Full wwPDB EM Validation Report (i)

Mar 11, 2024 – 08:15 AM EDT

PDB ID	:	6U0M
EMDB ID	:	EMD-20607
Title	:	Structure of the S. cerevisiae replicative helicase CMG in complex with a forked DNA
Authors	:	Yuan, Z.; Georgescu, R.; Bai, L.; Zhang, D.; O'Donnell, M.; Li, H.
Deposited on	:	2019-08-14
Resolution	:	3.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

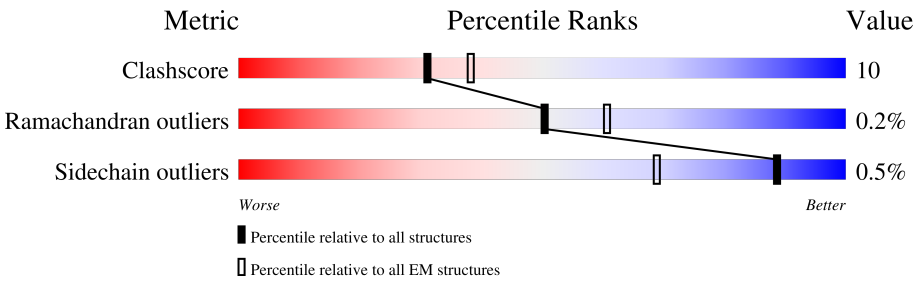
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.90 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	208	48% 72% 27%
2	B	198	22% 74% 18% 9%
3	C	191	35% 63% 19% • 17%
4	D	291	26% 59% 16% 24%
5	E	646	21% 62% 23% • 14%
6	2	664	26% 73% 22% 5%
7	3	722	32% 64% 18% 18%
8	4	753	42% 69% 21% 10%

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Mol	Chain	Length	Quality of chain
9	5	670	24% 69% 19% 11%
10	6	667	29% 72% 20% 8%
11	7	729	54% 72% 19% 9%
12	F	23	65% 57% 43%
13	G	15	73% 33% 40% 27%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 41146 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	208	1690	1062	287	331	10	0	0

- Molecule 2 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	181	1507	975	258	270	4	0	0

- Molecule 3 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	159	1288	843	207	232	6	0	0

- Molecule 4 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	221	1820	1159	300	348	13	0	0

- Molecule 5 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	553	4472	2853	763	843	13	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	634	4957	3110	897	933	17	0	0

- Molecule 7 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	3	594	4653	2933	829	878	13	0	0

- Molecule 8 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	4	681	5404	3394	945	1037	28	0	0

- Molecule 9 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	5	597	4663	2931	799	910	23	0	0

- Molecule 10 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	6	614	4691	2953	829	889	20	0	0

- Molecule 11 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	7	663	5212	3285	903	994	30	0	0

- Molecule 12 is a DNA chain called DNA (26-MER).

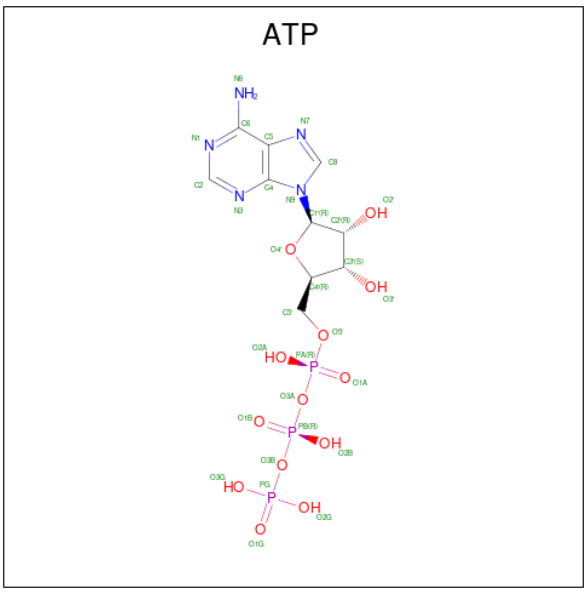
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
12	F	23	472	228	78	143	23	0	0

- Molecule 13 is a DNA chain called DNA (15-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
13	G	11	224	107	40	66	11	0	0

- Molecule 14 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

$C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



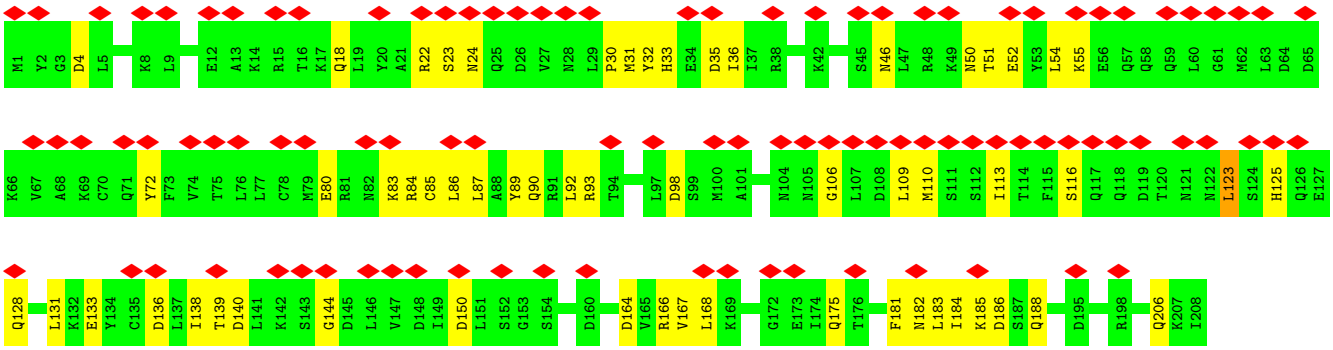
Mol	Chain	Residues	Atoms					AltConf
14	2	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	3	1	Total	C	N	O	P	0
			31	10	5	13	3	
14	5	1	Total	C	N	O	P	0
			31	10	5	13	3	

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.

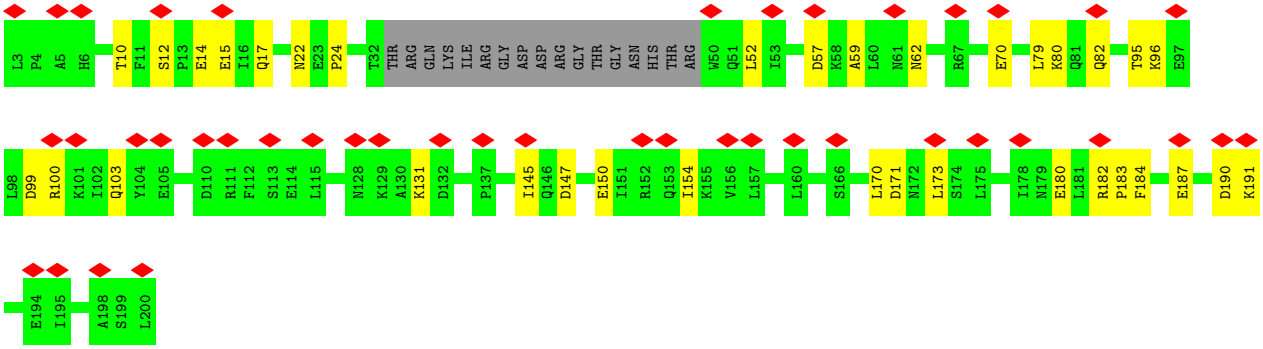
• Molecule 1: DNA replication complex GINS protein PSF1

Chain A:



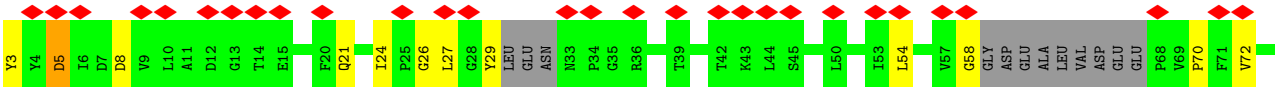
• Molecule 2: DNA replication complex GINS protein PSF2

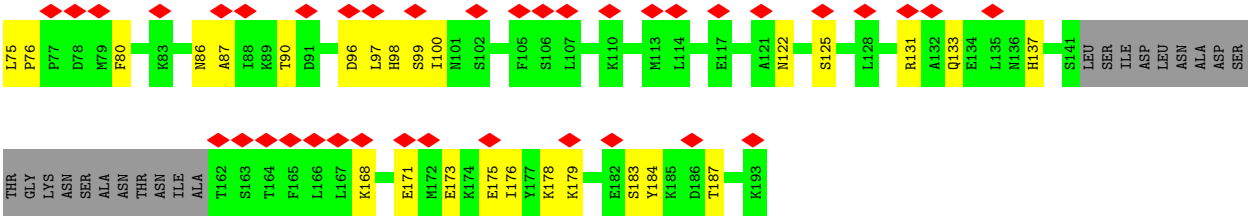
Chain B:



• Molecule 3: DNA replication complex GINS protein PSF3

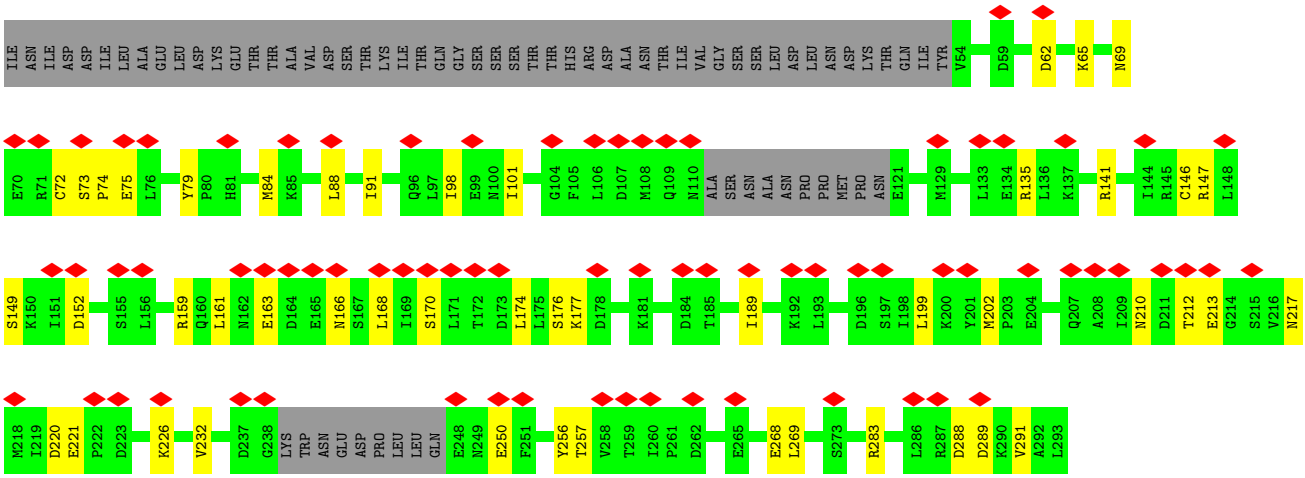
Chain C:





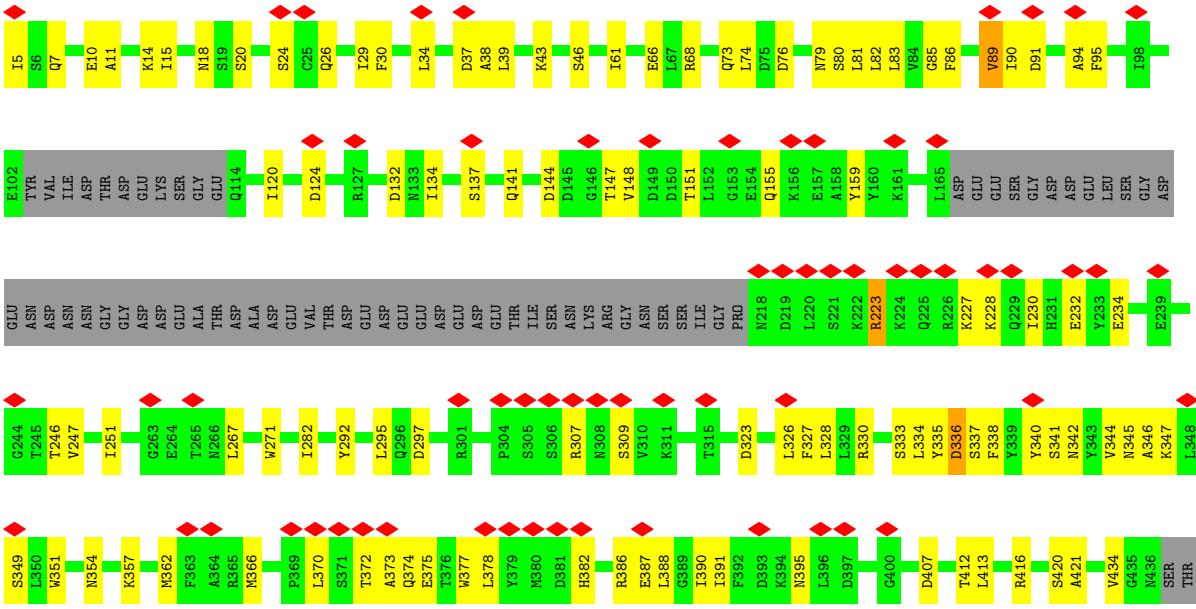
• Molecule 4: DNA replication complex GINS protein SLD5

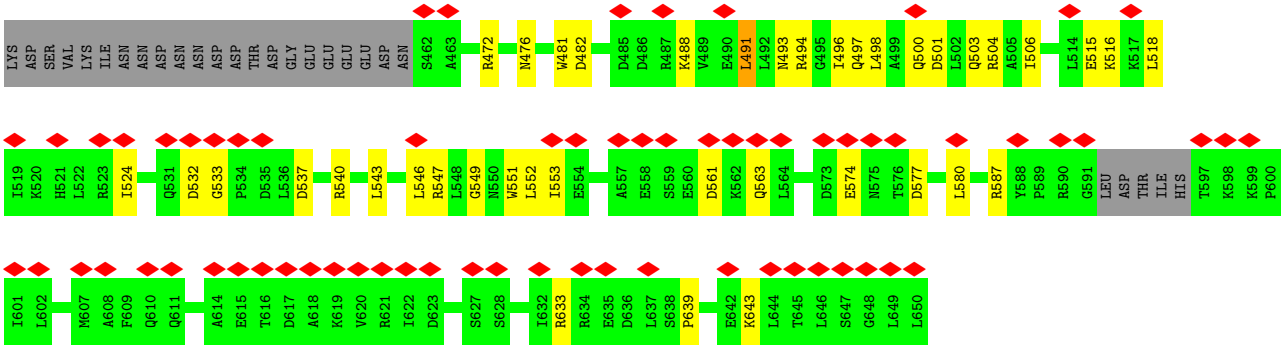
Chain D:



• Molecule 5: Cell division control protein 45

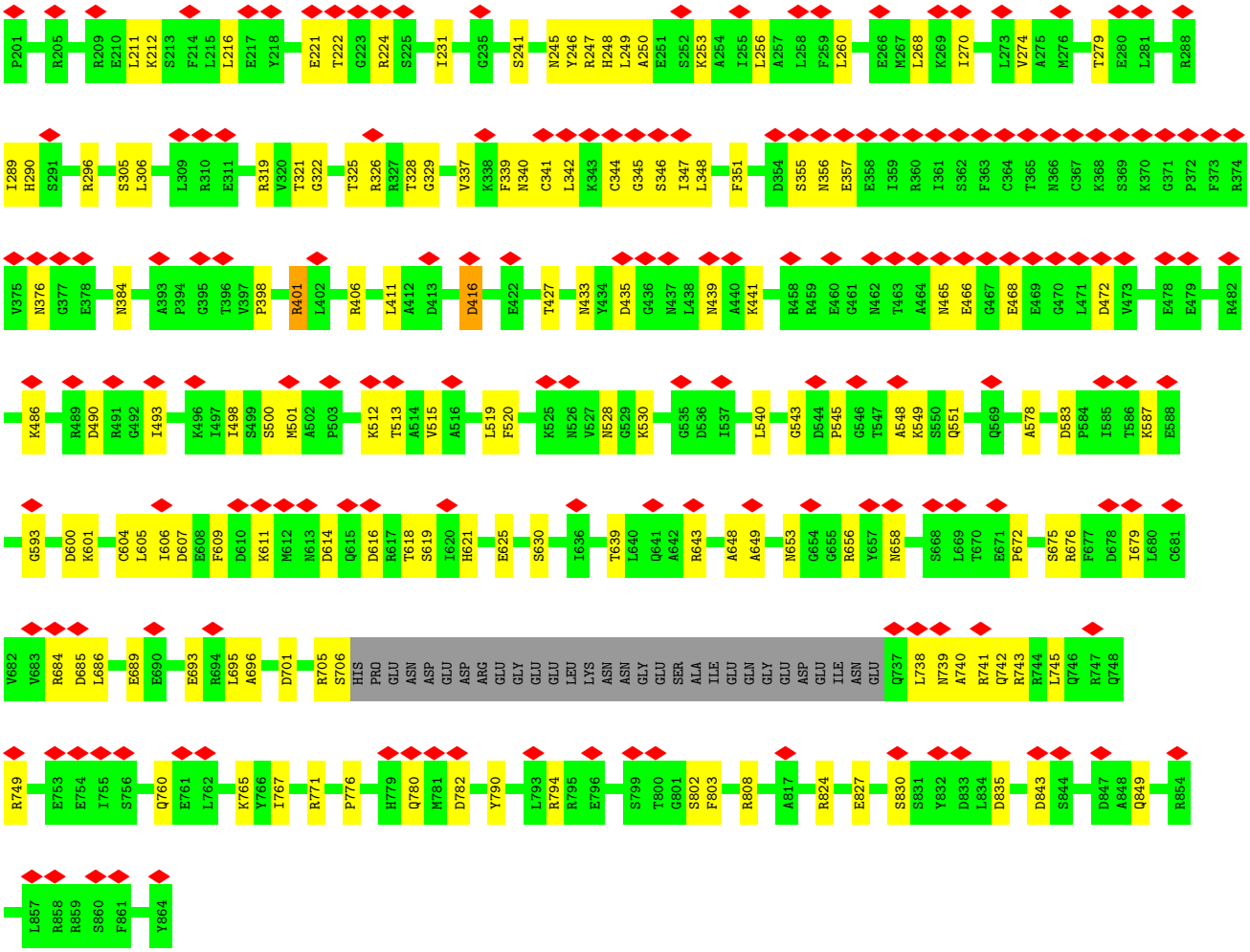
Chain E:





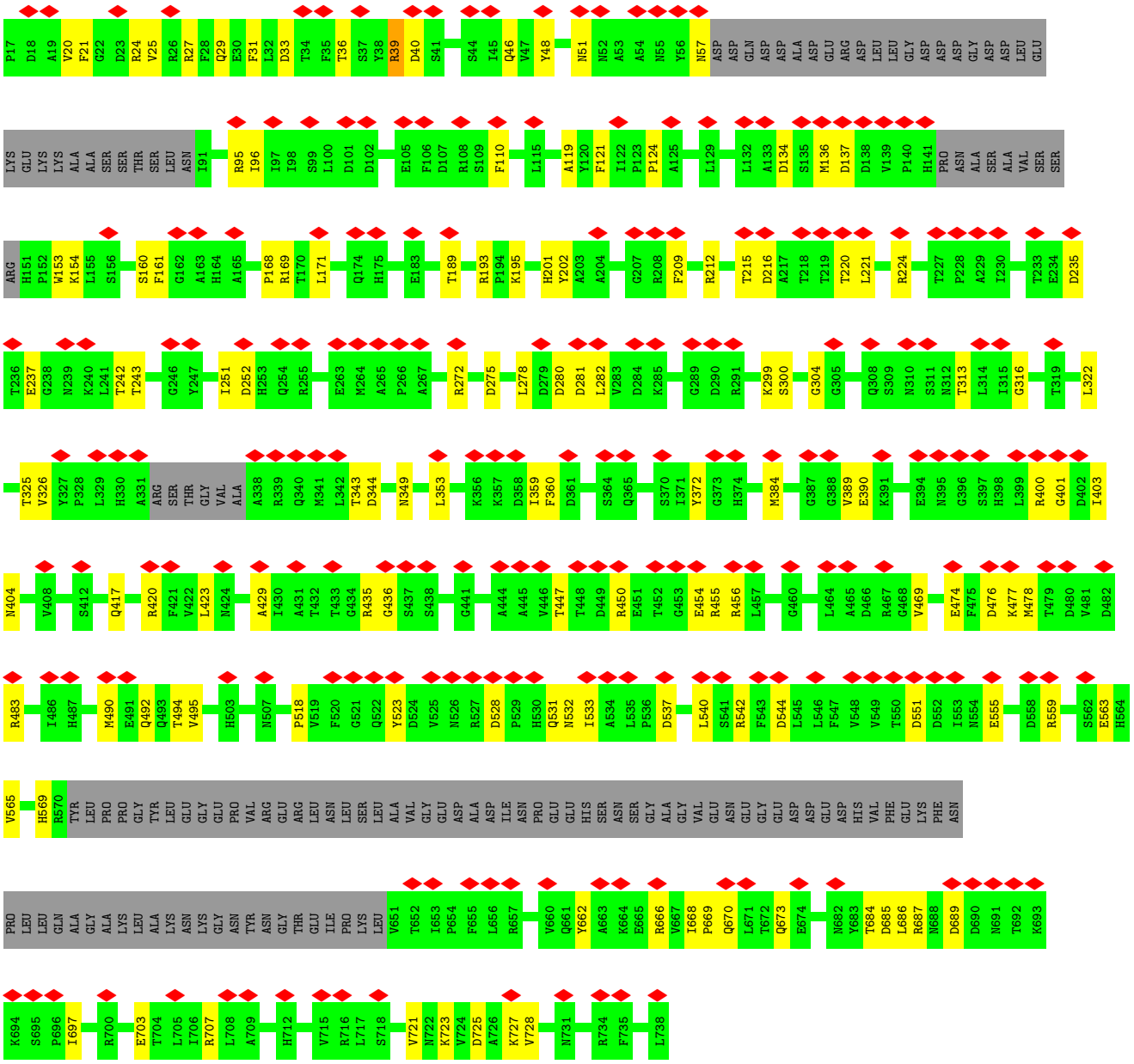
• Molecule 6: DNA replication licensing factor MCM2

Chain 2:



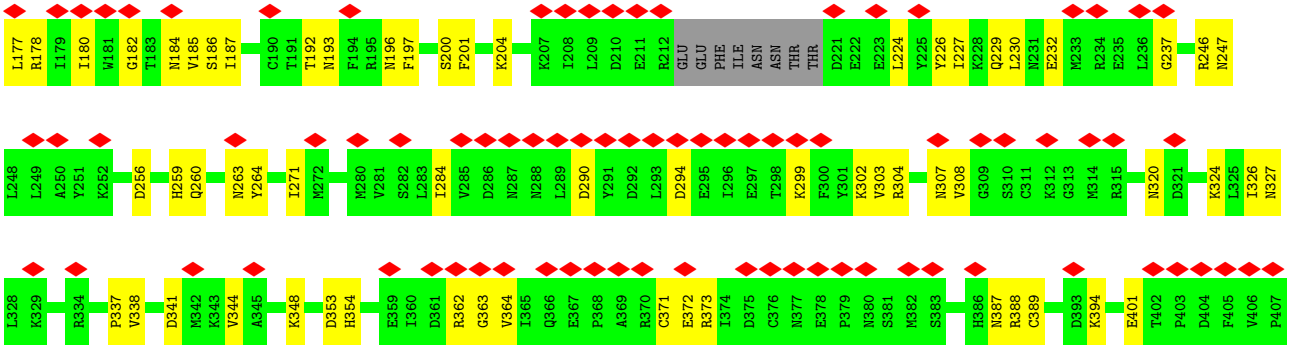
• Molecule 7: DNA replication licensing factor MCM3

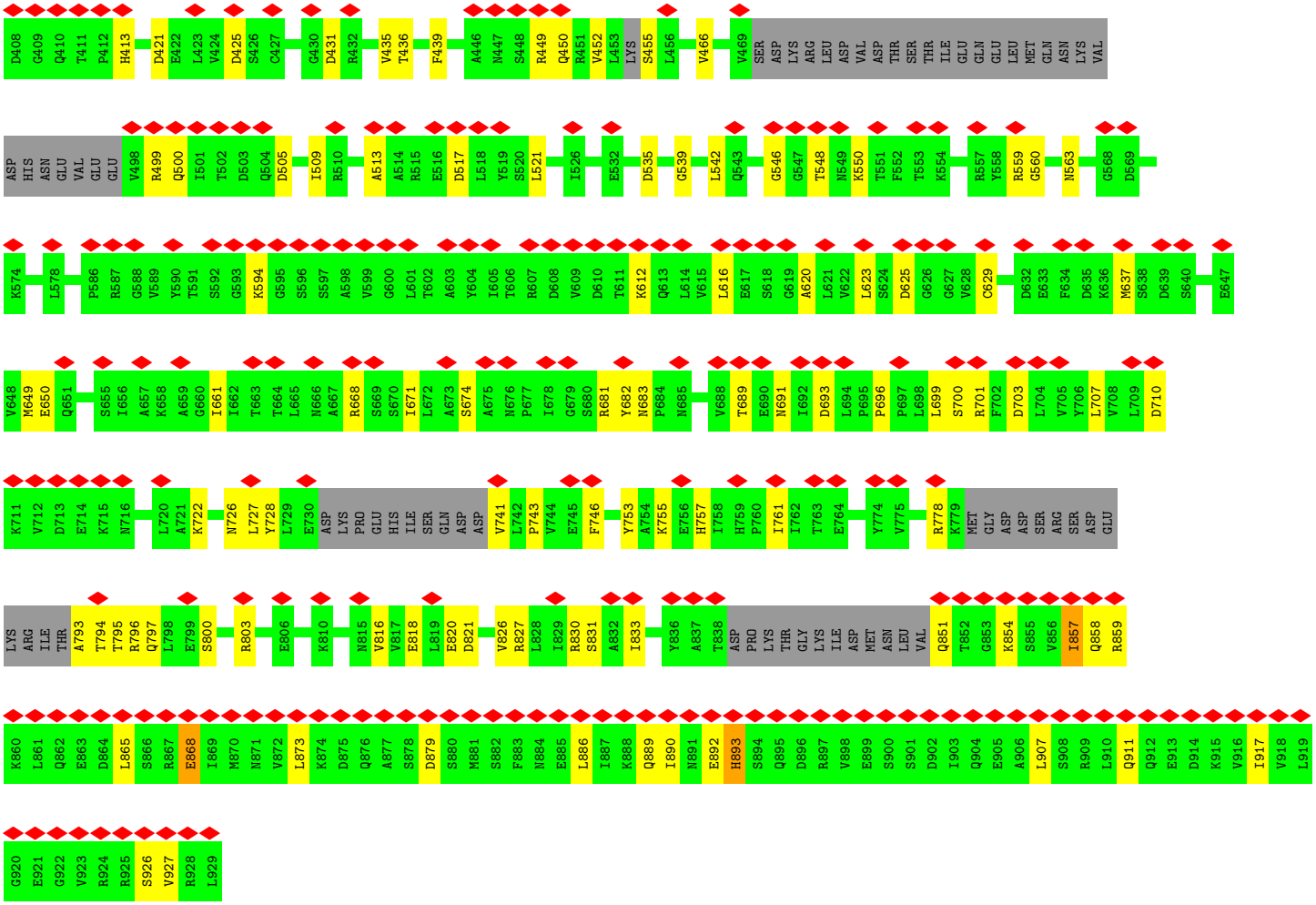
Chain 3:



- Molecule 8: DNA replication licensing factor MCM4

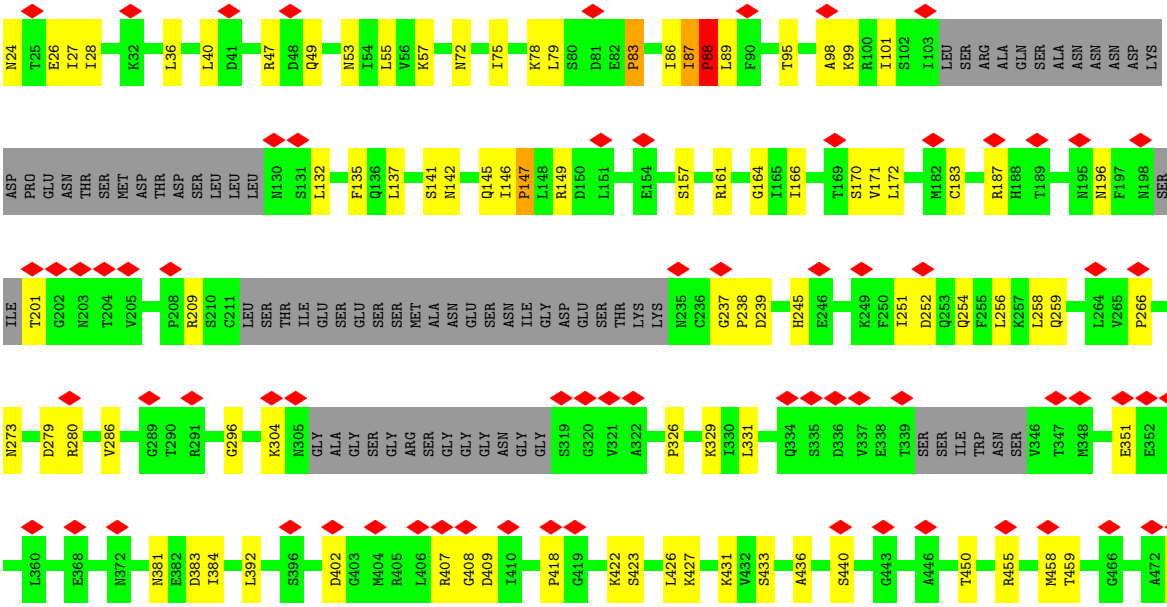
Chain 4:

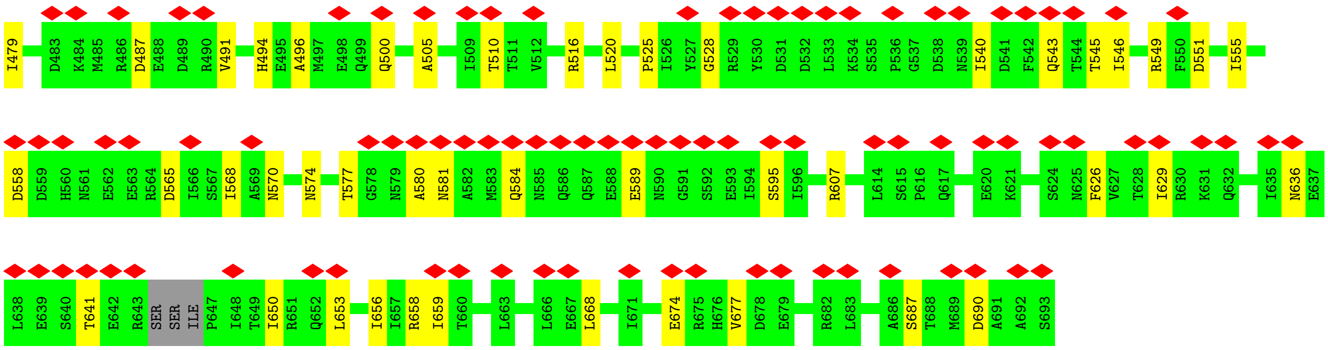




- Molecule 9: Minichromosome maintenance protein 5

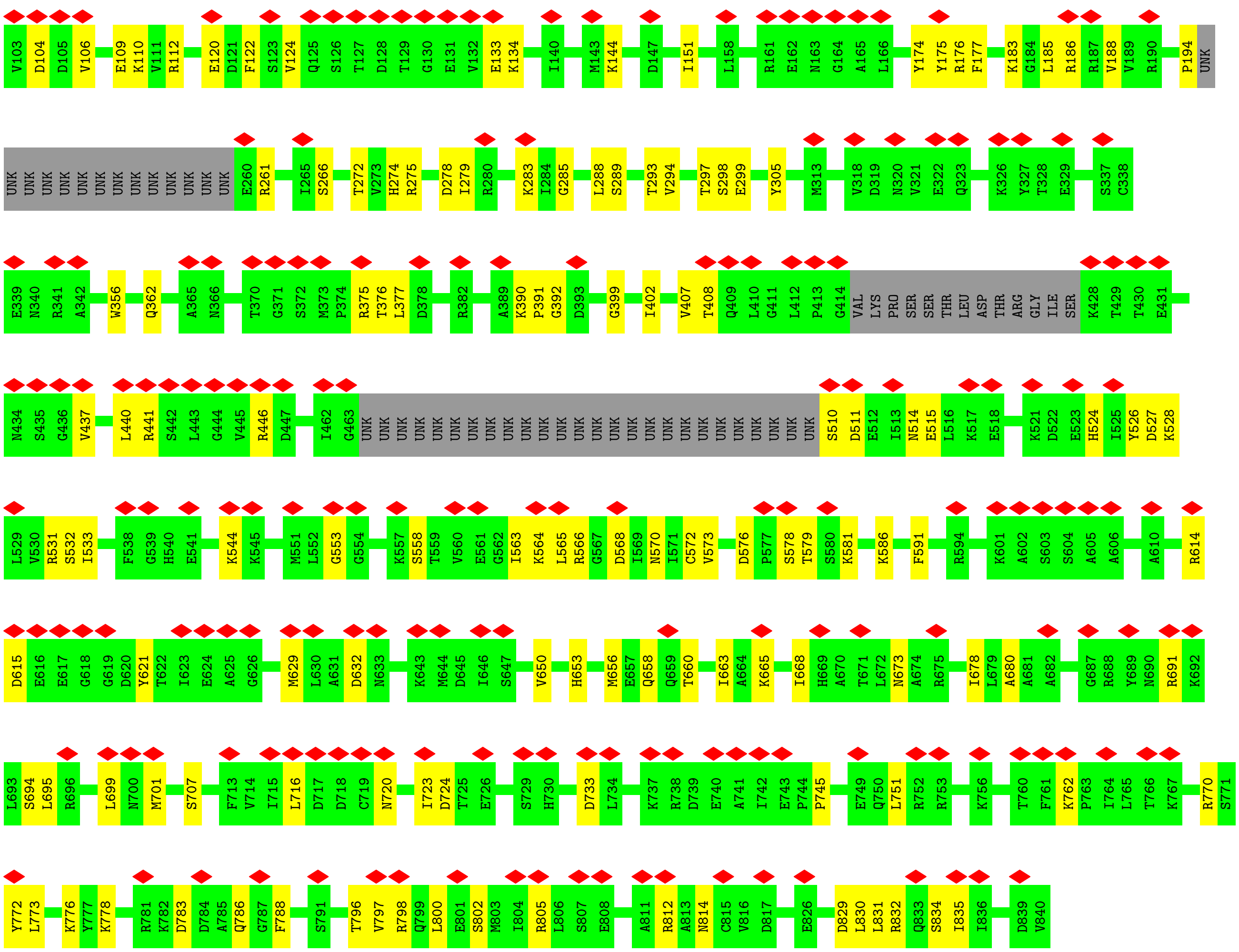
Chain 5:





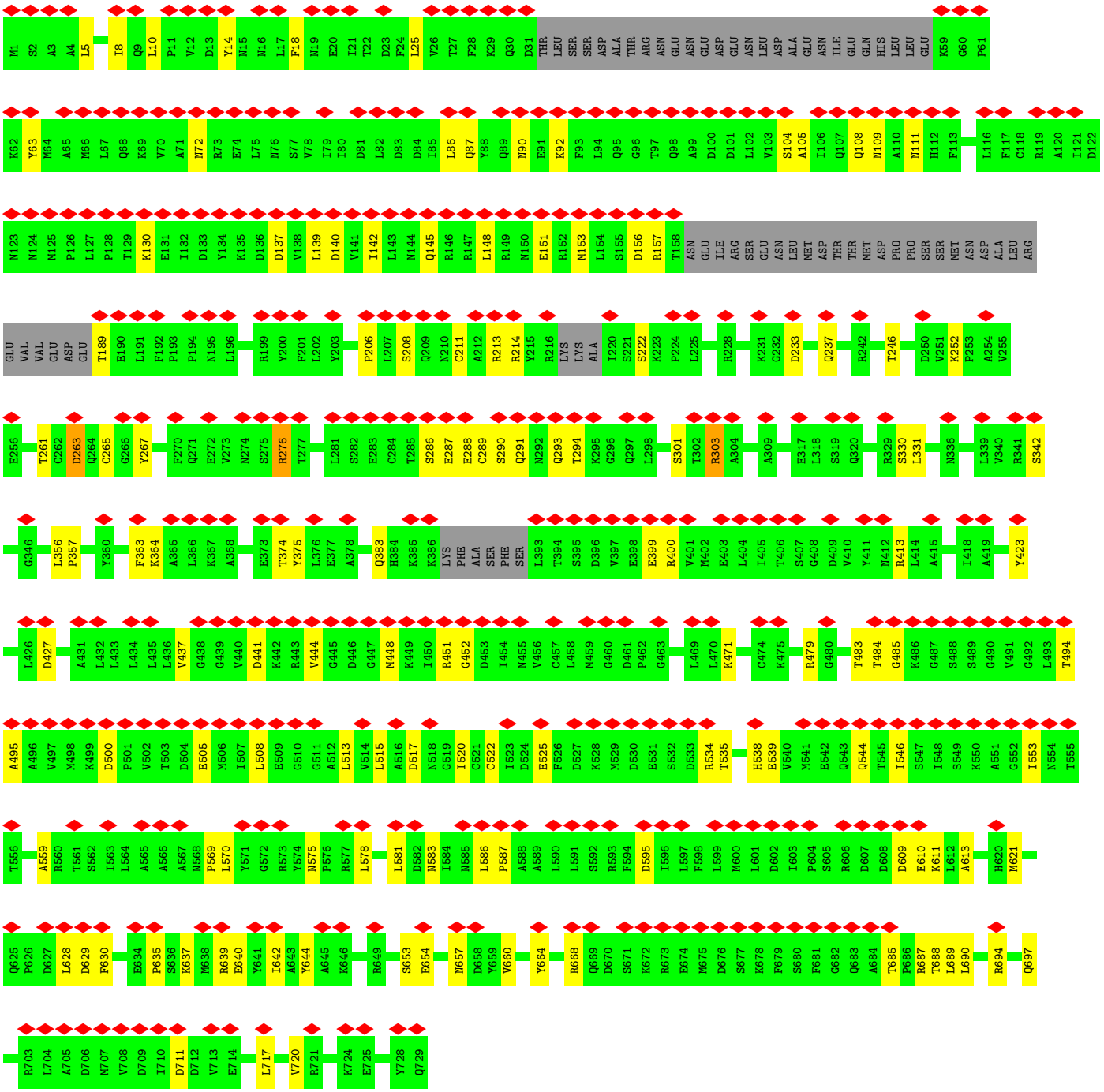
- Molecule 10: DNA replication licensing factor MCM6

Chain 6:



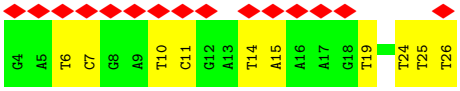
- Molecule 11: DNA replication licensing factor MCM7

Chain 7:



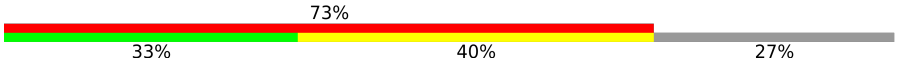
- Molecule 12: DNA (26-MER)

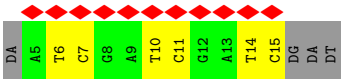
Chain F:



- Molecule 13: DNA (15-MER)

Chain G:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	162550	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	274.944, 274.944, 274.944	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.074, 1.074, 1.074	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.31	0/1712	0.61	2/2307 (0.1%)
2	B	0.32	0/1539	0.57	0/2085
3	C	0.33	0/1320	0.54	0/1784
4	D	0.33	0/1853	0.51	0/2500
5	E	0.33	0/4552	0.59	3/6158 (0.0%)
6	2	0.32	0/5036	0.57	1/6801 (0.0%)
7	3	0.32	0/4733	0.58	0/6418
8	4	0.30	0/5473	0.58	2/7384 (0.0%)
9	5	0.34	0/4724	0.61	3/6381 (0.0%)
10	6	0.32	0/4759	0.58	1/6428 (0.0%)
11	7	0.29	0/5291	0.59	4/7151 (0.1%)
12	F	0.81	4/527 (0.8%)	1.22	0/812
13	G	1.07	6/250 (2.4%)	1.29	0/383
All	All	0.34	10/41769 (0.0%)	0.60	16/56592 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	10	DT	C1'-N1	5.26	1.56	1.49
12	F	6	DT	C1'-N1	5.25	1.56	1.49
12	F	7	DC	C1'-N1	5.23	1.56	1.49
13	G	14	DT	C1'-N1	5.22	1.56	1.49
12	F	10	DT	C1'-N1	5.20	1.56	1.49
12	F	11	DC	C1'-N1	5.18	1.55	1.49
13	G	15	DC	C1'-N1	5.15	1.55	1.49
13	G	11	DC	C1'-N1	5.11	1.55	1.49
13	G	7	DC	C1'-N1	5.09	1.55	1.49
13	G	6	DT	C1'-N1	5.09	1.55	1.49

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	7	263	ASP	CB-CG-OD1	8.71	126.14	118.30
10	6	440	LEU	CA-CB-CG	8.01	133.71	115.30
11	7	628	LEU	CA-CB-CG	7.17	131.79	115.30
9	5	88	PRO	CA-N-CD	-7.10	101.56	111.50
1	A	109	LEU	CA-CB-CG	6.97	131.34	115.30
9	5	668	LEU	CA-CB-CG	6.94	131.26	115.30
8	4	727	LEU	CA-CB-CG	6.82	130.99	115.30
9	5	87	ILE	C-N-CD	-6.60	106.08	120.60
8	4	707	LEU	CA-CB-CG	6.11	129.35	115.30
5	E	328	LEU	CA-CB-CG	5.85	128.76	115.30
11	7	629	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	123	LEU	CA-CB-CG	5.62	128.22	115.30
6	2	416	ASP	CB-CG-OD1	5.57	123.31	118.30
5	E	491	LEU	CA-CB-CG	5.48	127.91	115.30
5	E	580	LEU	CA-CB-CG	5.47	127.87	115.30
11	7	139	LEU	CA-CB-CG	5.35	127.60	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1690	0	1687	41	0
2	B	1507	0	1547	22	0
3	C	1288	0	1298	27	0
4	D	1820	0	1824	33	0
5	E	4472	0	4483	92	0
6	2	4957	0	4968	102	0
7	3	4653	0	4709	93	0
8	4	5404	0	5485	118	0
9	5	4663	0	4709	124	0
10	6	4691	0	4617	88	0
11	7	5212	0	5285	95	0
12	F	472	0	265	13	0
13	G	224	0	125	0	0
14	2	31	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	3	31	0	12	1	0
14	5	31	0	12	4	0
All	All	41146	0	41038	799	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 10.

