15	26,33,33	0.71	1 (3%)	26,52,52	1.07	2 (7%)
17	AGS	E	501	15	26,33,33	0.72	1 (3%)	26,52,52	0.98	2 (7%)
17	AGS	6	901	15	26,33,33	0.72	1 (3%)	26,52,52	1.01	2 (7%)
17	AGS	A	901	15	26,33,33	0.72	1 (3%)	26,52,52	1.01	2 (7%)

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
17	AGS	6	902	15	-	6/17/38/38	0/3/3/3
17	AGS	D	901	15	-	3/17/38/38	0/3/3/3
17	AGS	E	501	15	-	4/17/38/38	0/3/3/3
17	AGS	6	901	15	-	3/17/38/38	0/3/3/3
17	AGS	A	901	15	-	3/17/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	E	501	AGS	PG-S1G	2.19	1.95	1.90
17	D	901	AGS	PG-S1G	2.17	1.95	1.90
17	6	901	AGS	PG-S1G	2.17	1.95	1.90
17	6	902	AGS	PG-S1G	2.17	1.95	1.90
17	A	901	AGS	PG-S1G	2.17	1.95	1.90

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	D	901	AGS	PA-O3A-PB	-3.75	119.96	132.83
17	6	902	AGS	PA-O3A-PB	-3.38	121.24	132.83
17	A	901	AGS	PA-O3A-PB	-3.36	121.31	132.83
17	E	501	AGS	PA-O3A-PB	-2.99	122.57	132.83
17	6	901	AGS	PA-O3A-PB	-2.97	122.62	132.83
17	D	901	AGS	C5-C6-N6	2.30	123.84	120.35
17	6	902	AGS	C5-C6-N6	2.29	123.83	120.35
17	E	501	AGS	C5-C6-N6	2.27	123.81	120.35
17	A	901	AGS	C5-C6-N6	2.26	123.78	120.35
17	6	901	AGS	C5-C6-N6	2.24	123.76	120.35

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	6	901	AGS	C5'-O5'-PA-O3A
17	6	902	AGS	C5'-O5'-PA-O3A
17	6	902	AGS	O4'-C4'-C5'-O5'
17	A	901	AGS	C5'-O5'-PA-O3A
17	D	901	AGS	C5'-O5'-PA-O1A
17	D	901	AGS	C5'-O5'-PA-O2A
17	E	501	AGS	C5'-O5'-PA-O2A
17	6	902	AGS	C3'-C4'-C5'-O5'
17	A	901	AGS	O4'-C4'-C5'-O5'
17	A	901	AGS	C3'-C4'-C5'-O5'
17	E	501	AGS	C5'-O5'-PA-O3A
17	6	901	AGS	PA-O3A-PB-O1B
17	6	902	AGS	PA-O3A-PB-O1B
17	6	901	AGS	C5'-O5'-PA-O1A
17	E	501	AGS	C5'-O5'-PA-O1A
17	6	902	AGS	PG-O3B-PB-O1B
17	6	902	AGS	PG-O3B-PB-O2B
17	D	901	AGS	C5'-O5'-PA-O3A
17	E	501	AGS	PA-O3A-PB-O2B

There are no ring outliers.

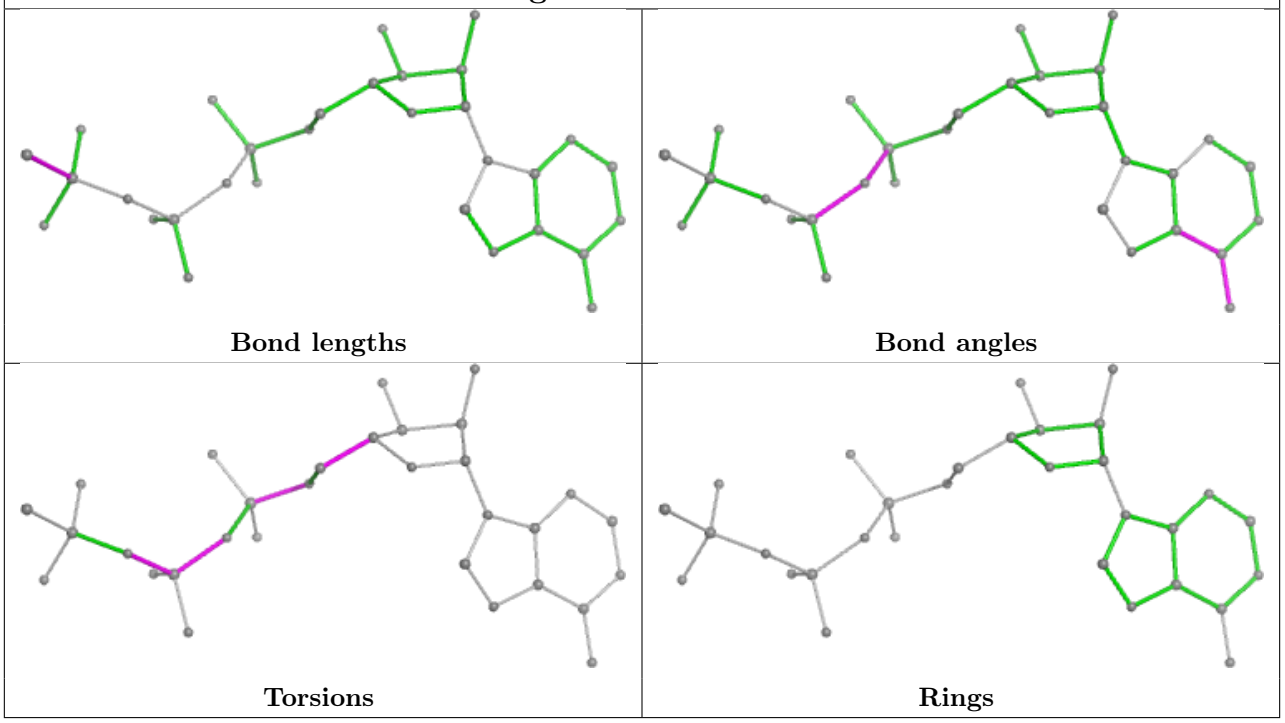
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	6	902	AGS	3	0
17	D	901	AGS	1	0
17	E	501	AGS	2	0
17	A	901	AGS	2	0

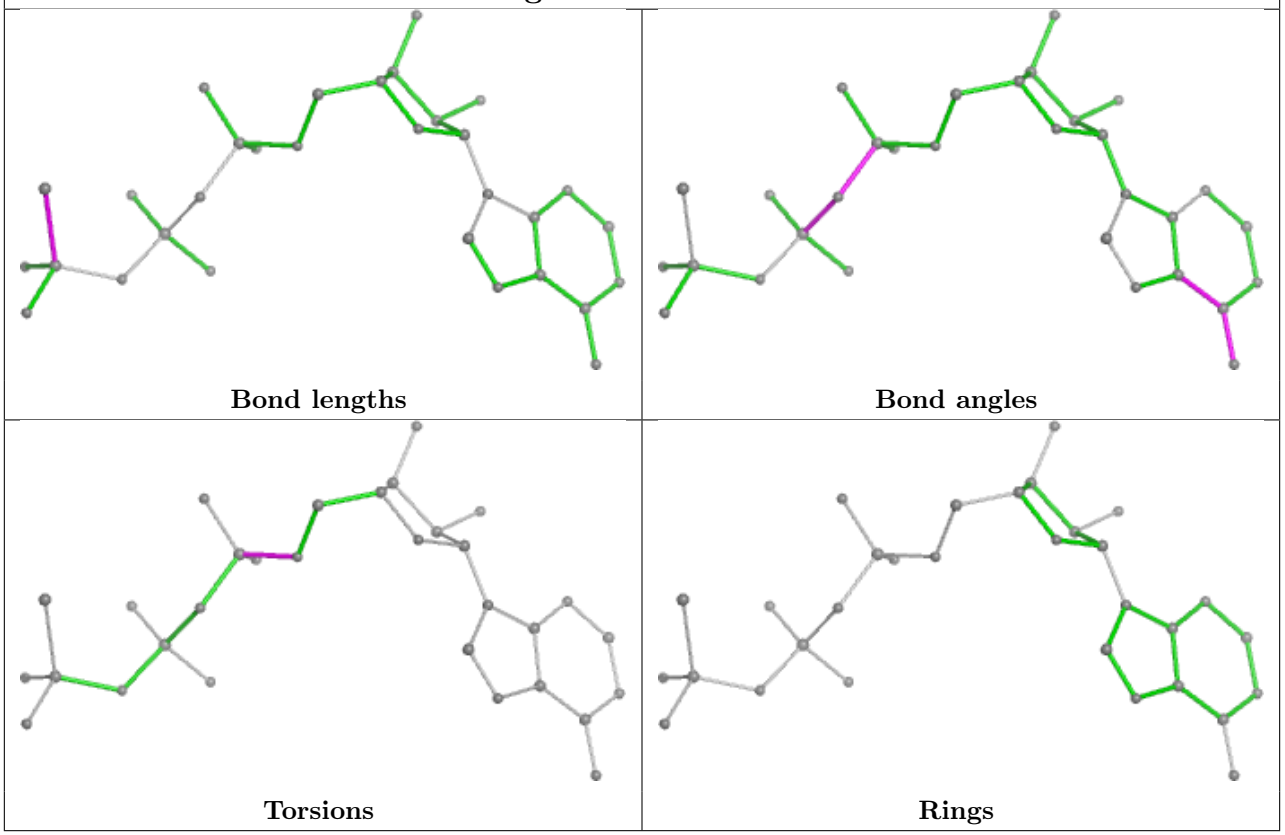
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