All (799) 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)
11:7:265:CYS:SG	11:7:288:GLU:CB	2.59	0.90
9:5:87:ILE:HD12	9:5:137:LEU:HD21	1.56	0.86
8:4:865:LEU:HD12	8:4:868:GLU:OE2	1.74	0.85
9:5:87:ILE:HB	9:5:88:PRO:HD2	1.56	0.85
9:5:87:ILE:HG22	9:5:88:PRO:HD3	1.59	0.82
9:5:95:THR:HG22	9:5:135:PHE:HD1	1.42	0.82
11:7:265:CYS:HB2	11:7:289:CYS:HB3	1.63	0.81
10:6:665:LYS:HE2	12:F:25:DT:OP1	1.83	0.78
9:5:87:ILE:HD12	9:5:137:LEU:CD2	2.14	0.77
9:5:79:LEU:HD12	9:5:86:ILE:HG21	1.66	0.77
12:F:24:DT:H2"	12:F:25:DT:H5'	1.67	0.76
9:5:87:ILE:HG23	9:5:137:LEU:CD2	2.19	0.73
9:5:95:THR:HG22	9:5:135:PHE:CD1	2.24	0.72
8:4:873:LEU:CD2	8:4:927:VAL:HG12	2.20	0.71
11:7:265:CYS:HB3	11:7:289:CYS:SG	2.32	0.69
9:5:145:GLN:HE21	9:5:161:ARG:HE	1.40	0.69
11:7:363:PHE:CZ	12:F:15:DA:H2'	2.28	0.68
8:4:873:LEU:HD21	8:4:927:VAL:HG12	1.76	0.68
9:5:166:ILE:HD12	9:5:286:VAL:HG21	1.77	0.67
7:3:304:GLY:HA3	7:3:316:GLY:HA3	1.77	0.67
11:7:265:CYS:SG	11:7:267:TYR:HD2	2.18	0.67
9:5:87:ILE:HG23	9:5:137:LEU:HD21	1.76	0.66
11:7:265:CYS:SG	11:7:267:TYR:CD2	2.87	0.66
3:C:27:LEU:HD23	3:C:29:TYR:H	1.60	0.66
9:5:95:THR:HA	9:5:135:PHE:CE1	2.30	0.66
9:5:137:LEU:HD11	9:5:331:LEU:HD12	1.78	0.66
1:A:86:LEU:HD12	1:A:87:LEU:HD12	1.77	0.65
9:5:88:PRO:HD2	9:5:196:ASN:HD22	1.61	0.65
8:4:681:ARG:HG3	8:4:683:ASN:H	1.62	0.65
9:5:79:LEU:HD12	9:5:86:ILE:CG2	2.27	0.65
6:2:253:LYS:HA	6:2:256:LEU:HB2	1.80	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:6:829:ASP:HA	10:6:832:ARG:HB3	1.79	0.65
8:4:892:GLU:OE1	8:4:892:GLU:HA	1.98	0.64
7:3:390:GLU:HB2	7:3:401:GLY:HA3	1.81	0.63
10:6:407:VAL:HG13	10:6:408:THR:HG23	1.80	0.63
9:5:28:ILE:HD11	9:5:89:LEU:HD12	1.81	0.62
8:4:683:ASN:HD21	8:4:691:ASN:HB2	1.65	0.61
8:4:387:ASN:HD22	10:6:402:ILE:HD11	1.65	0.61
1:A:133:GLU:HG2	4:D:189:ILE:HG12	1.81	0.61
8:4:911:GLN:HE22	8:4:917:ILE:HD12	1.66	0.61
6:2:398:PRO:HB2	6:2:401:ARG:HH21	1.65	0.61
9:5:87:ILE:CB	9:5:88:PRO:CD	2.79	0.60
5:E:375:GLU:HA	5:E:378:LEU:HB2	1.84	0.60
5:E:482:ASP:N	5:E:482:ASP:OD1	2.34	0.60
11:7:451:ARG:O	11:7:694:ARG:NH2	2.35	0.60
11:7:538:HIS:ND1	11:7:539:GLU:OE2	2.35	0.60
10:6:802:SER:HA	10:6:805:ARG:HG2	1.83	0.60
11:7:265:CYS:CB	11:7:289:CYS:HB3	2.30	0.60
6:2:319:ARG:HG3	6:2:427:THR:HG22	1.84	0.60
9:5:87:ILE:HG22	9:5:88:PRO:CD	2.30	0.60
3:C:97:LEU:HD23	3:C:98:HIS:HD2	1.67	0.60
9:5:98:ALA:CB	9:5:135:PHE:CZ	2.85	0.59
9:5:426:LEU:HD11	9:5:520:LEU:HD22	1.83	0.59
5:E:342:ASN:O	5:E:346:ALA:N	2.34	0.59
9:5:87:ILE:CB	9:5:88:PRO:HD2	2.30	0.59
7:3:673:GLN:NE2	11:7:621:MET:SD	2.76	0.59
5:E:7:GLN:HB3	5:E:10:GLU:HG2	1.85	0.58
8:4:455:SER:N	11:7:276:ARG:O	2.36	0.58
8:4:594:LYS:NZ	8:4:637:MET:SD	2.76	0.58
6:2:305:SER:OG	6:2:306:LEU:N	2.37	0.58
6:2:706:SER:O	10:6:762:LYS:NZ	2.36	0.58
8:4:616:LEU:H	10:6:362:GLN:HE22	1.50	0.58
8:4:563:ASN:ND2	8:4:701:ARG:O	2.35	0.58
9:5:88:PRO:HG3	9:5:196:ASN:HB2	1.85	0.58
9:5:172:LEU:HD22	9:5:254:GLN:HE22	1.68	0.58
9:5:88:PRO:CD	9:5:196:ASN:HD22	2.15	0.58
10:6:194:PRO:O	10:6:261:ARG:NH2	2.36	0.58
10:6:441:ARG:HH12	10:6:446:ARG:HB2	1.68	0.58
2:B:99:ASP:O	2:B:103:GLN:NE2	2.37	0.58
5:E:362:MET:SD	5:E:362:MET:N	2.77	0.57
7:3:40:ASP:OD1	7:3:40:ASP:N	2.36	0.57
4:D:72:CYS:O	4:D:226:LYS:NZ	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:5:101:ILE:HG22	9:5:101:ILE:O	2.02	0.57
1:A:164:ASP:OD2	1:A:166:ARG:NH2	2.38	0.57
3:C:5:ASP:HB3	3:C:8:ASP:OD1	2.05	0.57
8:4:560:GLY:HA2	8:4:803:ARG:HD2	1.85	0.57
7:3:39:ARG:NH1	7:3:136:MET:SD	2.77	0.57
7:3:168:PRO:O	7:3:272:ARG:NH2	2.34	0.57
7:3:300:SER:HG	9:5:245:HIS:HD1	1.52	0.57
3:C:24:ILE:HG22	3:C:26:GLY:H	1.70	0.57
8:4:337:PRO:HG3	10:6:375:ARG:HD3	1.87	0.57
1:A:86:LEU:HD12	1:A:87:LEU:CD1	2.34	0.57
8:4:284:ILE:HG23	8:4:290:ASP:HB2	1.87	0.57
10:6:629:MET:SD	10:6:629:MET:N	2.78	0.57
7:3:450:ARG:HB2	7:3:454:GLU:HB2	1.87	0.57
9:5:79:LEU:CD1	9:5:86:ILE:HG21	2.35	0.57
9:5:87:ILE:HB	9:5:88:PRO:CD	2.30	0.57
5:E:493:ASN:O	5:E:497:GLN:NE2	2.38	0.56
3:C:3:TYR:O	4:D:217:ASN:ND2	2.34	0.56
6:2:551:GLN:HE21	10:6:563:ILE:HG12	1.68	0.56
7:3:189:THR:O	7:3:456:ARG:NH2	2.37	0.56
11:7:399:GLU:OE2	11:7:400:ARG:NH2	2.38	0.56
6:2:490:ASP:H	6:2:493:ILE:HD11	1.70	0.56
6:2:604:CYS:SG	6:2:605:LEU:N	2.78	0.56
8:4:450:GLN:HB2	8:4:452:VAL:HG22	1.86	0.56
5:E:85:GLY:HA2	5:E:124:ASP:HA	1.85	0.56
5:E:540:ARG:NH2	5:E:574:GLU:OE1	2.38	0.56
9:5:87:ILE:HG23	9:5:137:LEU:HD23	1.88	0.56
7:3:478:MET:O	7:3:483:ARG:NH1	2.38	0.56
9:5:27:ILE:HD11	9:5:78:LYS:NZ	2.21	0.56
9:5:27:ILE:HD11	9:5:78:LYS:HZ1	1.70	0.56
11:7:657:ASN:HA	11:7:660:VAL:HG22	1.86	0.56
6:2:222:THR:OG1	6:2:224:ARG:NH2	2.39	0.56
7:3:119:ALA:HA	7:3:221:LEU:HD22	1.88	0.56
8:4:192:THR:O	8:4:196:ASN:ND2	2.39	0.56
9:5:95:THR:HA	9:5:135:PHE:HE1	1.70	0.56
7:3:400:ARG:NH1	7:3:490:MET:O	2.38	0.56
10:6:527:ASP:OD2	10:6:531:ARG:NH1	2.39	0.56
5:E:561:ASP:N	5:E:561:ASP:OD1	2.38	0.55
6:2:347:ILE:HD11	6:2:376:ASN:HD21	1.72	0.55
6:2:356:ASN:O	6:2:433:ASN:ND2	2.39	0.55
6:2:689:GLU:O	10:6:778:LYS:NZ	2.38	0.55
9:5:392:LEU:O	9:5:607:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:4:873:LEU:HD13	8:4:927:VAL:CG1	2.36	0.55
6:2:843:ASP:OD1	6:2:843:ASP:N	2.40	0.55
5:E:5:ILE:N	5:E:144:ASP:O	2.39	0.55
6:2:465:ASN:ND2	6:2:468:GLU:O	2.38	0.55
8:4:180:ILE:HG22	8:4:182:GLY:H	1.72	0.55
8:4:873:LEU:CD1	8:4:927:VAL:CG1	2.85	0.55
1:A:52:GLU:HA	1:A:55:LYS:HB2	1.88	0.55
3:C:131:ARG:NH1	3:C:173:GLU:OE1	2.40	0.55
5:E:333:SER:HB2	5:E:377:TRP:CZ3	2.41	0.55
5:E:387:GLU:O	5:E:391:ILE:N	2.39	0.55
6:2:625:GLU:OE2	9:5:422:LYS:NZ	2.39	0.55
1:A:167:VAL:HG21	1:A:183:LEU:HD11	1.88	0.55
8:4:851:GLN:HE21	8:4:857:ILE:HD13	1.71	0.55
5:E:382:HIS:O	5:E:386:ARG:NE	2.30	0.55
5:E:532:ASP:OD2	6:2:780:GLN:NE2	2.38	0.55
6:2:341:CYS:SG	6:2:342:LEU:N	2.80	0.55
7:3:275:ASP:OD1	7:3:275:ASP:N	2.38	0.55
8:4:256:ASP:N	8:4:256:ASP:OD1	2.40	0.55
10:6:526:TYR:HB2	10:6:814:ASN:HD21	1.70	0.55
4:D:152:ASP:N	4:D:152:ASP:OD1	2.40	0.55
6:2:643:ARG:HH12	9:5:266:PRO:HB2	1.71	0.55
6:2:676:ARG:HA	6:2:808:ARG:HH22	1.72	0.55
5:E:68:ARG:NH1	5:E:95:PHE:O	2.41	0.54
7:3:216:ASP:OD1	7:3:216:ASP:N	2.40	0.54
7:3:685:ASP:N	7:3:685:ASP:OD2	2.40	0.54
9:5:496:ALA:O	9:5:500:GLN:NE2	2.40	0.54
2:B:99:ASP:OD1	2:B:99:ASP:N	2.39	0.54
6:2:321:THR:OG1	6:2:322:GLY:N	2.39	0.54
8:4:320:ASN:O	8:4:324:LYS:NZ	2.40	0.54
8:4:873:LEU:CD2	8:4:927:VAL:CG1	2.86	0.54
9:5:28:ILE:HD11	9:5:89:LEU:CD1	2.37	0.54
5:E:76:ASP:OD1	5:E:76:ASP:N	2.39	0.54
5:E:345:ASN:O	5:E:349:SER:N	2.40	0.54
10:6:106:VAL:O	10:6:110:LYS:N	2.40	0.54
10:6:275:ARG:NH1	10:6:278:ASP:OD2	2.40	0.54
10:6:288:LEU:H	10:6:399:GLY:HA3	1.72	0.54
5:E:388:LEU:HA	5:E:391:ILE:HB	1.89	0.54
6:2:656:ARG:HE	6:2:684:ARG:HD3	1.73	0.54
8:4:246:ARG:NH1	8:4:307:ASN:O	2.40	0.54
9:5:146:ILE:HD12	9:5:147:PRO:HD2	1.89	0.54
10:6:298:SER:OG	10:6:299:GLU:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:6:510:SER:O	10:6:514:ASN:ND2	2.40	0.54
11:7:148:LEU:HA	11:7:151:GLU:HB2	1.89	0.54
1:A:140:ASP:O	1:A:144:GLY:N	2.39	0.54
5:E:297:ASP:OD1	5:E:297:ASP:N	2.41	0.54
5:E:327:PHE:O	5:E:340:TYR:OH	2.21	0.54
5:E:407:ASP:N	5:E:407:ASP:OD1	2.41	0.54
8:4:344:VAL:HG13	8:4:389:CYS:HB2	1.90	0.54
9:5:79:LEU:HA	9:5:86:ILE:HG13	1.90	0.54
10:6:144:LYS:NZ	10:6:194:PRO:O	2.39	0.54
8:4:778:ARG:NH2	8:4:793:ALA:O	2.41	0.54
9:5:49:GLN:O	9:5:53:ASN:ND2	2.40	0.54
5:E:416:ARG:HH21	9:5:40:LEU:HB2	1.72	0.54
5:E:537:ASP:OD1	5:E:537:ASP:N	2.40	0.54
7:3:57:ASN:OD1	11:7:213:ARG:NH1	2.41	0.54
8:4:499:ARG:NH2	8:4:500:GLN:O	2.41	0.54
1:A:35:ASP:OD1	1:A:35:ASP:N	2.40	0.54
1:A:46:ASN:O	1:A:50:ASN:ND2	2.41	0.54
2:B:147:ASP:OD1	2:B:147:ASP:N	2.39	0.54
5:E:282:ILE:O	5:E:587:ARG:NH1	2.41	0.54
7:3:46:GLN:NE2	7:3:137:ASP:OD2	2.41	0.54
7:3:447:THR:O	7:3:450:ARG:NE	2.38	0.54
8:4:371:CYS:SG	8:4:372:GLU:N	2.79	0.54
10:6:570:ASN:ND2	10:6:656:MET:SD	2.77	0.54
11:7:479:ARG:NH2	11:7:515:LEU:O	2.41	0.54
3:C:175:GLU:O	3:C:179:LYS:NZ	2.41	0.54
8:4:693:ASP:N	8:4:693:ASP:OD1	2.40	0.54
8:4:722:LYS:O	8:4:726:ASN:ND2	2.41	0.54
10:6:831:LEU:O	10:6:835:ILE:N	2.41	0.54
4:D:250:GLU:HA	4:D:256:TYR:HB2	1.89	0.53
7:3:282:LEU:HD13	7:3:326:VAL:H	1.72	0.53
11:7:153:MET:HA	11:7:156:ASP:HB2	1.90	0.53
5:E:524:ILE:HA	5:E:563:GLN:HE22	1.73	0.53
8:4:873:LEU:HD22	8:4:927:VAL:CG1	2.37	0.53
9:5:141:SER:O	9:5:161:ARG:NH1	2.42	0.53
10:6:174:TYR:HA	10:6:177:PHE:HB2	1.90	0.53
6:2:247:ARG:HH12	6:2:738:LEU:HG	1.71	0.53
8:4:753:TYR:O	8:4:757:HIS:ND1	2.39	0.53
9:5:83:PRO:HG3	9:5:157:SER:HB2	1.90	0.53
9:5:383:ASP:OD1	9:5:383:ASP:N	2.41	0.53
1:A:128:GLN:HG2	1:A:131:LEU:HD23	1.90	0.53
9:5:427:LYS:O	9:5:431:LYS:NZ	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:7:86:LEU:O	11:7:90:ASN:N	2.41	0.53
1:A:85:CYS:SG	1:A:86:LEU:N	2.82	0.53
1:A:150:ASP:OD1	4:D:141:ARG:NH1	2.42	0.53
5:E:148:VAL:O	5:E:151:THR:OG1	2.26	0.53
9:5:458:MET:HG3	9:5:459:THR:HG23	1.91	0.53
10:6:691:ARG:HH12	10:6:716:LEU:HB2	1.73	0.53
10:6:124:VAL:HG21	10:6:133:GLU:HA	1.91	0.53
6:2:340:ASN:ND2	6:2:346:SER:O	2.41	0.53
6:2:790:TYR:OH	6:2:794:ARG:NH2	2.42	0.53
5:E:81:LEU:HB3	5:E:120:ILE:HG22	1.91	0.53
9:5:402:ASP:OD1	9:5:402:ASP:N	2.42	0.53
6:2:212:LYS:HG2	6:2:216:LEU:HD13	1.91	0.52
10:6:632:ASP:OD1	10:6:632:ASP:N	2.39	0.52
8:4:259:HIS:O	8:4:263:ASN:ND2	2.42	0.52
10:6:572:CYS:SG	10:6:573:VAL:N	2.82	0.52
7:3:20:VAL:O	7:3:24:ARG:NE	2.41	0.52
5:E:543:LEU:HD13	5:E:546:LEU:HD21	1.92	0.52
7:3:300:SER:OG	9:5:245:HIS:ND1	2.41	0.52
7:3:723:LYS:O	7:3:727:LYS:NZ	2.42	0.52
9:5:570:ASN:O	9:5:574:ASN:ND2	2.42	0.52
10:6:783:ASP:O	10:6:786:GLN:NE2	2.42	0.52
6:2:519:LEU:O	6:2:771:ARG:NH1	2.43	0.52
7:3:212:ARG:HH21	11:7:5:LEU:HD21	1.72	0.52
8:4:373:ARG:O	8:4:373:ARG:NH2	2.39	0.52
8:4:625:ASP:OD1	8:4:625:ASP:N	2.40	0.52
8:4:800:SER:HA	8:4:803:ARG:HG3	1.90	0.52
6:2:685:ASP:N	6:2:685:ASP:OD1	2.40	0.52
7:3:669:PRO:HB2	7:3:721:VAL:HG23	1.92	0.52
9:5:137:LEU:C	9:5:137:LEU:HD12	2.30	0.52
9:5:494:HIS:O	9:5:549:ARG:NH2	2.43	0.52
1:A:31:MET:O	1:A:93:ARG:NH2	2.42	0.52
1:A:32:TYR:HB2	1:A:123:LEU:HG	1.91	0.52
1:A:32:TYR:OH	1:A:90:GLN:NE2	2.41	0.52
1:A:175:GLN:HG3	1:A:181:PHE:HD2	1.75	0.52
2:B:150:GLU:O	2:B:154:ILE:N	2.42	0.52
5:E:533:GLY:O	6:2:780:GLN:NE2	2.43	0.52
10:6:294:VAL:HG13	10:6:392:GLY:H	1.75	0.52
12:F:14:DT:H2”	12:F:15:DA:H5”	1.92	0.52
12:F:25:DT:H2”	12:F:26:DT:H5’	1.91	0.52
8:4:425:ASP:OD1	10:6:375:ARG:NH2	2.43	0.52
10:6:658:GLN:NE2	10:6:660:THR:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:LYS:O	2:B:100:ARG:NH1	2.43	0.52
6:2:693:GLU:HA	6:2:696:ALA:HB3	1.92	0.52
7:3:201:HIS:ND1	7:3:243:THR:OG1	2.41	0.52
9:5:137:LEU:CD1	9:5:331:LEU:HD12	2.39	0.52
7:3:33:ASP:HA	7:3:36:THR:HG23	1.91	0.52
7:3:195:LYS:N	7:3:251:ILE:O	2.43	0.52
3:C:97:LEU:HD22	3:C:131:ARG:HH22	1.76	0.51
4:D:170:SER:HA	4:D:174:LEU:HD23	1.90	0.51
6:2:520:PHE:HE1	6:2:767:ILE:HD12	1.75	0.51
5:E:501:ASP:N	5:E:501:ASP:OD1	2.41	0.51
2:B:10:THR:HG21	2:B:183:PRO:HB3	1.91	0.51
5:E:639:PRO:O	5:E:643:LYS:NZ	2.42	0.51
7:3:252:ASP:N	7:3:252:ASP:OD1	2.43	0.51
7:3:523:TYR:OH	7:3:532:ASN:O	2.28	0.51
11:7:265:CYS:HB2	11:7:289:CYS:CB	2.35	0.51
7:3:349:ASN:O	7:3:353:LEU:N	2.43	0.51
8:4:353:ASP:OD1	8:4:353:ASP:N	2.43	0.51
1:A:128:GLN:HA	1:A:131:LEU:HB3	1.91	0.51
9:5:88:PRO:CG	9:5:196:ASN:HB2	2.40	0.51
9:5:525:PRO:HG2	9:5:528:GLY:HA2	1.92	0.51
7:3:220:THR:HG22	7:3:322:LEU:HD22	1.92	0.51
8:4:649:MET:HG2	8:4:701:ARG:HB3	1.91	0.51
8:4:793:ALA:O	8:4:797:GLN:NE2	2.43	0.51
8:4:827:ARG:O	8:4:827:ARG:NH2	2.43	0.51
10:6:566:ARG:NH1	10:6:656:MET:O	2.44	0.51
5:E:73:GLN:HG2	5:E:74:LEU:HG	1.93	0.51
5:E:86:PHE:N	5:E:124:ASP:OD2	2.44	0.51
11:7:717:LEU:HA	11:7:720:VAL:HG12	1.93	0.51
8:4:701:ARG:HA	8:4:796:ARG:HH11	1.75	0.51
8:4:826:VAL:HB	8:4:830:ARG:HH21	1.76	0.51
8:4:830:ARG:HD3	8:4:833:ILE:HD11	1.92	0.51
9:5:259:GLN:NE2	9:5:272:ARG:O	2.42	0.51
9:5:423:SER:OG	14:5:801:ATP:O2B	2.29	0.51
11:7:664:TYR:OH	11:7:668:ARG:NH2	2.44	0.51
9:5:55:LEU:O	9:5:57:LYS:NZ	2.39	0.51
10:6:796:THR:OG1	10:6:797:VAL:N	2.44	0.51
11:7:427:ASP:N	11:7:427:ASP:OD1	2.43	0.51
4:D:176:SER:OG	4:D:177:LYS:N	2.44	0.51
5:E:577:ASP:OD2	5:E:633:ARG:NH1	2.44	0.51
6:2:607:ASP:OD1	6:2:607:ASP:N	2.35	0.51
9:5:581:ASN:HA	9:5:584:GLN:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:7:342:SER:O	11:7:383:GLN:NE2	2.44	0.50
5:E:516:LYS:HB3	5:E:518:LEU:HG	1.93	0.50
6:2:337:VAL:HB	6:2:351:PHE:HB2	1.93	0.50
7:3:384:MET:HG2	7:3:403:ILE:HG23	1.93	0.50
8:4:197:PHE:HZ	8:4:247:ASN:HB3	1.76	0.50
9:5:142:ASN:N	9:5:142:ASN:OD1	2.44	0.50
9:5:551:ASP:OD1	9:5:551:ASP:N	2.43	0.50
8:4:224:LEU:HD23	8:4:227:ILE:HG12	1.94	0.50
8:4:559:ARG:O	8:4:803:ARG:NH1	2.45	0.50
4:D:69:ASN:N	4:D:69:ASN:OD1	2.45	0.50
4:D:79:TYR:HB2	4:D:147:ARG:HH22	1.77	0.50
4:D:232:VAL:HA	4:D:291:VAL:HG23	1.93	0.50
6:2:435:ASP:OD1	6:2:435:ASP:N	2.42	0.50
7:3:518:PRO:HA	7:3:533:ILE:HD13	1.94	0.50
8:4:338:VAL:HG23	8:4:394:LYS:H	1.75	0.50
8:4:728:TYR:OH	11:7:697:GLN:OE1	2.29	0.50
10:6:699:LEU:HD12	10:6:701:MET:H	1.76	0.50
11:7:87:GLN:HA	11:7:90:ASN:HB2	1.94	0.50
3:C:21:GLN:NE2	3:C:70:PRO:O	2.45	0.50
6:2:653:ASN:O	6:2:658:ASN:ND2	2.44	0.50
7:3:537:ASP:N	7:3:537:ASP:OD1	2.43	0.50
7:3:544:ASP:OD1	7:3:544:ASP:N	2.42	0.50
11:7:233:ASP:O	11:7:237:GLN:NE2	2.44	0.50
5:E:24:SER:HA	5:E:26:GLN:HE21	1.76	0.50
9:5:28:ILE:CG1	9:5:89:LEU:HD12	2.42	0.50
11:7:363:PHE:HZ	12:F:15:DA:H2'	1.76	0.50
7:3:668:ILE:HB	7:3:670:GLN:HE22	1.75	0.50
8:4:696:PRO:HA	8:4:699:LEU:HD13	1.92	0.50
8:4:827:ARG:HH22	8:4:831:SER:HB3	1.76	0.50
6:2:605:LEU:HG	6:2:649:ALA:HB3	1.94	0.50
6:2:740:ALA:HA	6:2:743:ARG:HB2	1.94	0.50
9:5:674:GLU:HA	9:5:677:VAL:HG12	1.93	0.50
10:6:591:PHE:HZ	10:6:751:LEU:HD22	1.77	0.50
1:A:23:SER:OG	1:A:24:ASN:N	2.45	0.49
7:3:169:ARG:HA	7:3:272:ARG:HE	1.77	0.49
8:4:431:ASP:OD1	8:4:431:ASP:N	2.45	0.49
8:4:794:THR:OG1	8:4:795:THR:N	2.45	0.49
11:7:544:GLN:OE1	11:7:559:ALA:N	2.43	0.49
5:E:323:ASP:OD1	5:E:330:ARG:NH2	2.45	0.49
5:E:488:LYS:HD3	5:E:491:LEU:HB3	1.94	0.49
6:2:630:SER:HB2	6:2:639:THR:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:4:237:GLY:O	8:4:299:LYS:NZ	2.45	0.49
10:6:109:GLU:OE1	10:6:112:ARG:NH2	2.45	0.49
1:A:89:TYR:OH	1:A:93:ARG:NH2	2.45	0.49
6:2:221:GLU:OE2	6:2:742:GLN:NE2	2.45	0.49
6:2:245:ASN:HD22	6:2:248:HIS:HD2	1.60	0.49
6:2:606:ILE:HA	6:2:609:PHE:HE1	1.78	0.49
1:A:54:LEU:O	1:A:72:TYR:OH	2.29	0.49
4:D:75:GLU:OE2	4:D:283:ARG:NH2	2.40	0.49
5:E:434:VAL:HB	5:E:498:LEU:HD11	1.94	0.49
7:3:686:LEU:HA	7:3:689:ASP:HB2	1.94	0.49
8:4:818:GLU:HG3	8:4:821:ASP:H	1.77	0.49
9:5:98:ALA:CB	9:5:135:PHE:HZ	2.25	0.49
11:7:301:SER:OG	11:7:303:ARG:NH1	2.45	0.49
1:A:125:HIS:HA	1:A:128:GLN:HB2	1.94	0.49
5:E:491:LEU:HA	5:E:494:ARG:HG3	1.93	0.49
5:E:493:ASN:HA	5:E:496:ILE:HD12	1.93	0.49
7:3:528:ASP:HB2	7:3:531:GLN:HE21	1.77	0.49
5:E:29:ILE:HG22	5:E:82:LEU:HB3	1.95	0.49
7:3:343:THR:OG1	7:3:344:ASP:N	2.45	0.49
5:E:500:GLN:O	5:E:504:ARG:NH2	2.45	0.49
6:2:211:LEU:HD11	6:2:274:VAL:HG11	1.93	0.49
9:5:440:SER:HA	9:5:479:ILE:HA	1.95	0.49
11:7:437:VAL:HG23	11:7:642:ILE:HG23	1.94	0.49
3:C:58:GLY:HA2	3:C:70:PRO:HA	1.93	0.49
6:2:384:ASN:OD1	6:2:384:ASN:N	2.41	0.49
1:A:140:ASP:N	1:A:140:ASP:OD1	2.43	0.49
1:A:164:ASP:OD1	1:A:188:GLN:NE2	2.32	0.49
4:D:73:SER:OG	4:D:75:GLU:O	2.30	0.49
6:2:231:ILE:HD11	6:2:279:THR:HB	1.94	0.49
7:3:121:PHE:HA	7:3:124:PRO:HG2	1.94	0.49
7:3:193:ARG:NH2	7:3:454:GLU:OE2	2.39	0.49
11:7:687:ARG:HD3	11:7:690:LEU:HD21	1.95	0.49
6:2:782:ASP:OD1	6:2:782:ASP:N	2.42	0.49
9:5:407:ARG:O	9:5:658:ARG:NH1	2.45	0.49
2:B:14:GLU:O	2:B:17:GLN:NE2	2.39	0.48
2:B:187:GLU:HA	2:B:190:ASP:HB3	1.95	0.48
5:E:132:ASP:N	5:E:132:ASP:OD1	2.45	0.48
11:7:451:ARG:NE	11:7:452:GLY:O	2.45	0.48
12:F:24:DT:OP2	12:F:24:DT:H6	1.95	0.48
1:A:84:ARG:NH2	4:D:217:ASN:OD1	2.47	0.48
5:E:134:ILE:O	5:E:137:SER:OG	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:439:ASN:OD1	6:2:439:ASN:N	2.45	0.48
7:3:27:ARG:NH1	7:3:110:PHE:O	2.45	0.48
7:3:281:ASP:OD1	7:3:281:ASP:N	2.45	0.48
8:4:761:ILE:HG22	8:4:816:VAL:HG12	1.94	0.48
11:7:413:ARG:HG3	11:7:630:PHE:HE1	1.78	0.48
3:C:86:ASN:OD1	3:C:86:ASN:N	2.38	0.48
5:E:351:TRP:NE1	5:E:515:GLU:OE2	2.43	0.48
6:2:341:CYS:H	6:2:346:SER:HA	1.78	0.48
9:5:137:LEU:HD11	9:5:331:LEU:CD1	2.42	0.48
10:6:558:SER:HB3	10:6:565:LEU:HD23	1.94	0.48
11:7:293:GLN:NE2	11:7:294:THR:OG1	2.46	0.48
11:7:484:THR:OG1	11:7:525:GLU:OE1	2.29	0.48
9:5:273:ASN:OD1	9:5:273:ASN:N	2.46	0.48
11:7:330:SER:OG	11:7:331:LEU:N	2.46	0.48
1:A:80:GLU:HA	1:A:83:LYS:HB3	1.95	0.48
6:2:686:LEU:HD11	10:6:788:PHE:HA	1.95	0.48
7:3:134:ASP:OD1	7:3:134:ASP:N	2.47	0.48
1:A:106:GLY:HA2	1:A:110:MET:HB2	1.95	0.48
2:B:12:SER:OG	2:B:15:GLU:OE1	2.29	0.48
6:2:441:LYS:HE3	10:6:356:TRP:HH2	1.78	0.48
8:4:548:THR:O	8:4:550:LYS:NZ	2.46	0.48
9:5:36:LEU:HB2	9:5:47:ARG:HH11	1.79	0.48
10:6:733:ASP:N	10:6:733:ASP:OD2	2.47	0.48
2:B:10:THR:HG22	2:B:182:ARG:HD2	1.94	0.48
8:4:682:TYR:OH	8:4:710:ASP:N	2.47	0.48
5:E:366:MET:HG3	6:2:289:ILE:HD12	1.96	0.48
7:3:417:GLN:HE22	7:3:420:ARG:HH12	1.60	0.48
9:5:407:ARG:HA	9:5:407:ARG:HD2	1.69	0.48
4:D:79:TYR:OH	4:D:84:MET:SD	2.69	0.48
8:4:620:ALA:HA	8:4:623:LEU:HB2	1.96	0.48
9:5:87:ILE:CG2	9:5:88:PRO:CD	2.92	0.48
9:5:543:GLN:HB2	9:5:545:THR:HG22	1.95	0.48
6:2:466:GLU:OE1	6:2:741:ARG:NH1	2.44	0.47
4:D:98:ILE:HA	4:D:101:ILE:HG22	1.95	0.47
8:4:184:ASN:ND2	8:4:264:TYR:OH	2.47	0.47
8:4:341:ASP:N	8:4:341:ASP:OD1	2.44	0.47
8:4:517:ASP:O	8:4:521:LEU:N	2.45	0.47
10:6:104:ASP:OD2	10:6:176:ARG:NH1	2.46	0.47
11:7:8:ILE:HG13	11:7:10:LEU:HG	1.96	0.47
11:7:685:THR:HG23	11:7:688:THR:H	1.78	0.47
4:D:159:ARG:O	4:D:163:GLU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:246:TYR:HA	6:2:249:LEU:HB3	1.96	0.47
6:2:614:ASP:OD1	6:2:614:ASP:N	2.35	0.47
6:2:675:SER:O	6:2:808:ARG:NH2	2.48	0.47
8:4:304:ARG:NH2	8:4:421:ASP:OD2	2.47	0.47
9:5:487:ASP:OD1	9:5:487:ASP:N	2.46	0.47
5:E:326:LEU:HD22	5:E:337:SER:HB2	1.95	0.47
5:E:420:SER:OG	5:E:421:ALA:N	2.48	0.47