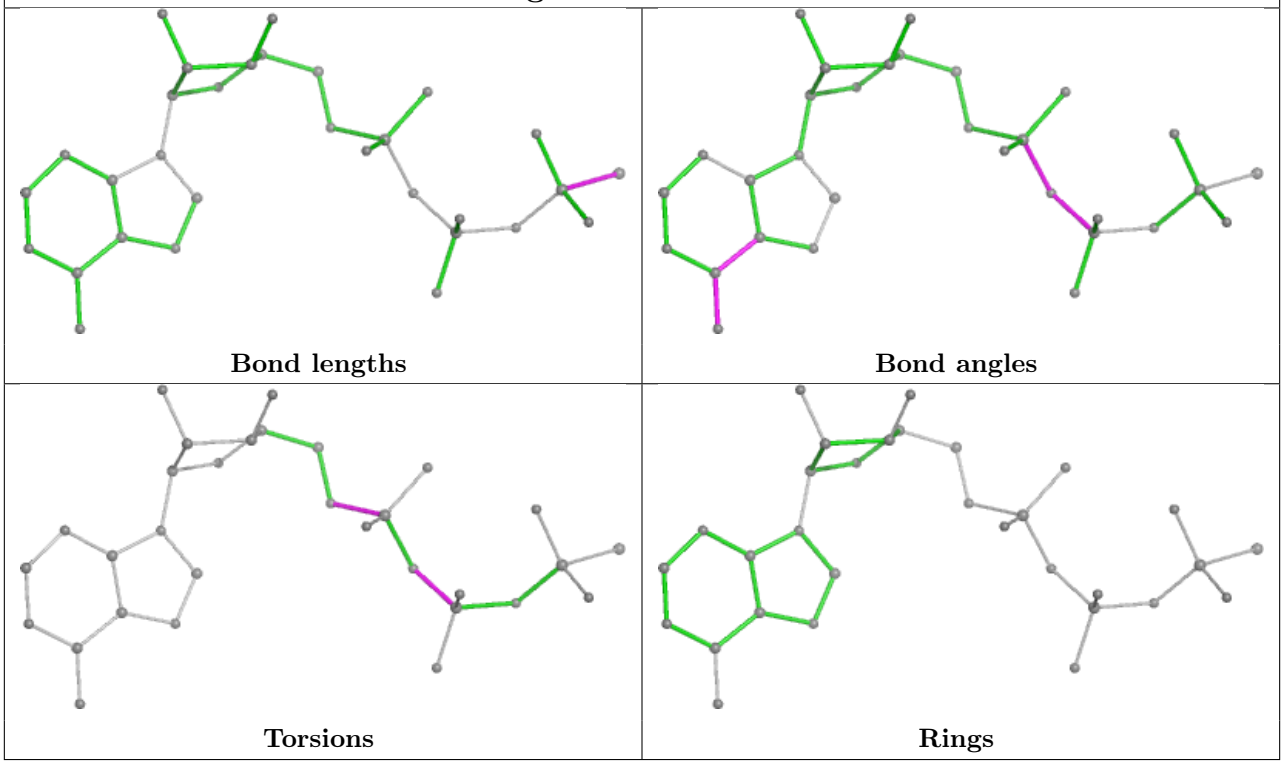
Ligand AGS 6 902



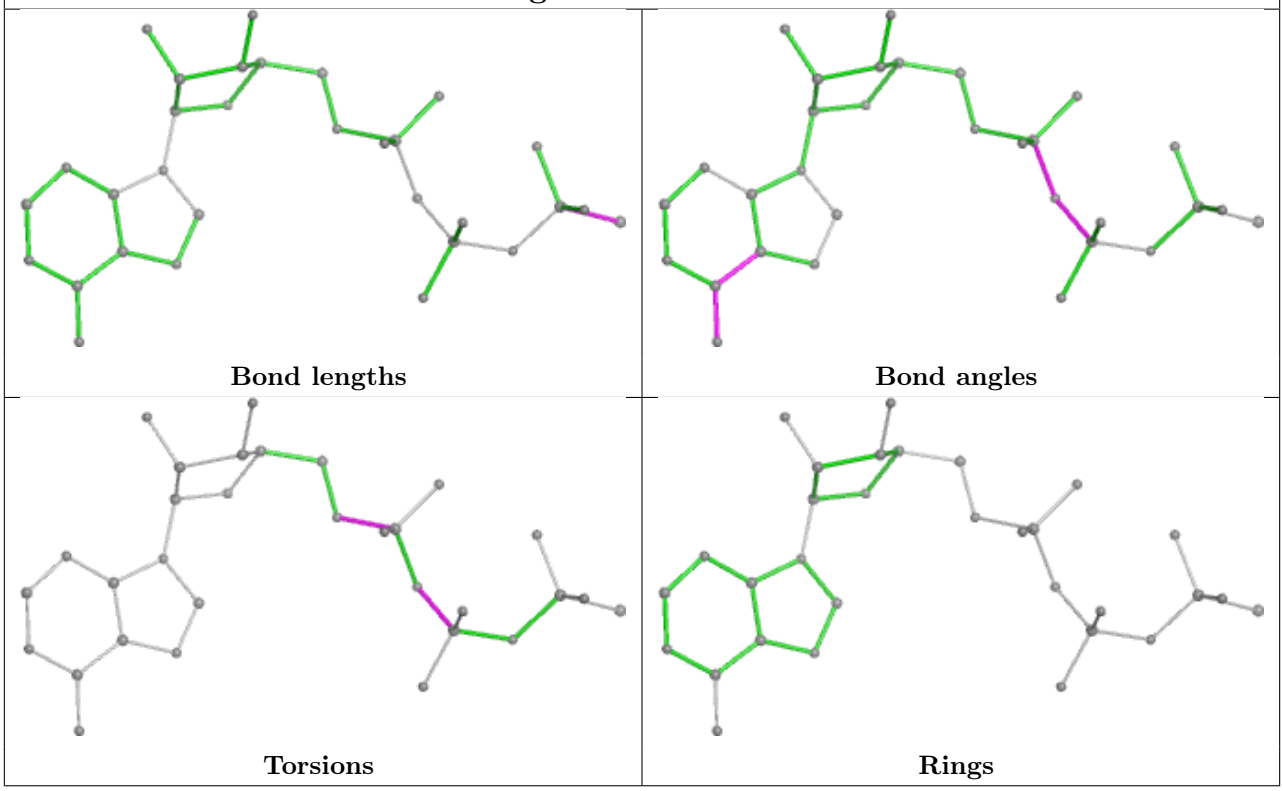
Ligand AGS D 901



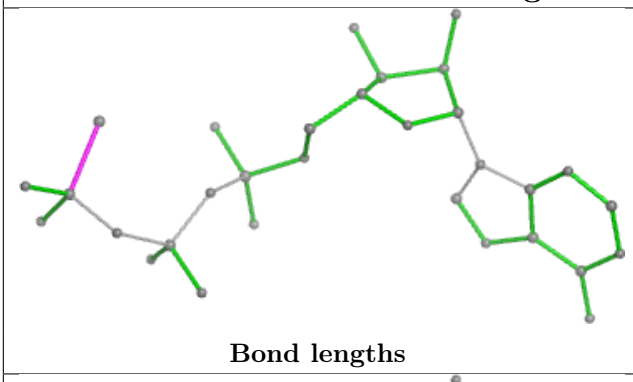
Ligand AGS E 501



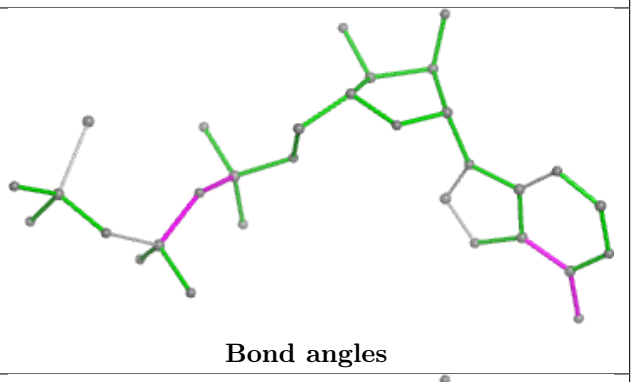
Ligand AGS 6 901



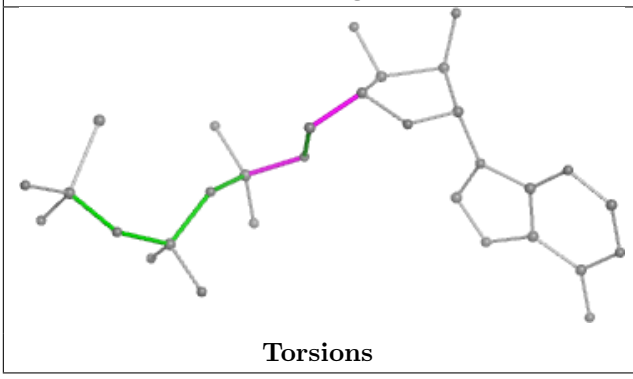
Ligand AGS A 901



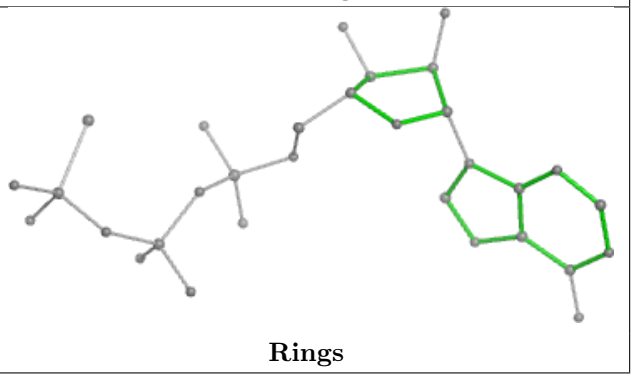
Bond lengths



Bond angles



Torsions



Rings

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.

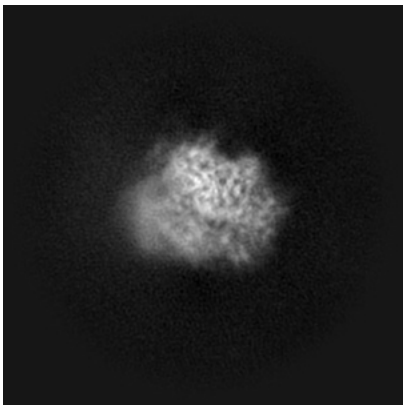
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19624. These allow visual inspection of the internal detail of the map and identification of artifacts.

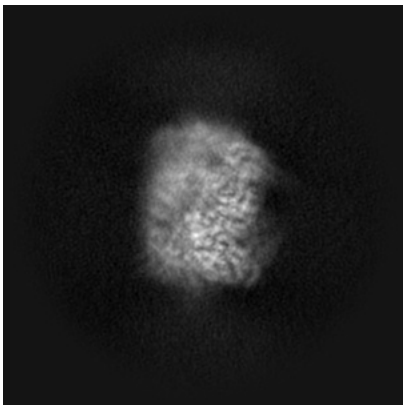
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

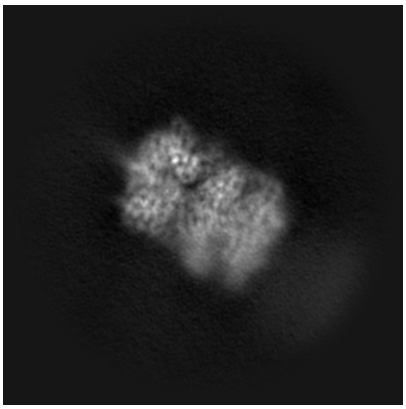
6.1.1 Primary map



X

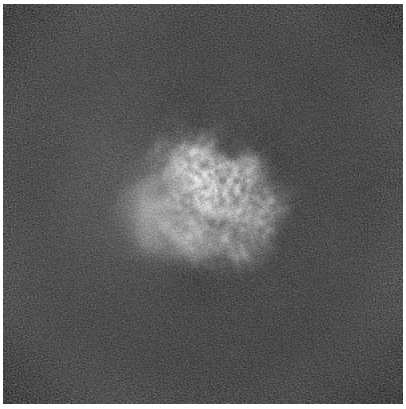


Y

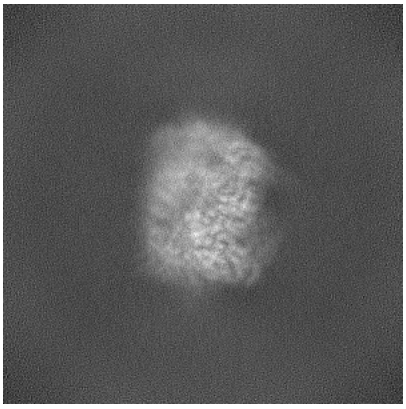


Z

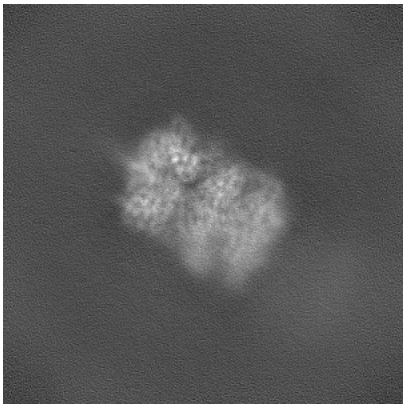
6.1.2 Raw map



X



Y

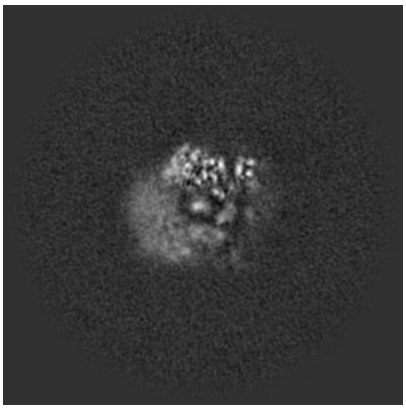


Z

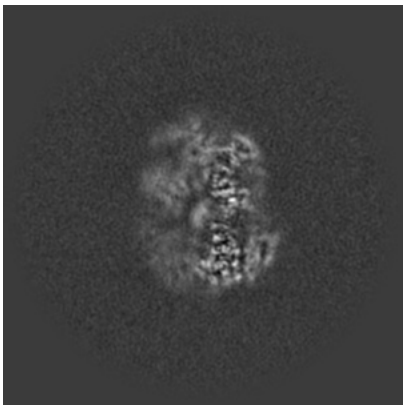
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