11:7:441:ASP:N	11:7:441:ASP:OD1	2.43	0.47
3:C:168:LYS:HA	3:C:171:GLU:HB2	1.97	0.47
4:D:161:LEU:HD21	4:D:168:LEU:HB3	1.96	0.47
7:3:494:THR:OG1	7:3:495:VAL:N	2.48	0.47
9:5:505:ALA:HA	9:5:510:THR:HG22	1.96	0.47
9:5:555:ILE:HD12	9:5:690:ASP:HB2	1.96	0.47
10:6:832:ARG:HA	10:6:835:ILE:HG22	1.97	0.47
11:7:105:ALA:HA	11:7:108:GLN:HB2	1.97	0.47
11:7:485:GLY:N	11:7:525:GLU:OE1	2.46	0.47
5:E:89:VAL:HG23	5:E:90:ILE:HD12	1.97	0.47
8:4:436:THR:O	8:4:436:THR:OG1	2.32	0.47
9:5:209:ARG:HH21	9:5:239:ASP:HA	1.79	0.47
10:6:553:GLY:O	10:6:812:ARG:NH1	2.46	0.47
5:E:246:THR:OG1	5:E:247:VAL:N	2.48	0.47
6:2:245:ASN:HD21	6:2:247:ARG:HB2	1.80	0.47
6:2:339:PHE:HB2	6:2:348:LEU:HB2	1.95	0.47
6:2:498:ILE:HD12	6:2:513:THR:HG22	1.97	0.47
9:5:196:ASN:OD1	9:5:329:LYS:NZ	2.47	0.47
9:5:409:ASP:O	9:5:658:ARG:NH1	2.47	0.47
11:7:479:ARG:NE	11:7:517:ASP:O	2.46	0.47
11:7:581:LEU:HD21	11:7:587:PRO:HB3	1.97	0.47
2:B:57:ASP:OD1	2:B:57:ASP:N	2.47	0.47
4:D:288:ASP:OD1	4:D:288:ASP:N	2.39	0.47
6:2:548:ALA:HB2	14:2:901:ATP:C5	2.50	0.47
7:3:202:TYR:N	7:3:242:THR:O	2.48	0.47
8:4:505:ASP:N	8:4:505:ASP:OD1	2.41	0.47
8:4:700:SER:OG	8:4:701:ARG:NH1	2.48	0.46
11:7:104:SER:O	11:7:108:GLN:N	2.44	0.46
5:E:370:LEU:HA	5:E:373:ALA:HB2	1.98	0.46
5:E:503:GLN:HA	5:E:506:ILE:HG22	1.97	0.46
9:5:687:SER:O	9:5:687:SER:OG	2.32	0.46
10:6:797:VAL:HA	10:6:800:LEU:HD23	1.98	0.46
11:7:286:SER:N	11:7:290:SER:OG	2.48	0.46
11:7:640:GLU:O	11:7:644:TYR:N	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:88:LEU:HD23	4:D:91:ILE:HD11	1.96	0.46
6:2:411:LEU:HD23	6:2:411:LEU:HA	1.77	0.46
6:2:578:ALA:HA	6:2:593:GLY:HA2	1.97	0.46
7:3:404:ASN:OD1	7:3:404:ASN:N	2.49	0.46
10:6:830:LEU:O	10:6:834:SER:OG	2.31	0.46
3:C:80:PHE:HE1	3:C:100:ILE:HB	1.81	0.46
6:2:344:CYS:SG	6:2:345:GLY:N	2.86	0.46
6:2:676:ARG:NH1	14:5:801:ATP:O1B	2.48	0.46
8:4:354:HIS:NE2	8:4:372:GLU:OE2	2.43	0.46
3:C:21:GLN:NE2	3:C:72:VAL:O	2.49	0.46
8:4:308:VAL:O	8:4:327:ASN:ND2	2.48	0.46
11:7:72:ASN:HA	11:7:130:LYS:HD3	1.96	0.46
1:A:98:ASP:OD1	1:A:98:ASP:N	2.48	0.46
2:B:79:LEU:O	2:B:82:GLN:NE2	2.37	0.46
4:D:199:LEU:HD22	4:D:202:MET:HB2	1.97	0.46
4:D:257:THR:OG1	4:D:268:GLU:OE2	2.33	0.46
5:E:38:ALA:HA	5:E:251:ILE:HD11	1.97	0.46
9:5:580:ALA:O	9:5:584:GLN:N	2.48	0.46
4:D:166:ASN:OD1	4:D:166:ASN:N	2.49	0.46
6:2:501:MET:O	6:2:760:GLN:NE2	2.48	0.46
5:E:354:ASN:HA	5:E:357:LYS:HE2	1.97	0.46
9:5:381:ASN:HD21	9:5:384:ILE:HD12	1.80	0.46
10:6:724:ASP:OD1	10:6:724:ASP:N	2.48	0.46
6:2:325:THR:OG1	6:2:326:ARG:N	2.49	0.46
7:3:96:ILE:HD11	7:3:153:TRP:HE3	1.81	0.46
7:3:551:ASP:OD1	7:3:551:ASP:N	2.48	0.46
9:5:565:ASP:HA	9:5:568:ILE:HD12	1.98	0.46
11:7:374:THR:OG1	11:7:375:TYR:N	2.48	0.46
7:3:202:TYR:HA	7:3:209:PHE:HA	1.98	0.46
9:5:558:ASP:OD1	9:5:558:ASP:N	2.44	0.46
10:6:376:THR:OG1	10:6:377:LEU:N	2.49	0.46
2:B:22:ASN:OD1	4:D:135:ARG:NH1	2.49	0.45
7:3:435:ARG:NE	7:3:436:GLY:H	2.15	0.45
9:5:251:ILE:HA	9:5:280:ARG:HE	1.81	0.45
11:7:137:ASP:HB3	11:7:140:ASP:HB2	1.97	0.45
5:E:15:ILE:HD11	5:E:80:SER:HB3	1.98	0.45
5:E:155:GLN:HB2	5:E:159:TYR:HE1	1.80	0.45
6:2:246:TYR:O	6:2:250:ALA:N	2.43	0.45
8:4:326:ILE:HD11	8:4:439:PHE:HB2	1.98	0.45
8:4:449:ARG:NH2	12:F:14:DT:O3'	2.49	0.45
10:6:293:THR:O	10:6:362:GLN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:7:479:ARG:HH21	11:7:517:ASP:H	1.64	0.45
2:B:180:GLU:HB3	3:C:184:TYR:HE1	1.81	0.45
4:D:74:PRO:HB3	4:D:226:LYS:HE3	1.98	0.45
5:E:547:ARG:HE	5:E:547:ARG:HB3	1.60	0.45
6:2:695:LEU:HD23	10:6:797:VAL:HG11	1.98	0.45
7:3:555:GLU:O	7:3:559:ARG:NH1	2.50	0.45
6:2:465:ASN:OD1	6:2:465:ASN:N	2.49	0.45
6:2:500:SER:OG	6:2:500:SER:O	2.34	0.45
6:2:600:ASP:HB3	6:2:601:LYS:HD2	1.98	0.45
8:4:177:LEU:HD22	8:4:186:SER:HB2	1.99	0.45
11:7:444:VAL:HB	11:7:448:MET:HG3	1.99	0.45
1:A:51:THR:O	1:A:55:LYS:N	2.45	0.45
3:C:96:ASP:OD1	3:C:99:SER:N	2.43	0.45
5:E:336:ASP:C	5:E:338:PHE:N	2.70	0.45
6:2:739:ASN:O	6:2:743:ARG:N	2.45	0.45
8:4:229:GLN:HA	8:4:232:GLU:HB2	1.98	0.45
8:4:539:GLY:HA2	8:4:542:LEU:HB2	1.99	0.45
8:4:700:SER:O	8:4:796:ARG:NE	2.49	0.45
8:4:907:LEU:O	8:4:911:GLN:N	2.50	0.45
9:5:304:LYS:HA	9:5:304:LYS:HD3	1.76	0.45
4:D:220:ASP:OD1	4:D:221:GLU:N	2.49	0.45
10:6:570:ASN:OD1	10:6:678:ILE:N	2.50	0.45
11:7:520:ILE:HG22	11:7:522:CYS:SG	2.57	0.45
11:7:534:ARG:HD3	11:7:586:LEU:HD21	1.99	0.45
5:E:34:LEU:HD12	5:E:543:LEU:HD23	1.99	0.45
5:E:292:TYR:HD1	5:E:295:LEU:HD21	1.81	0.45
9:5:28:ILE:CD1	9:5:89:LEU:HD12	2.45	0.45
9:5:164:GLY:HA3	9:5:258:LEU:HD11	1.98	0.45
1:A:4:ASP:OD1	1:A:4:ASP:N	2.42	0.45
6:2:328:THR:OG1	6:2:329:GLY:N	2.50	0.45
7:3:477:LYS:HB3	9:5:491:VAL:HG12	1.99	0.45
9:5:455:ARG:HH12	12:F:19:DT:H4'	1.82	0.45
10:6:572:CYS:HB2	10:6:680:ALA:HB3	1.98	0.45
4:D:65:LYS:NZ	4:D:289:ASP:OD2	2.49	0.45
6:2:802:SER:HB3	6:2:849:GLN:HE22	1.82	0.45
8:4:674:SER:OG	8:4:674:SER:O	2.34	0.45
9:5:408:GLY:HA2	9:5:658:ARG:HD3	1.99	0.45
9:5:473:ASP:OD2	9:5:516:ARG:N	2.49	0.45
10:6:707:SER:O	10:6:798:ARG:NH1	2.50	0.45
7:3:48:TYR:HA	7:3:51:ASN:HB2	1.99	0.45
7:3:420:ARG:HA	7:3:423:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:6:720:ASN:HB3	10:6:723:ILE:HG12	1.98	0.45
11:7:25:LEU:O	11:7:63:TYR:OH	2.35	0.45
11:7:109:ASN:ND2	11:7:111:ASN:OD1	2.50	0.45
11:7:211:CYS:HA	11:7:214:ARG:HD3	1.98	0.45
1:A:113:ILE:O	1:A:116:SER:OG	2.34	0.44
6:2:765:LYS:HE2	6:2:765:LYS:HB3	1.72	0.44
7:3:389:VAL:HG21	7:3:668:ILE:HD13	2.00	0.44
8:4:178:ARG:H	8:4:187:ILE:HG23	1.82	0.44
1:A:136:ASP:O	1:A:139:THR:OG1	2.33	0.44
3:C:75:LEU:HD12	3:C:76:PRO:HD2	1.98	0.44
8:4:224:LEU:HG	8:4:226:TYR:H	1.82	0.44
8:4:546:GLY:H	8:4:755:LYS:HD2	1.82	0.44
8:4:612:LYS:HA	8:4:612:LYS:HD3	1.85	0.44
8:4:629:CYS:HB2	8:4:671:ILE:HG22	1.99	0.44
6:2:245:ASN:HD22	6:2:248:HIS:CD2	2.35	0.44
6:2:472:ASP:OD1	6:2:472:ASP:N	2.49	0.44
6:2:835:ASP:OD1	6:2:835:ASP:N	2.49	0.44
9:5:653:LEU:HA	9:5:656:ILE:HD12	2.00	0.44
11:7:569:PRO:HB3	11:7:583:ASN:HD22	1.82	0.44
4:D:257:THR:OG1	4:D:269:LEU:O	2.33	0.44
5:E:5:ILE:HD11	5:E:141:GLN:HE22	1.83	0.44
7:3:25:VAL:HG13	7:3:29:GLN:HE22	1.83	0.44
11:7:494:THR:OG1	11:7:495:ALA:N	2.49	0.44
12:F:19:DT:OP2	12:F:19:DT:C6	2.70	0.44
8:4:449:ARG:HH12	12:F:14:DT:H5”	1.83	0.44
9:5:565:ASP:N	9:5:565:ASP:OD1	2.51	0.44
10:6:185:LEU:HA	10:6:188:VAL:HG12	1.99	0.44
11:7:222:SER:O	11:7:222:SER:OG	2.33	0.44
5:E:412:THR:OG1	5:E:413:LEU:N	2.51	0.44
9:5:540:ILE:HG21	9:5:546:ILE:HD11	1.99	0.44
1:A:168:LEU:N	1:A:206:GLN:OE1	2.47	0.44
3:C:133:GLN:O	3:C:137:HIS:ND1	2.49	0.44
5:E:230:ILE:O	5:E:234:GLU:N	2.50	0.44
6:2:672:PRO:HB3	9:5:418:PRO:HG3	1.99	0.44
6:2:802:SER:OG	6:2:803:PHE:N	2.51	0.44
10:6:511:ASP:O	10:6:515:GLU:N	2.51	0.44
5:E:11:ALA:HA	5:E:14:LYS:HE2	2.00	0.44
6:2:543:GLY:HA3	6:2:549:LYS:HD3	2.00	0.44
8:4:890:ILE:HA	8:4:893:HIS:ND1	2.32	0.44
10:6:568:ASP:O	10:6:805:ARG:NE	2.45	0.44
11:7:142:ILE:HA	11:7:145:GLN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:30:PHE:HB2	5:E:83:LEU:HD23	2.00	0.43
5:E:307:ARG:HH21	5:E:309:SER:H	1.66	0.43
5:E:374:GLN:HG2	5:E:375:GLU:HG3	2.01	0.43
6:2:676:ARG:HA	6:2:808:ARG:HH12	1.83	0.43
8:4:348:LYS:HB3	8:4:348:LYS:HE2	1.76	0.43
9:5:170:SER:OG	9:5:171:VAL:N	2.50	0.43
7:3:687:ARG:HD3	7:3:697:ILE:HD11	1.99	0.43
9:5:636:ASN:O	9:5:641:THR:OG1	2.33	0.43
10:6:576:ASP:O	10:6:579:THR:OG1	2.29	0.43
5:E:228:LYS:O	5:E:232:GLU:N	2.46	0.43
7:3:21:PHE:HA	7:3:24:ARG:HE	1.83	0.43
8:4:201:PHE:CZ	8:4:204:LYS:HB2	2.53	0.43
10:6:694:SER:OG	10:6:695:LEU:N	2.51	0.43
11:7:483:THR:OG1	11:7:484:THR:N	2.51	0.43
11:7:520:ILE:CG2	11:7:522:CYS:SG	3.06	0.43
7:3:325:THR:O	7:3:325:THR:OG1	2.31	0.43
8:4:689:THR:HG21	8:4:854:LYS:HZ1	1.84	0.43
8:4:873:LEU:HD22	8:4:927:VAL:HG13	2.00	0.43
10:6:120:GLU:O	10:6:134:LYS:NZ	2.52	0.43
10:6:122:PHE:HD2	10:6:124:VAL:H	1.66	0.43
11:7:609:ASP:O	11:7:613:ALA:N	2.45	0.43
11:7:711:ASP:OD1	11:7:711:ASP:N	2.51	0.43
3:C:3:TYR:CE2	3:C:5:ASP:HA	2.53	0.43
3:C:178:LYS:HE3	3:C:178:LYS:HB3	1.88	0.43
6:2:618:THR:HA	6:2:621:HIS:CE1	2.54	0.43
8:4:743:PRO:HG3	8:4:746:PHE:HD2	1.83	0.43
9:5:99:LYS:HB2	9:5:99:LYS:NZ	2.33	0.43
11:7:261:THR:HG22	11:7:263:ASP:H	1.83	0.43
11:7:570:LEU:HB2	11:7:583:ASN:HB3	2.00	0.43
11:7:664:TYR:HB2	11:7:689:LEU:HD13	2.01	0.43
3:C:8:ASP:OD1	3:C:8:ASP:N	2.34	0.43
5:E:37:ASP:OD1	5:E:37:ASP:N	2.51	0.43
5:E:488:LYS:HD3	5:E:491:LEU:H	1.84	0.43
10:6:402:ILE:HD12	10:6:402:ILE:HA	1.88	0.43
11:7:685:THR:O	11:7:688:THR:OG1	2.31	0.43
5:E:20:SER:O	5:E:20:SER:OG	2.36	0.43
5:E:549:GLY:O	5:E:553:ILE:N	2.46	0.43
6:2:745:LEU:O	6:2:749:ARG:NH1	2.52	0.43
7:3:235:ASP:O	7:3:237:GLU:N	2.52	0.43
7:3:372:TYR:OH	7:3:563:GLU:OE2	2.37	0.43
11:7:423:TYR:HE1	11:7:611:LYS:HG2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:39:LEU:HD11	5:E:481:TRP:HD1	1.83	0.43
5:E:337:SER:O	5:E:341:SER:N	2.49	0.43
5:E:387:GLU:HA	5:E:390:ILE:HG12	2.00	0.43
1:A:18:GLN:HE21	1:A:22:ARG:HD2	1.84	0.43
5:E:342:ASN:ND2	5:E:351:TRP:O	2.52	0.43
6:2:306:LEU:HD11	6:2:406:ARG:HG3	2.00	0.43
6:2:656:ARG:CZ	6:2:685:ASP:H	2.32	0.43
7:3:224:ARG:HD3	7:3:224:ARG:HA	1.81	0.43
7:3:429:ALA:HB1	7:3:469:VAL:H	1.84	0.43
7:3:474:GLU:HB3	7:3:477:LYS:HB2	2.00	0.43
7:3:666:ARG:HA	7:3:666:ARG:HD3	1.83	0.43
8:4:185:VAL:HA	8:4:260:GLN:HE22	1.84	0.43
9:5:690:ASP:N	9:5:690:ASP:OD1	2.51	0.43
10:6:614:ARG:HD2	10:6:615:ASP:H	1.83	0.43
11:7:72:ASN:OD1	11:7:72:ASN:N	2.47	0.43
11:7:356:LEU:HD12	11:7:357:PRO:HD2	2.01	0.43
11:7:635:PRO:HG2	11:7:639:ARG:HH22	1.84	0.43
4:D:212:THR:OG1	4:D:213:GLU:N	2.52	0.42
5:E:551:TRP:HE3	5:E:552:LEU:HD22	1.83	0.42
6:2:289:ILE:HG12	6:2:290:HIS:CD2	2.54	0.42
8:4:761:ILE:HD12	8:4:761:ILE:HA	1.94	0.42
10:6:532:SER:HB3	10:6:745:PRO:HD2	2.01	0.42
10:6:829:ASP:OD1	10:6:829:ASP:N	2.48	0.42
11:7:553:ILE:HD12	11:7:553:ILE:HA	1.94	0.42
2:B:145:ILE:HD13	2:B:145:ILE:HA	1.88	0.42
2:B:171:ASP:OD1	2:B:171:ASP:N	2.47	0.42
6:2:512:LYS:HA	6:2:515:VAL:HG12	2.01	0.42
8:4:294:ASP:OD1	8:4:294:ASP:N	2.47	0.42
9:5:24:ASN:N	9:5:27:ILE:HD12	2.34	0.42
6:2:241:SER:OG	6:2:296:ARG:NH2	2.50	0.42
8:4:388:ARG:HG3	10:6:175:TYR:HE2	1.85	0.42
9:5:423:SER:OG	14:5:801:ATP:O1G	2.33	0.42
10:6:578:SER:O	10:6:578:SER:OG	2.35	0.42
11:7:364:LYS:HA	11:7:364:LYS:HD2	1.86	0.42
5:E:472:ARG:O	5:E:476:ASN:ND2	2.53	0.42
6:2:253:LYS:HG3	6:2:260:LEU:HD12	2.02	0.42
6:2:355:SER:O	6:2:357:GLU:N	2.53	0.42
7:3:160:SER:OG	7:3:161:PHE:N	2.51	0.42
7:3:360:PHE:HE2	7:3:728:VAL:HG21	1.84	0.42
9:5:146:ILE:HD11	9:5:149:ARG:HB2	2.01	0.42
10:6:533:ILE:HD12	10:6:544:LYS:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:6:673:ASN:OD1	10:6:673:ASN:N	2.51	0.42
11:7:252:LYS:HE2	11:7:252:LYS:HB2	1.85	0.42
1:A:182:ASN:HD21	5:E:74:LEU:HB3	1.83	0.42
5:E:61:ILE:HD11	5:E:66:GLU:HB3	2.01	0.42
5:E:333:SER:O	5:E:336:ASP:N	2.52	0.42
7:3:565:VAL:O	7:3:569:HIS:NE2	2.46	0.42
10:6:390:LYS:NZ	10:6:391:PRO:O	2.39	0.42
11:7:637:LYS:HE3	11:7:637:LYS:HB2	1.82	0.42
1:A:54:LEU:HD23	1:A:54:LEU:HA	1.89	0.42
2:B:187:GLU:O	2:B:191:LYS:NZ	2.50	0.42
5:E:372:THR:O	5:E:372:THR:OG1	2.36	0.42
7:3:278:LEU:HD12	7:3:282:LEU:HB2	2.02	0.42
9:5:79:LEU:CG	9:5:86:ILE:HG21	2.49	0.42
9:5:659:ILE:HD13	9:5:659:ILE:HA	1.91	0.42
3:C:122:ASN:O	3:C:125:SER:OG	2.32	0.42
4:D:62:ASP:OD1	4:D:62:ASP:N	2.52	0.42
6:2:540:LEU:HG	6:2:648:ALA:HB3	2.01	0.42
8:4:363:GLY:HA2	10:6:437:VAL:HG22	2.02	0.42
2:B:24:PRO:HB2	2:B:70:GLU:HG2	2.01	0.42
2:B:95:THR:HG23	2:B:96:LYS:HD3	2.02	0.42
7:3:533:ILE:HD12	7:3:533:ILE:HA	1.91	0.42
8:4:873:LEU:HD22	8:4:927:VAL:HG12	1.96	0.42
8:4:889:GLN:HG2	8:4:893:HIS:CE1	2.54	0.42
9:5:626:PHE:HA	9:5:629:ILE:HD12	2.02	0.42
10:6:272:THR:O	10:6:289:SER:OG	2.38	0.42
6:2:611:LYS:HA	6:2:611:LYS:HD3	1.86	0.42
6:2:701:ASP:OD2	6:2:705:ARG:NH2	2.53	0.42
7:3:703:GLU:HB3	7:3:707:ARG:HH22	1.84	0.42
10:6:663:ILE:HD12	10:6:663:ILE:HA	1.86	0.42
5:E:147:THR:OG1	5:E:148:VAL:N	2.53	0.41
6:2:268:LEU:HD23	6:2:268:LEU:HA	1.90	0.41
6:2:528:ASN:O	6:2:530:LYS:N	2.52	0.41
9:5:166:ILE:HG21	9:5:256:LEU:HD12	2.01	0.41
9:5:237:GLY:HA2	9:5:238:PRO:HD3	1.94	0.41
9:5:279:ASP:OD2	9:5:280:ARG:N	2.53	0.41
8:4:435:VAL:HG12	8:4:466:VAL:HG23	2.02	0.41
8:4:650:GLU:HB3	10:6:586:LYS:NZ	2.35	0.41
8:4:886:LEU:HB2	8:4:890:ILE:HD12	2.02	0.41
9:5:132:LEU:HD23	9:5:132:LEU:HA	1.90	0.41
9:5:252:ASP:HB3	9:5:280:ARG:HG2	2.03	0.41
11:7:208:SER:OG	11:7:222:SER:O	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:7:471:LYS:HZ2	11:7:522:CYS:HB3	1.85	0.41
2:B:62:ASN:OD1	2:B:62:ASN:N	2.53	0.41
4:D:146:CYS:HA	4:D:149:SER:HB2	2.01	0.41
6:2:679:ILE:HA	6:2:679:ILE:HD12	1.82	0.41
7:3:537:ASP:HA	7:3:540:LEU:HD13	2.02	0.41
8:4:401:GLU:OE2	8:4:413:HIS:N	2.53	0.41
10:6:524:HIS:O	10:6:528:LYS:N	2.48	0.41
10:6:621:TYR:OH	10:6:668:ILE:O	2.26	0.41
11:7:92:LYS:HE3	11:7:92:LYS:HB3	1.94	0.41
11:7:265:CYS:CB	11:7:289:CYS:SG	3.06	0.41
11:7:484:THR:OG1	11:7:485:GLY:N	2.54	0.41
1:A:33:HIS:HB3	1:A:36:ILE:HB	2.02	0.41
1:A:184:ILE:HD12	1:A:184:ILE:HA	1.94	0.41
3:C:173:GLU:HA	3:C:176:ILE:HD13	2.02	0.41
5:E:43:LYS:O	5:E:46:SER:OG	2.38	0.41
5:E:91:ASP:OD2	5:E:94:ALA:N	2.43	0.41
8:4:302:LYS:NZ	8:4:303:VAL:O	2.40	0.41
8:4:509:ILE:O	8:4:513:ALA:N	2.46	0.41
8:4:741:VAL:HG12	8:4:743:PRO:HD3	2.03	0.41
11:7:157:ARG:NH2	11:7:189:THR:OG1	2.44	0.41
11:7:500:ASP:HB2	11:7:505:GLU:HA	2.02	0.41
11:7:508:LEU:HD12	11:7:508:LEU:HA	1.91	0.41
1:A:185:LYS:HZ3	1:A:186:ASP:HB3	1.86	0.41
6:2:583:ASP:HB2	6:2:587:LYS:HB2	2.02	0.41
7:3:20:VAL:HG23	7:3:24:ARG:HH21	1.85	0.41
7:3:95:ARG:NH2	7:3:154:LYS:HG3	2.35	0.41
7:3:251:ILE:HD12	7:3:251:ILE:HA	1.98	0.41
7:3:476:ASP:HB3	7:3:477:LYS:HZ2	1.85	0.41
9:5:433:SER:HB3	9:5:436:ALA:HB2	2.02	0.41
2:B:170:LEU:HB3	2:B:173:LEU:HD23	2.02	0.41
6:2:245:ASN:HB3	6:2:248:HIS:HB2	2.03	0.41
6:2:289:ILE:HG12	6:2:290:HIS:HD2	1.85	0.41
8:4:668:ARG:H	8:4:668:ARG:HG2	1.70	0.41
8:4:873:LEU:CD1	8:4:927:VAL:HG11	2.50	0.41
9:5:296:GLY:HA2	9:5:331:LEU:HD23	2.02	0.41
10:6:175:TYR:HB3	10:6:285:GLY:HA2	2.01	0.41
10:6:564:LYS:HD3	10:6:564:LYS:HA	1.80	0.41
10:6:772:TYR:CZ	10:6:776:LYS:HD2	2.56	0.41
11:7:534:ARG:HB3	11:7:586:LEU:HD11	2.01	0.41
3:C:54:LEU:HD12	3:C:54:LEU:HA	1.91	0.41
6:2:545:PRO:O	10:6:798:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:616:ASP:O	6:2:619:SER:OG	2.33	0.41
7:3:542:ARG:HD3	7:3:542:ARG:HA	1.79	0.41
7:3:662:TYR:HE1	7:3:666:ARG:HH21	1.69	0.41
10:6:151:ILE:O	10:6:266:SER:OG	2.33	0.41
11:7:287:GLU:O	11:7:291:GLN:NE2	2.48	0.41
11:7:595:ASP:OD1	11:7:595:ASP:N	2.54	0.41
11:7:653:SER:OG	11:7:654:GLU:N	2.52	0.41
1:A:92:LEU:HD12	1:A:92:LEU:HA	1.88	0.41
3:C:3:TYR:CZ	3:C:5:ASP:HA	2.56	0.41
8:4:193:ASN:HA	8:4:196:ASN:HD21	1.85	0.41
8:4:661:ILE:HD12	8:4:661:ILE:HA	1.91	0.41
8:4:858:GLN:HA	8:4:858:GLN:OE1	2.21	0.41
9:5:422:LYS:HG2	14:5:801:ATP:PG	2.61	0.41
9:5:455:ARG:HH12	12:F:19:DT:C4'	2.34	0.41
2:B:52:LEU:HB2	2:B:59:ALA:HB2	2.03	0.41
3:C:87:ALA:O	3:C:90:THR:OG1	2.38	0.41
4:D:210:ASN:OD1	4:D:210:ASN:N	2.53	0.41
5:E:267:LEU:O	5:E:271:TRP:N	2.53	0.41
7:3:359:ILE:H	7:3:359:ILE:HG13	1.69	0.41
8:4:594:LYS:HA	8:4:594:LYS:HD3	1.81	0.41
8:4:879:ASP:HB3	8:4:926:SER:HB2	2.03	0.41
9:5:87:ILE:CG2	9:5:88:PRO:HD3	2.40	0.41
9:5:98:ALA:HB1	9:5:135:PHE:HZ	1.85	0.41
9:5:589:GLU:OE2	9:5:595:SER:OG	2.33	0.41
11:7:513:LEU:HB3	11:7:546:ILE:HD13	2.01	0.41
5:E:344:VAL:HA	5:E:347:LYS:HB2	2.02	0.41
7:3:492:GLN:HG3	7:3:494:THR:H	1.85	0.41
7:3:684:THR:HG21	11:7:610:GLU:HB3	2.02	0.41
9:5:72:ASN:HB3	9:5:75:ILE:HG22	2.02	0.41
10:6:279:ILE:HA	10:6:283:LYS:HE3	2.03	0.41
10:6:770:ARG:HA	10:6:773:LEU:HB3	2.02	0.41
11:7:575:ASN:HB3	11:7:578:LEU:HB2	2.03	0.41
7:3:455:ARG:NH2	12:F:19:DT:OP1	2.54	0.40
7:3:537:ASP:HA	7:3:540:LEU:HB2	2.03	0.40
7:3:725:ASP:N	7:3:725:ASP:OD1	2.54	0.40
8:4:196:ASN:O	8:4:200:SER:OG	2.32	0.40
8:4:227:ILE:HD13	8:4:230:LEU:HD21	2.03	0.40
9:5:183:CYS:SG	9:5:187:ARG:N	2.94	0.40
5:E:344:VAL:HG13	5:E:347:LYS:HE3	2.03	0.40
6:2:270:ILE:HD12	6:2:270:ILE:HA	1.95	0.40
6:2:824:ARG:HH22	6:2:830:SER:HB3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:3:171:LEU:HD23	9:5:280:ARG:HH12	1.85	0.40
9:5:351:GLU:H	9:5:351:GLU:HG3	1.73	0.40
1:A:84:ARG:NH1	4:D:217:ASN:HD21	2.19	0.40
5:E:223:ARG:O	5:E:227:LYS:N	2.42	0.40
5:E:391:ILE:O	5:E:395:ASN:N	2.52	0.40
7:3:313:THR:N	9:5:201:THR:OG1	2.54	0.40
8:4:362:ARG:HH11	8:4:364:VAL:HB	1.86	0.40
10:6:274:HIS:CG	10:6:288:LEU:HD11	2.57	0.40
11:7:206:PRO:HB2	11:7:222:SER:HB2	2.03	0.40
3:C:183:SER:O	3:C:187:THR:OG1	2.32	0.40
7:3:215:THR:HG21	7:3:224:ARG:HG3	2.04	0.40
7:3:299:LYS:HA	7:3:299:LYS:HD3	1.93	0.40
7:3:313:THR:N	9:5:201:THR:O	2.50	0.40
10:6:183:LYS:HG3	10:6:186:ARG:HH22	1.85	0.40
10:6:586:LYS:HA	10:6:586:LYS:HD3	1.80	0.40
10:6:650:VAL:HA	10:6:653:HIS:HB3	2.02	0.40
1:A:138:ILE:HD12	1:A:138:ILE:HA	1.91	0.40
5:E:18:ASN:O	5:E:79:ASN:ND2	2.54	0.40
6:2:776:PRO:HA	6:2:827:GLU:HA	2.04	0.40
7:3:280:ASP:N	7:3:280:ASP:OD1	2.54	0.40
14:3:1001:ATP:C8	9:5:650:ILE:HD11	2.56	0.40
8:4:271:ILE:HD13	8:4:271:ILE:HA	1.94	0.40
8:4:535:ASP:N	8:4:535:ASP:OD1	2.54	0.40
8:4:703:ASP:N	8:4:703:ASP:OD1	2.49	0.40
8:4:818:GLU:HG3	8:4:820:GLU:H	1.86	0.40
8:4:873:LEU:HD13	8:4:927:VAL:HG11	2.04	0.40
9:5:95:THR:CG2	9:5:135:PHE:HD1	2.21	0.40
10:6:297:THR:OG1	10:6:298:SER:N	2.54	0.40
11:7:14:TYR:O	11:7:18:PHE:N	2.55	0.40
11:7:265:CYS:CB	11:7:289:CYS:CB	2.97	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	206/208 (99%)	180 (87%)	25 (12%)	1 (0%)	29	67
2	B	177/198 (89%)	147 (83%)	30 (17%)	0	100	100
3	C	151/191 (79%)	131 (87%)	20 (13%)	0	100	100
4	D	215/291 (74%)	188 (87%)	27 (13%)	0	100	100
5	E	543/646 (84%)	470 (87%)	70 (13%)	3 (1%)	25	63
6	2	630/664 (95%)	543 (86%)	86 (14%)	1 (0%)	47	79
7	3	584/722 (81%)	517 (88%)	67 (12%)	0	100	100
8	4	667/753 (89%)	575 (86%)	91 (14%)	1 (0%)	51	84
9	5	583/670 (87%)	500 (86%)	81 (14%)	2 (0%)	41	75
10	6	606/667 (91%)	530 (88%)	75 (12%)	1 (0%)	47	79
11	7	653/729 (90%)	565 (86%)	88 (14%)	0	100	100
All	All	5015/5739 (87%)	4346 (87%)	660 (13%)	9 (0%)	50	79