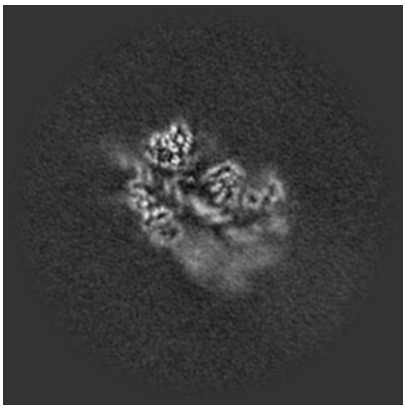
6.2.1 Primary map



X Index: 200

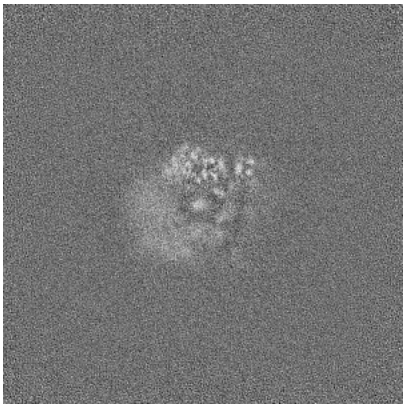


Y Index: 200

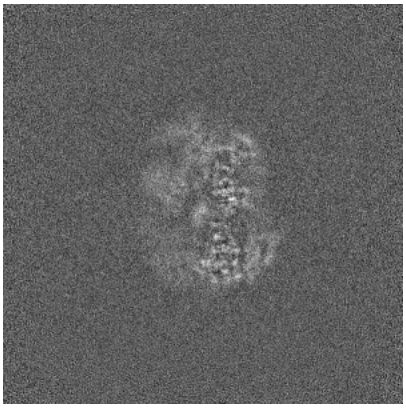


Z Index: 200

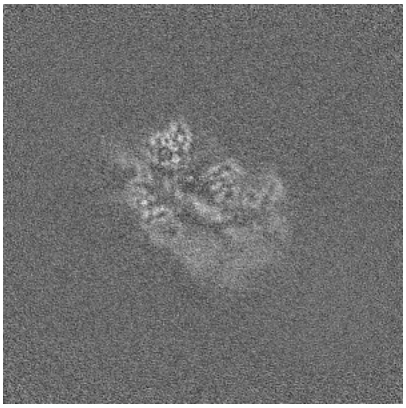
6.2.2 Raw map



X Index: 200



Y Index: 200

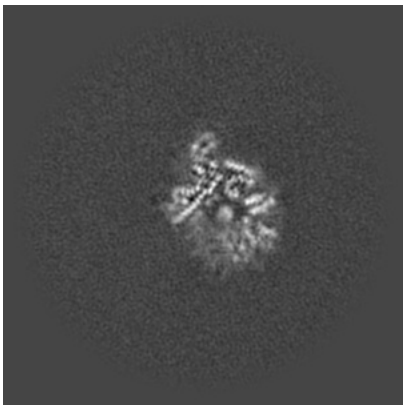


Z Index: 200

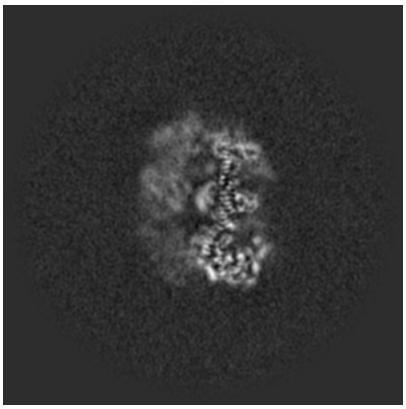
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

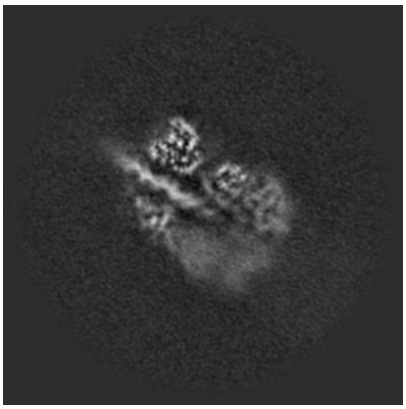
6.3.1 Primary map



X Index: 151

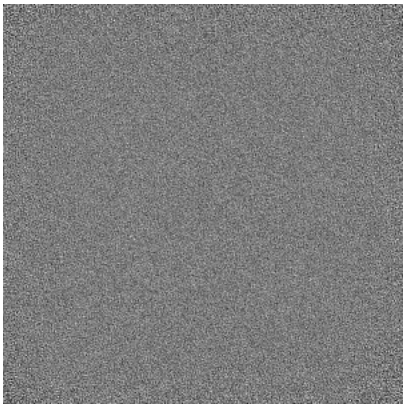


Y Index: 193

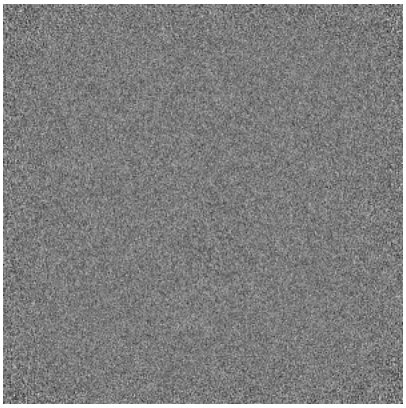


Z Index: 193

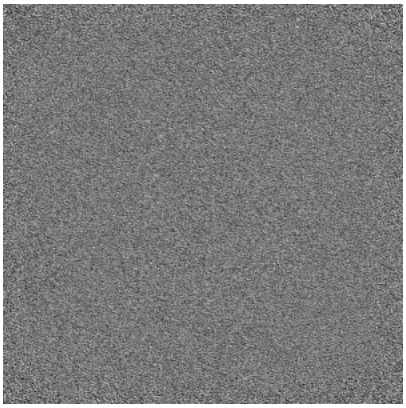
6.3.2 Raw map



X Index: 0



Y Index: 0

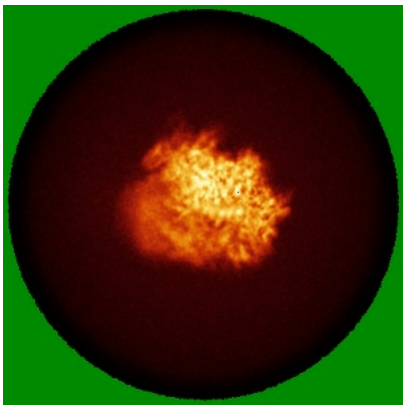


Z Index: 0

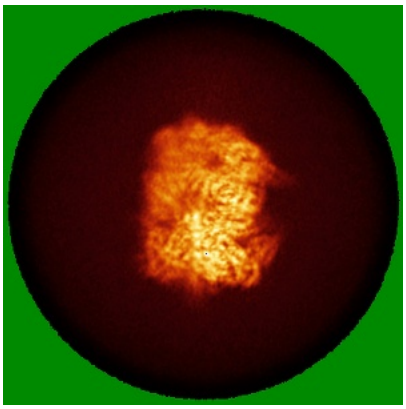
The images above show the largest variance slices of the map in three orthogonal directions.

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

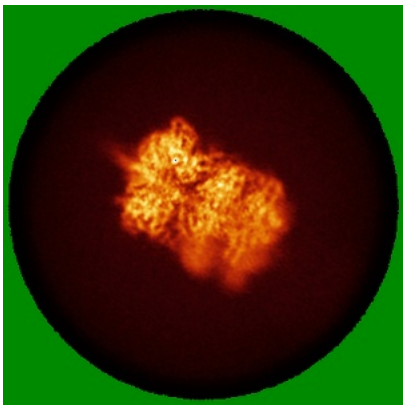
6.4.1 Primary map



X

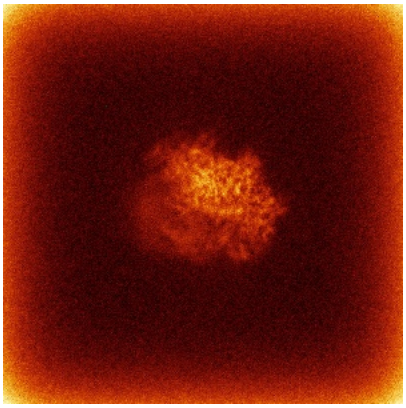


Y

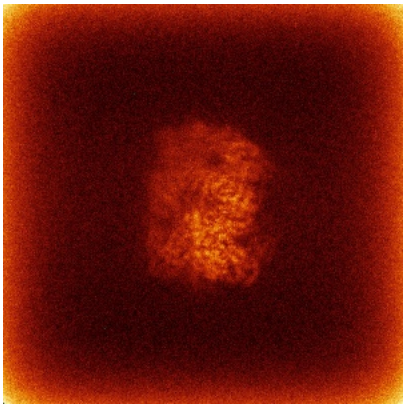


Z

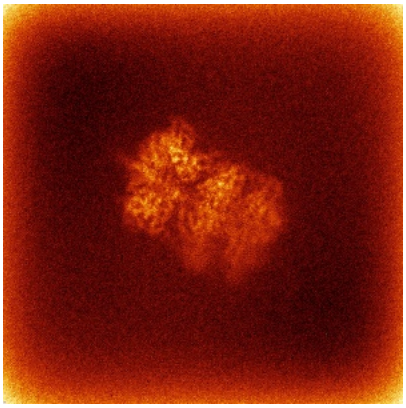
6.4.2 Raw map



X



Y

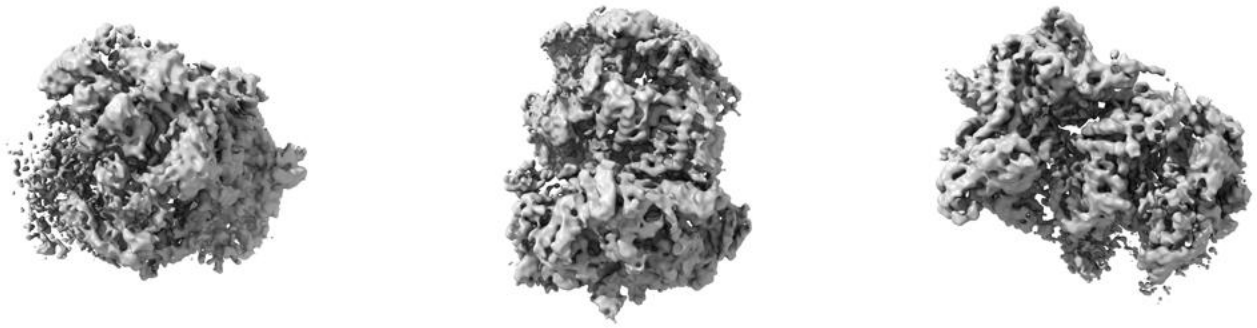


Z

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)

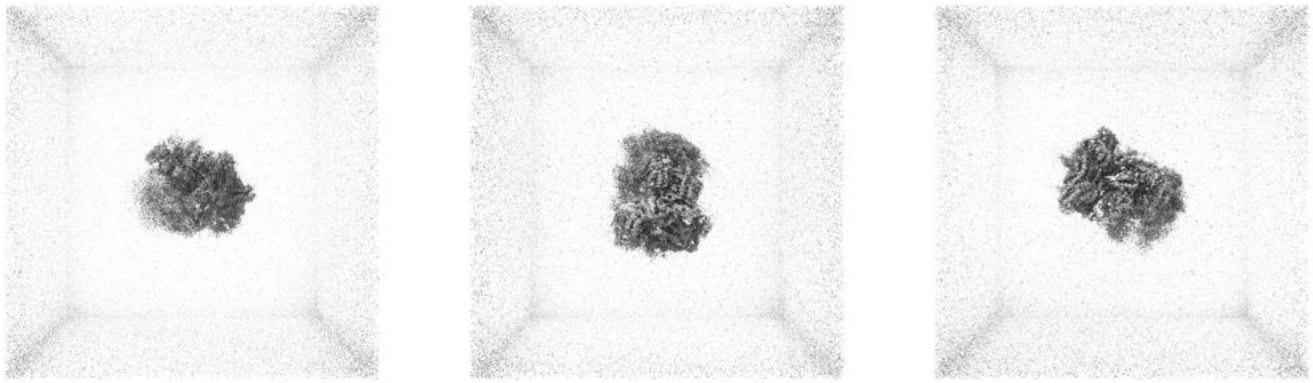
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

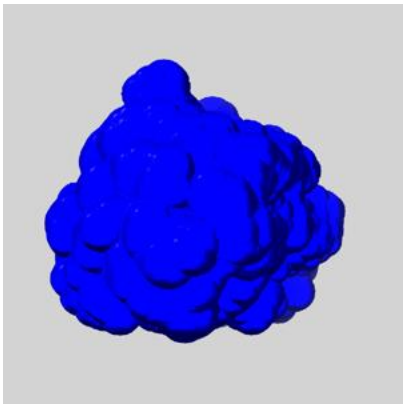
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

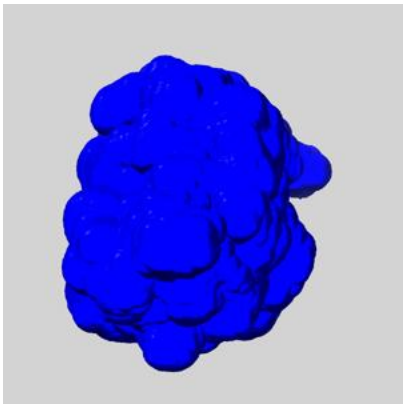
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

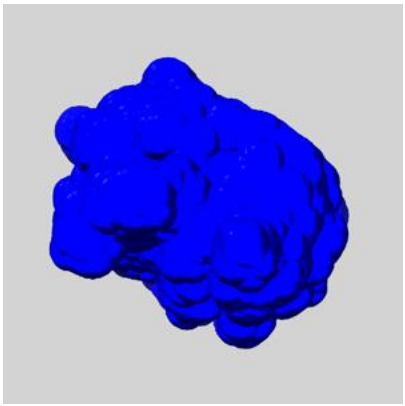
6.6.1 emd_19624_msk_1.map (i)