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	336	ASP
5	E	334	LEU
5	E	335	TYR
8	4	893	HIS
9	5	83	PRO
10	6	305	TYR
6	2	416	ASP
1	A	30	PRO
9	5	147	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	192/193 (100%)	192 (100%)	0	100	100
2	B	170/185 (92%)	167 (98%)	3 (2%)	59	77
3	C	144/171 (84%)	143 (99%)	1 (1%)	84	90
4	D	213/276 (77%)	213 (100%)	0	100	100
5	E	497/583 (85%)	495 (100%)	2 (0%)	91	94
6	2	533/580 (92%)	531 (100%)	2 (0%)	91	94
7	3	514/619 (83%)	512 (100%)	2 (0%)	91	94
8	4	609/687 (89%)	606 (100%)	3 (0%)	88	93
9	5	529/595 (89%)	524 (99%)	5 (1%)	78	87
10	6	487/545 (89%)	486 (100%)	1 (0%)	93	96
11	7	583/646 (90%)	579 (99%)	4 (1%)	84	90
All	All	4471/5080 (88%)	4448 (100%)	23 (0%)	89	93

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	80	LYS
2	B	131	LYS
2	B	184	PHE
3	C	5	ASP
5	E	89	VAL
5	E	223	ARG
6	2	401	ARG
6	2	486	LYS
7	3	31	PHE
7	3	39	ARG
8	4	857	ILE
8	4	859	ARG
8	4	868	GLU
9	5	26	GLU
9	5	88	PRO
9	5	326	PRO
9	5	450	THR
9	5	577	THR
10	6	581	LYS
11	7	246	THR
11	7	276	ARG
11	7	303	ARG
11	7	535	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
2	B	103	GLN
2	B	128	ASN
3	C	21	GLN
3	C	41	ASN
3	C	133	GLN
4	D	58	GLN
4	D	249	ASN
5	E	22	HIS
5	E	57	GLN
5	E	141	GLN
5	E	468	ASN
5	E	497	GLN
5	E	563	GLN
6	2	202	ASN
6	2	245	ASN
6	2	340	ASN
6	2	551	GLN
6	2	849	GLN
7	3	29	GLN
7	3	351	ASN
7	3	417	GLN
7	3	531	GLN
7	3	554	ASN
7	3	677	ASN
8	4	184	ASN
8	4	193	ASN
8	4	196	ASN
8	4	231	ASN
8	4	247	ASN
8	4	260	GLN
8	4	274	GLN
8	4	413	HIS
8	4	579	GLN
8	4	646	HIS
8	4	683	ASN
8	4	797	GLN
8	4	851	GLN
8	4	889	GLN
8	4	911	GLN
9	5	145	GLN