X



Y

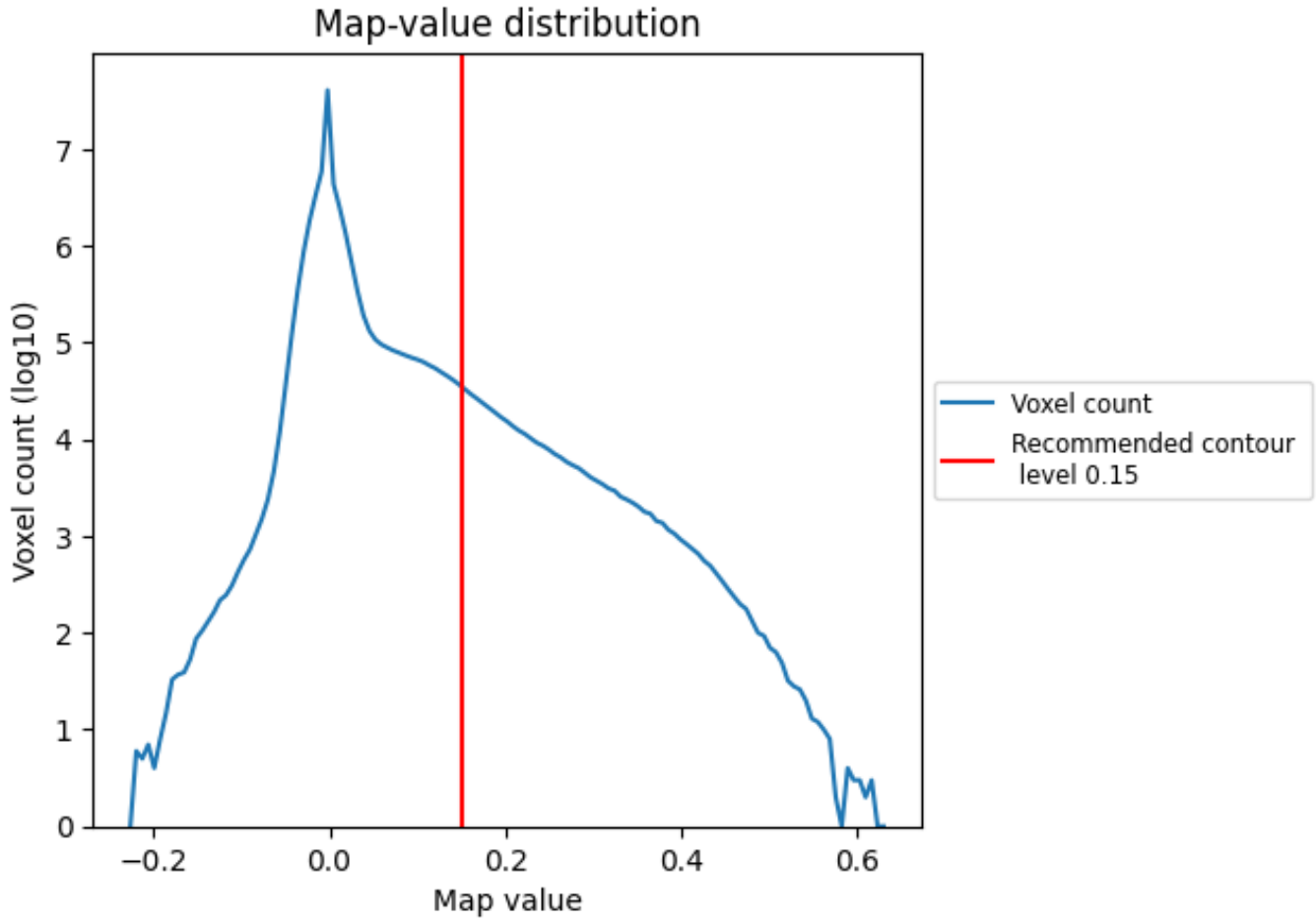


Z

7 Map analysis

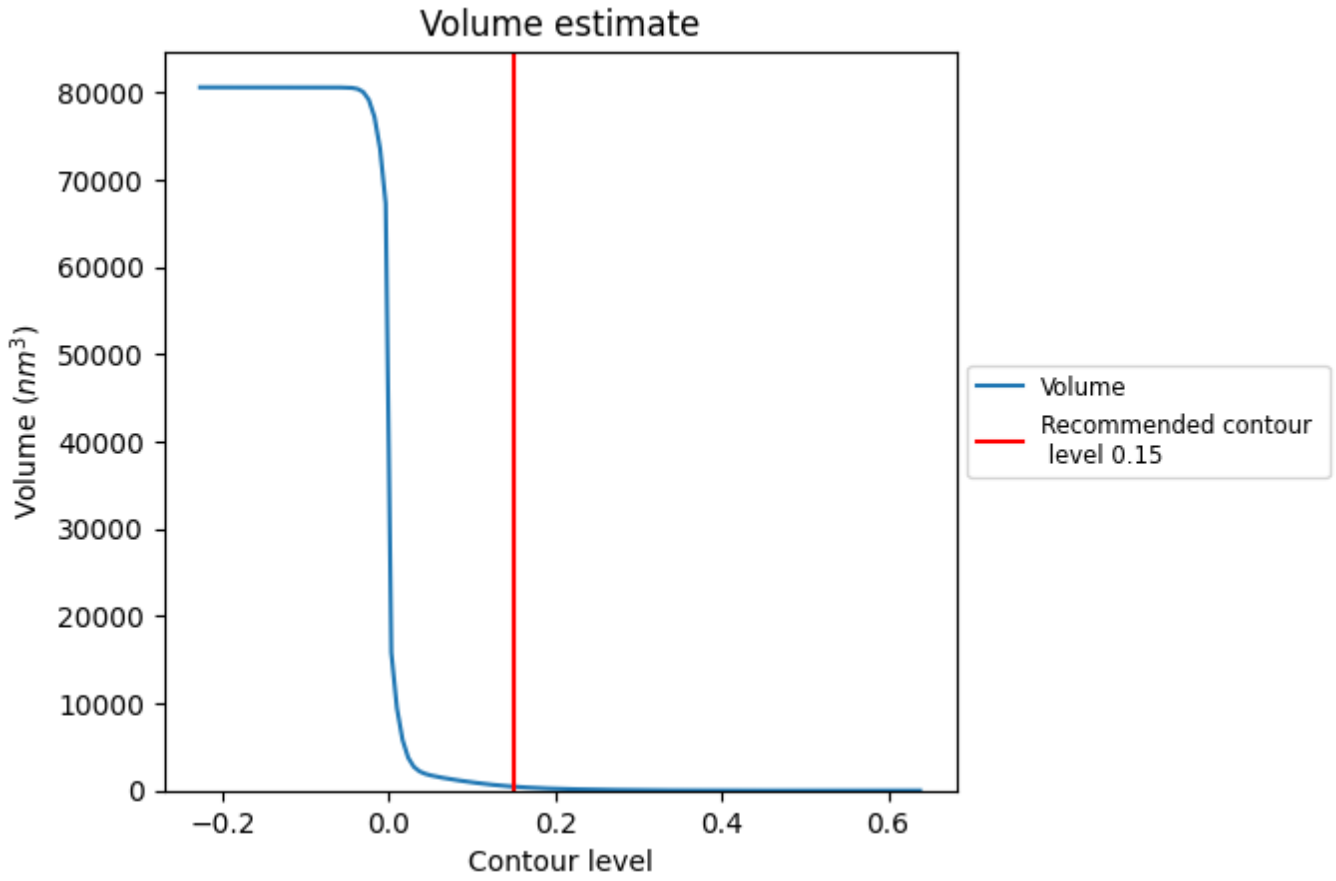
This section contains the results of statistical analysis of the map.

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.

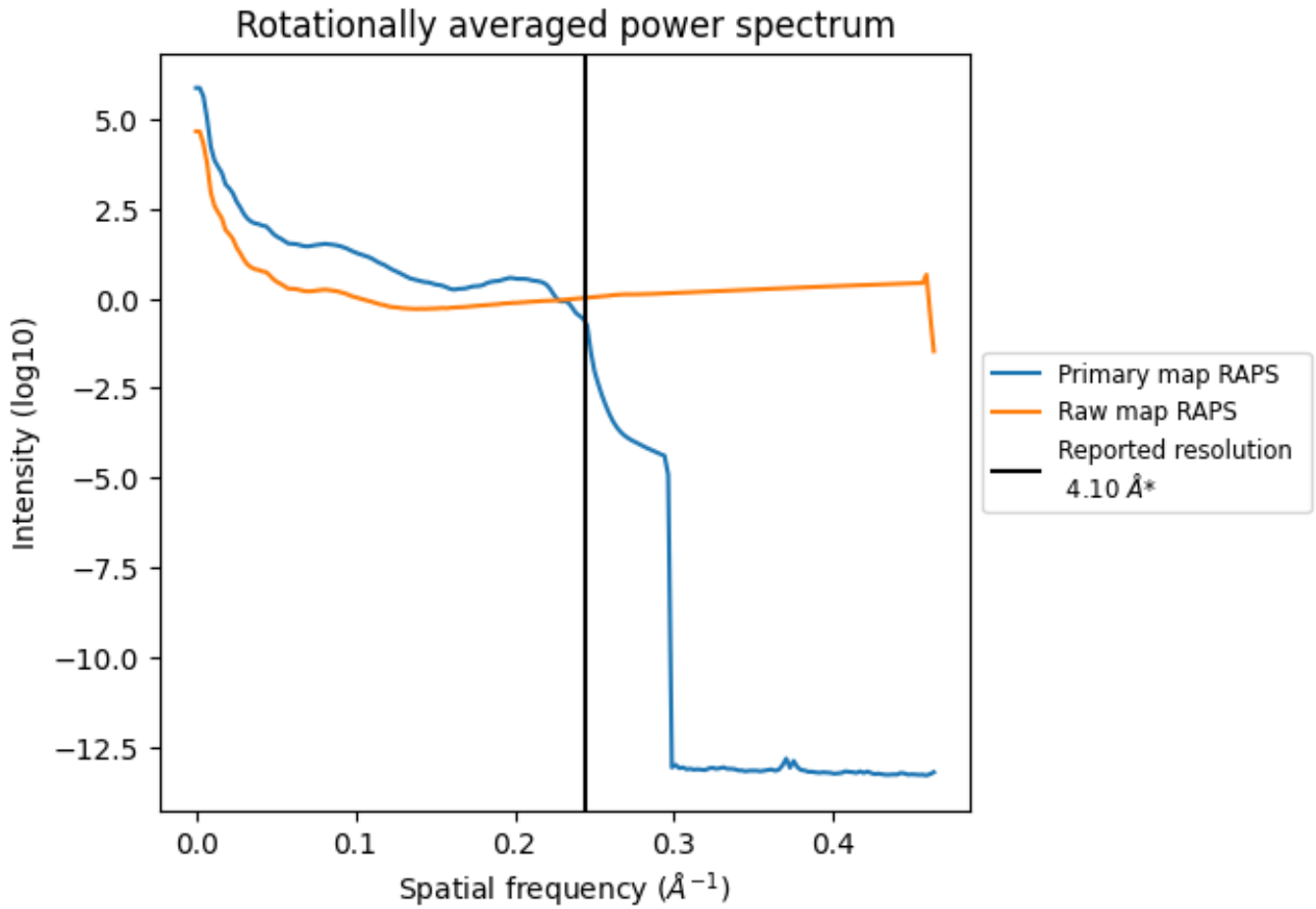
7.2 Volume estimate



The volume at the recommended contour level is 452 nm^3; this corresponds to an approximate mass of 408 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)

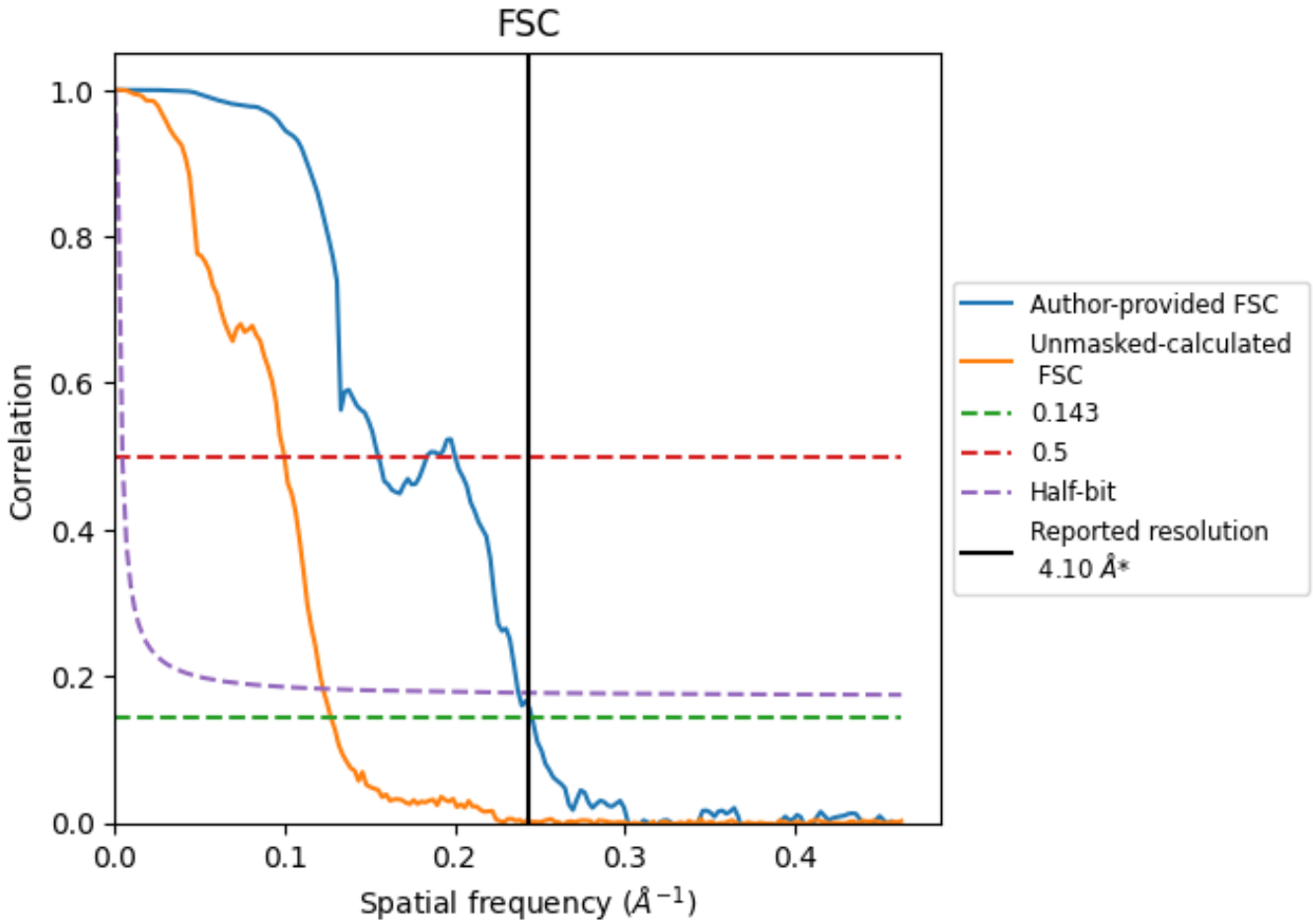


*Reported resolution corresponds to spatial frequency of 0.244 $Å^{-1}$

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 0.244 Å^{-1}

8.2 Resolution estimates (i)

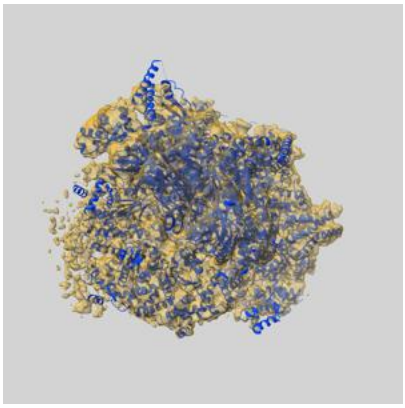
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.07	6.44	4.21
Unmasked-calculated*	7.86	10.02	8.16

*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 7.86 differs from the reported value 4.1 by more than 10 %

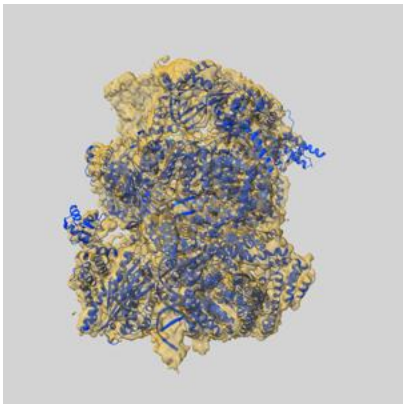
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19624 and PDB model 8S0F. Per-residue inclusion information can be found in section 3 on page 8.