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Mol	Chain	Res	Type
9	5	254	GLN
9	5	574	ASN
9	5	581	ASN
10	6	139	GLN
10	6	357	GLN
10	6	362	GLN
10	6	434	ASN
10	6	514	ASN
10	6	550	GLN
10	6	750	GLN
10	6	814	ASN
11	7	87	GLN
11	7	293	GLN
11	7	554	ASN
11	7	615	HIS
11	7	683	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands 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	$\#\|Z\| > 2$
14	ATP	2	901	-	26,33,33	0.91	1 (3%)	31,52,52	1.62	5 (16%)
14	ATP	5	801	-	26,33,33	0.89	1 (3%)	31,52,52	1.66	5 (16%)
14	ATP	3	1001	-	26,33,33	0.91	1 (3%)	31,52,52	1.84	5 (16%)

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
14	ATP	2	901	-	-	6/18/38/38	0/3/3/3
14	ATP	5	801	-	-	4/18/38/38	0/3/3/3
14	ATP	3	1001	-	-	4/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	3	1001	ATP	C5-C4	2.33	1.47	1.40
14	2	901	ATP	C5-C4	2.24	1.46	1.40
14	5	801	ATP	C5-C4	2.20	1.46	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	3	1001	ATP	PA-O3A-PB	-5.51	113.91	132.83
14	5	801	ATP	PB-O3B-PG	-4.69	116.73	132.83
14	3	1001	ATP	PB-O3B-PG	-4.54	117.25	132.83
14	2	901	ATP	PA-O3A-PB	-4.33	117.98	132.83
14	5	801	ATP	N3-C2-N1	-3.49	123.22	128.68
14	3	1001	ATP	C3'-C2'-C1'	3.39	106.08	100.98
14	2	901	ATP	PB-O3B-PG	-3.34	121.36	132.83
14	2	901	ATP	C3'-C2'-C1'	3.32	105.98	100.98
14	3	1001	ATP	N3-C2-N1	-3.20	123.67	128.68
14	2	901	ATP	N3-C2-N1	-3.03	123.95	128.68
14	5	801	ATP	C4-C5-N7	-2.85	106.42	109.40
14	5	801	ATP	PA-O3A-PB	-2.71	123.54	132.83
14	5	801	ATP	C3'-C2'-C1'	2.60	104.90	100.98
14	2	901	ATP	C4-C5-N7	-2.57	106.72	109.40
14	3	1001	ATP	C4-C5-N7	-2.18	107.12	109.40

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	2	901	ATP	C5'-O5'-PA-O1A
14	2	901	ATP	C5'-O5'-PA-O2A
14	3	1001	ATP	C5'-O5'-PA-O3A
14	3	1001	ATP	O4'-C4'-C5'-O5'
14	5	801	ATP	C5'-O5'-PA-O2A
14	5	801	ATP	C5'-O5'-PA-O3A
14	2	901	ATP	C3'-C4'-C5'-O5'
14	3	1001	ATP	C3'-C4'-C5'-O5'
14	2	901	ATP	O4'-C4'-C5'-O5'
14	5	801	ATP	O4'-C4'-C5'-O5'
14	5	801	ATP	C3'-C4'-C5'-O5'
14	3	1001	ATP	C5'-O5'-PA-O2A
14	2	901	ATP	C4'-C5'-O5'-PA
14	2	901	ATP	C5'-O5'-PA-O3A

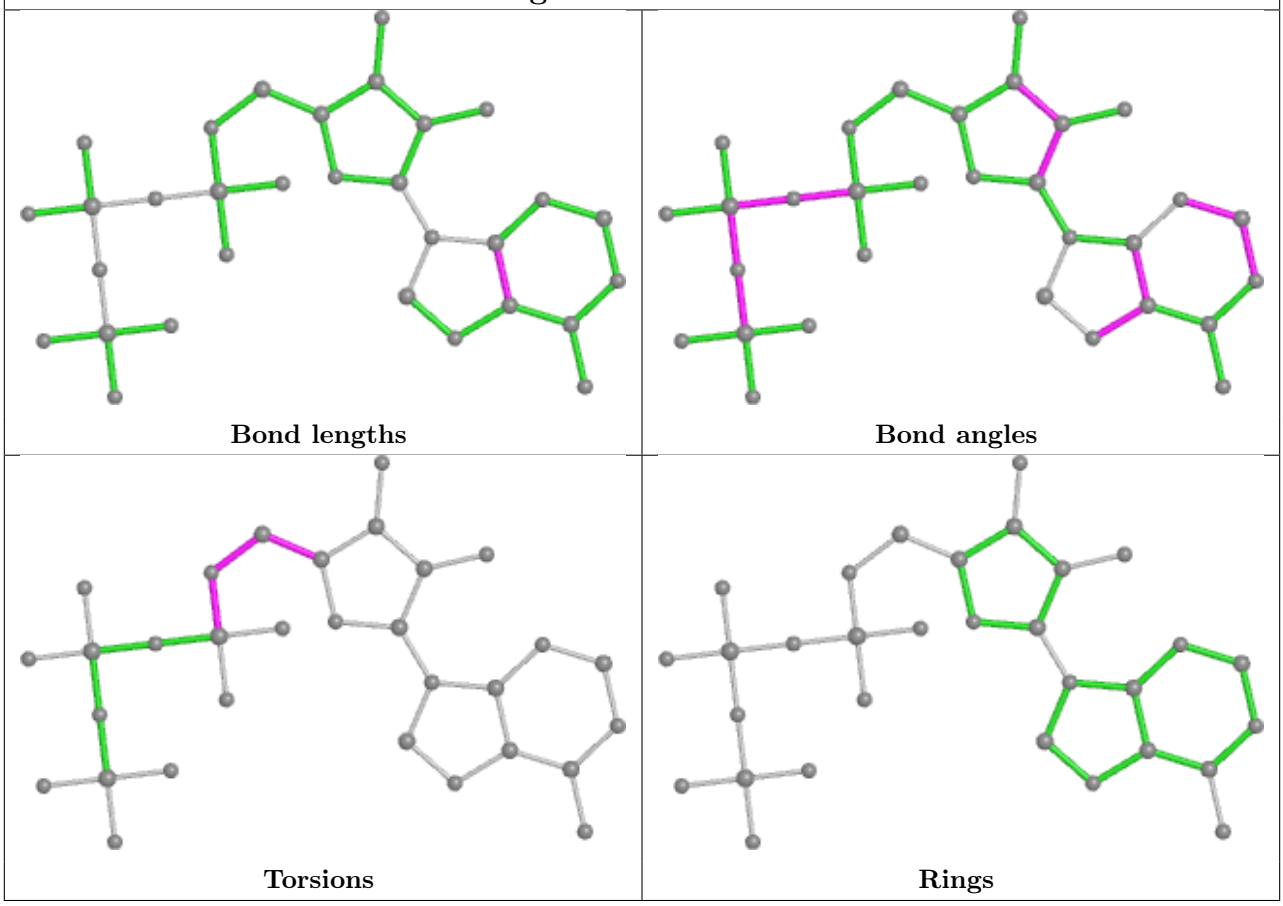
There are no ring outliers.