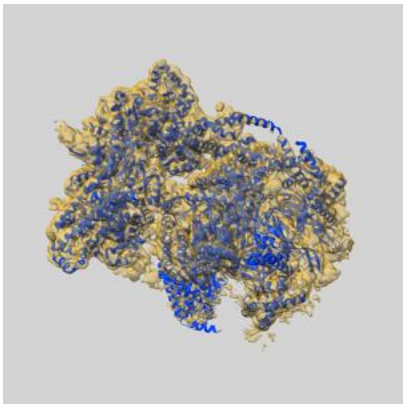
9.1 Map-model overlay



X



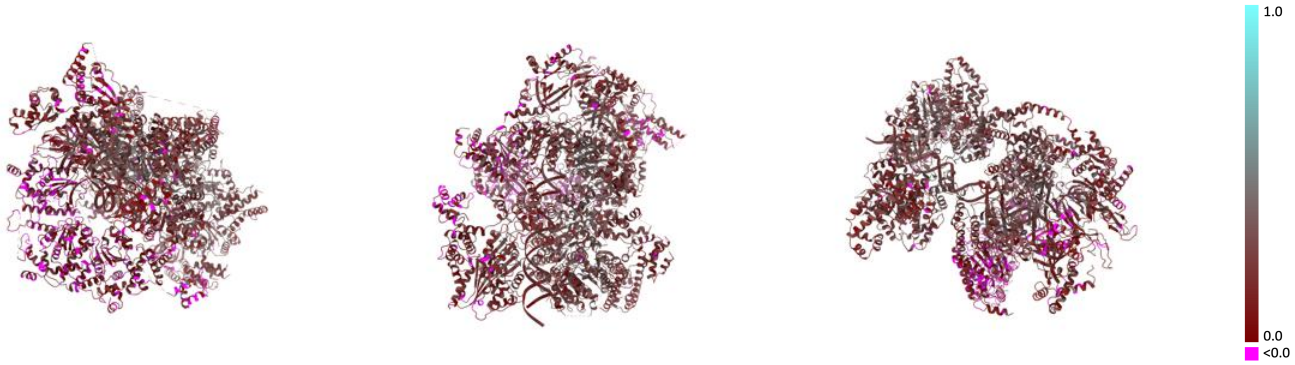
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

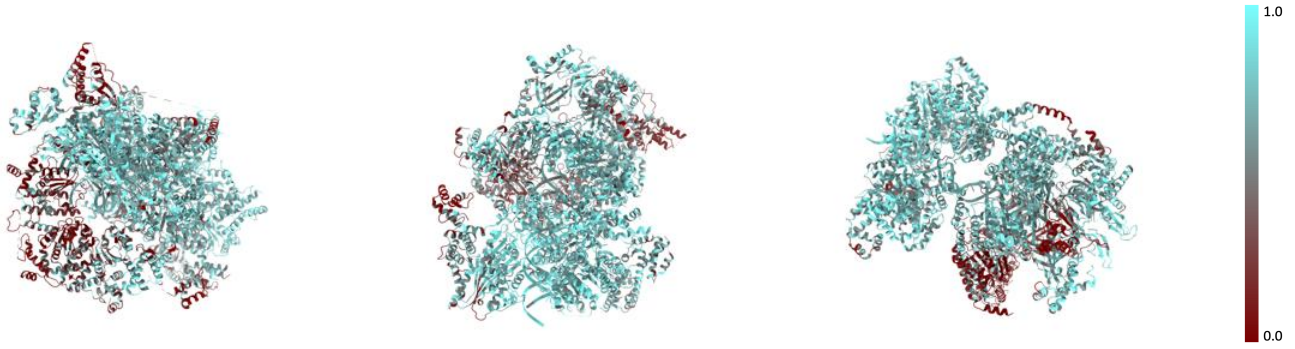
9.2 Q-score mapped to coordinate model (i)



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.

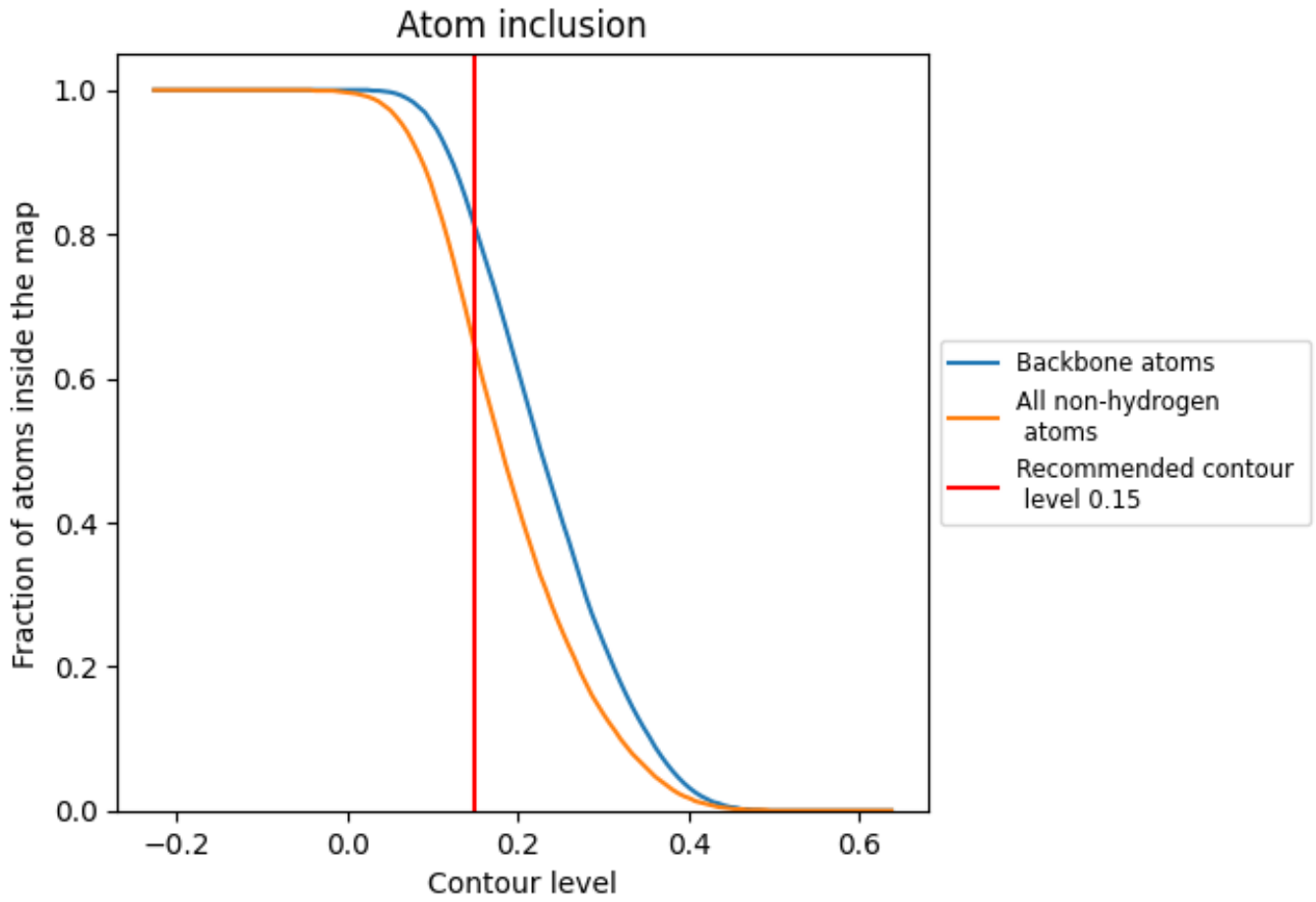
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 64% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6390	0.2120
2	0.7140	0.2270
3	0.2070	0.0620
4	0.6910	0.2080
5	0.1760	0.0430
6	0.7650	0.2860
7	0.4840	0.1120
8	0.3280	0.1520
A	0.6370	0.1920
B	0.8170	0.2880
C	0.7510	0.2460
D	0.7910	0.2770
E	0.7940	0.3240
X	0.8240	0.1870
Y	0.7810	0.1930