3 monomers are involved in 6 short contacts:

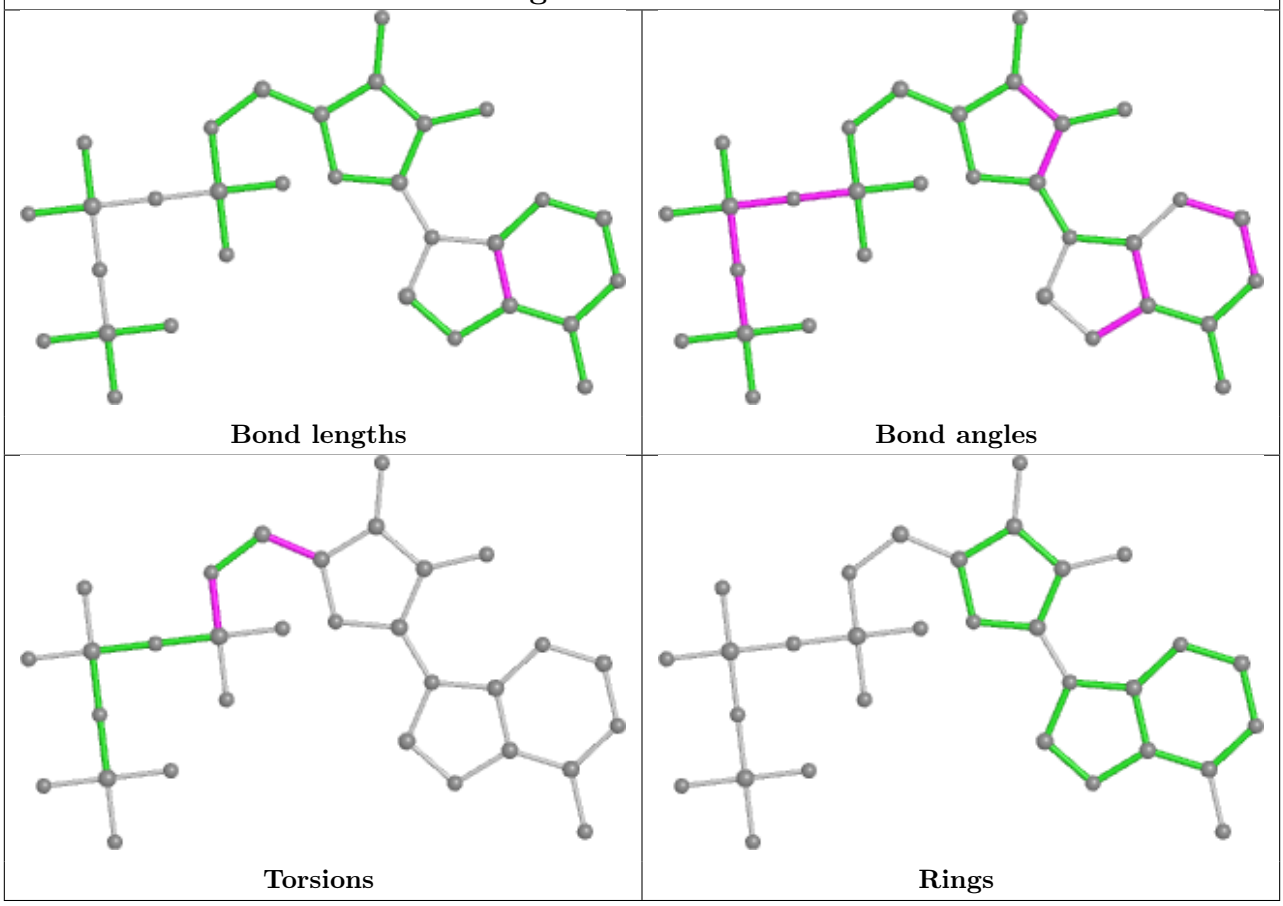
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	2	901	ATP	1	0
14	5	801	ATP	4	0
14	3	1001	ATP	1	0

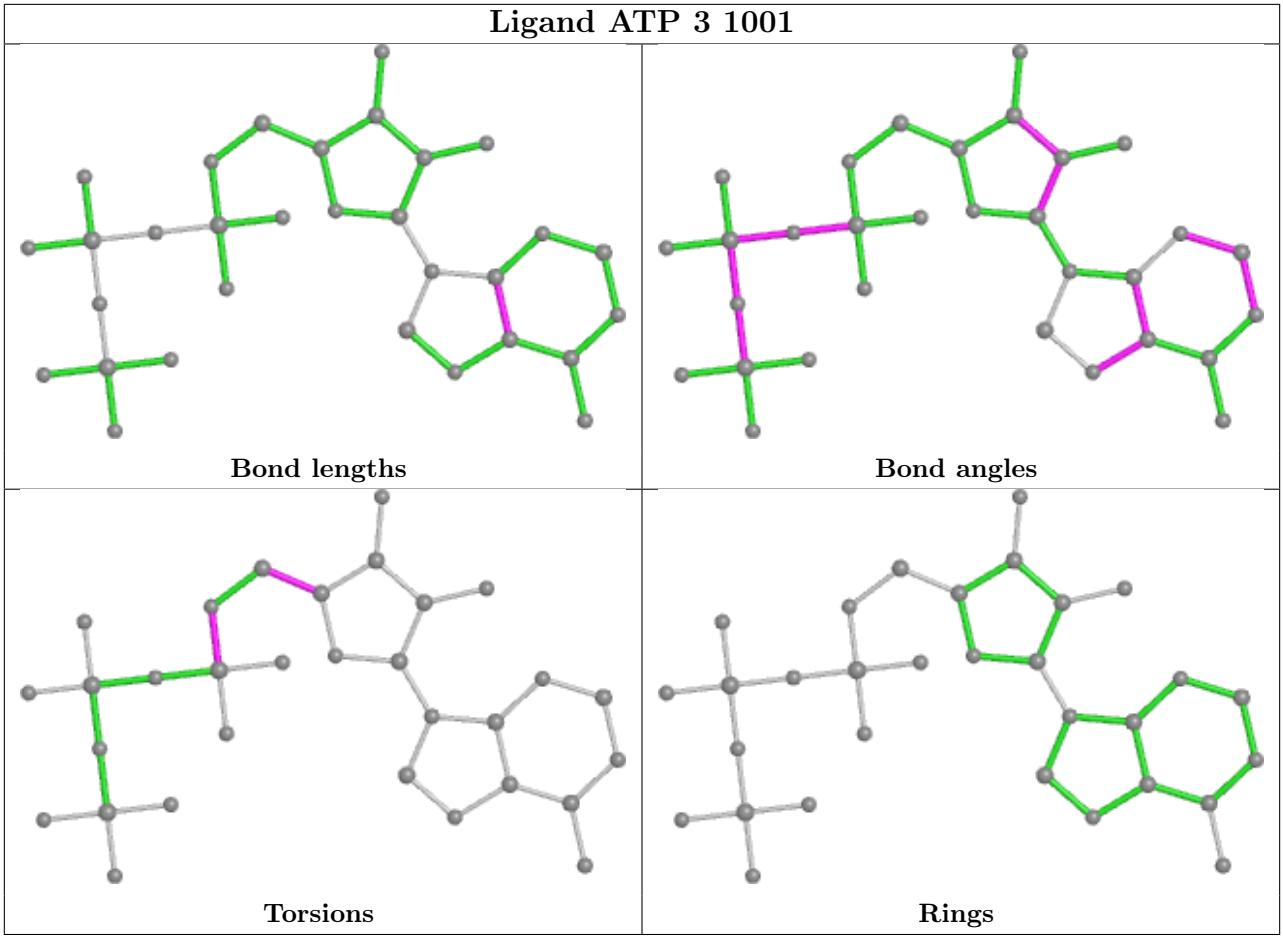
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 ATP 2 901



Ligand ATP 5 801





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

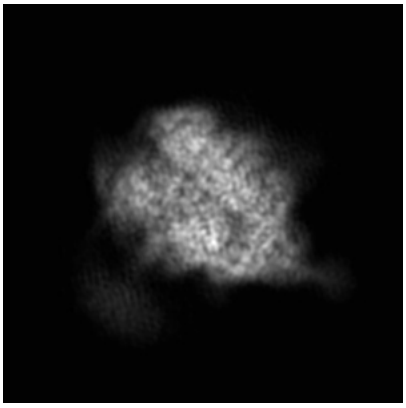
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20607. These allow visual inspection of the internal detail of the map and identification of artifacts.

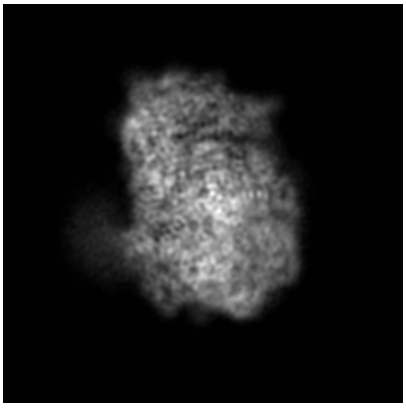
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

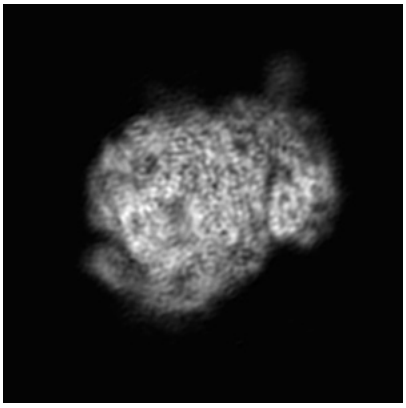
6.1.1 Primary map



X



Y

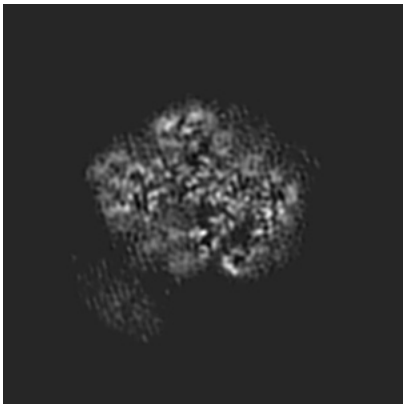


Z

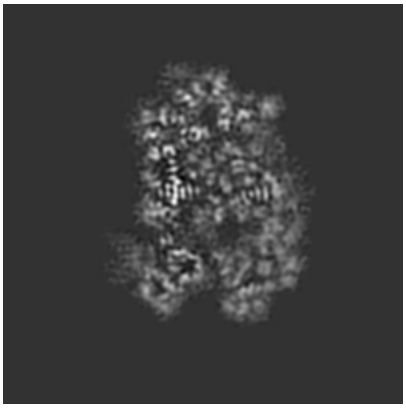
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

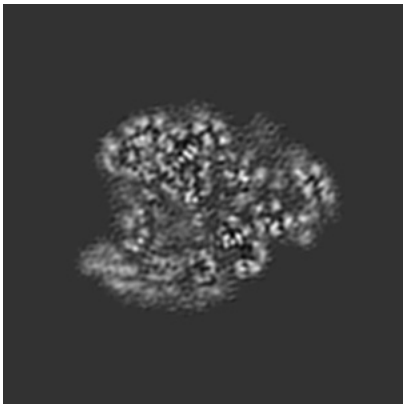
6.2.1 Primary map



X Index: 128



Y Index: 128

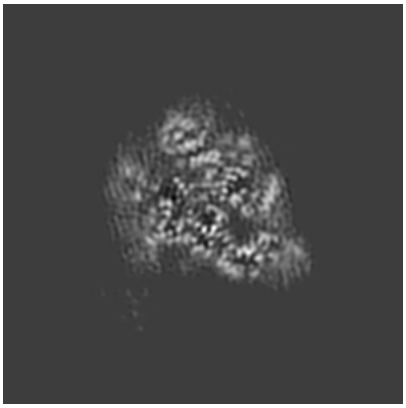


Z Index: 128

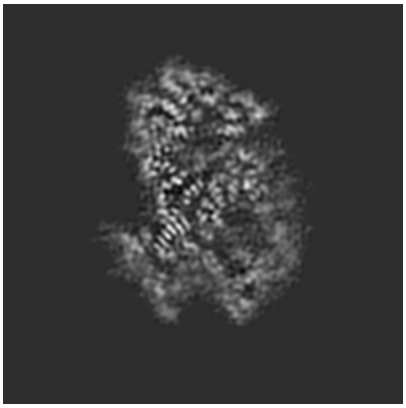
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

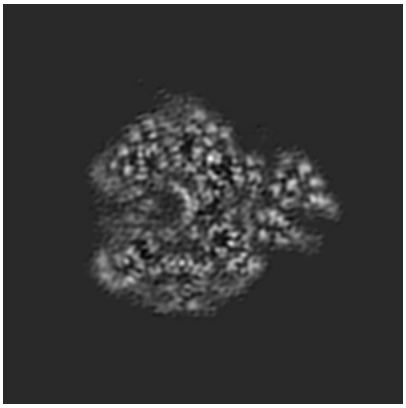
6.3.1 Primary map



X Index: 142



Y Index: 134

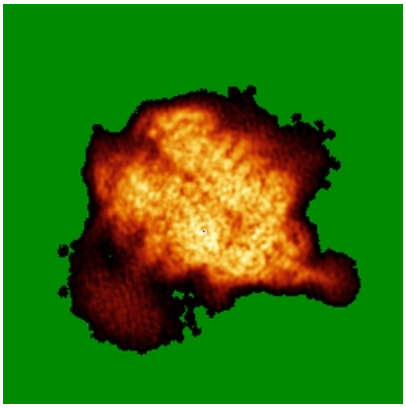


Z Index: 138

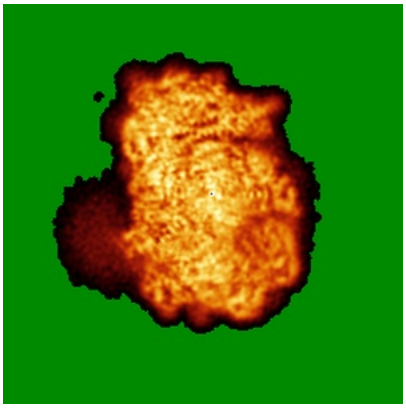
The images above show the largest variance slices of the map in three orthogonal directions.

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

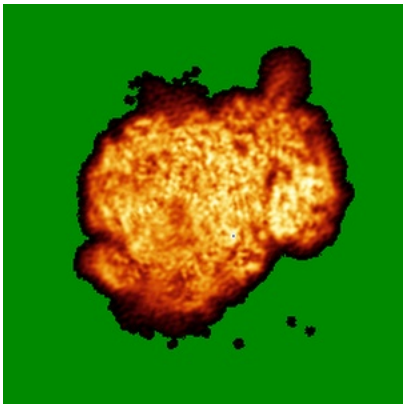
6.4.1 Primary map



X



Y

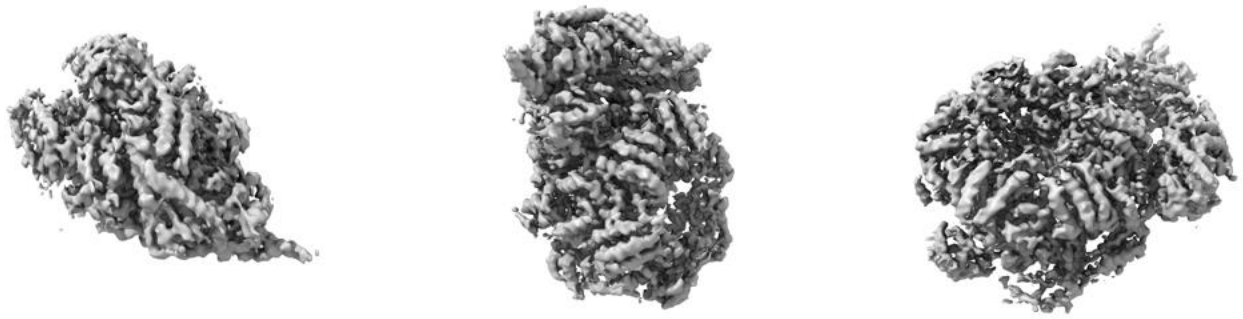


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

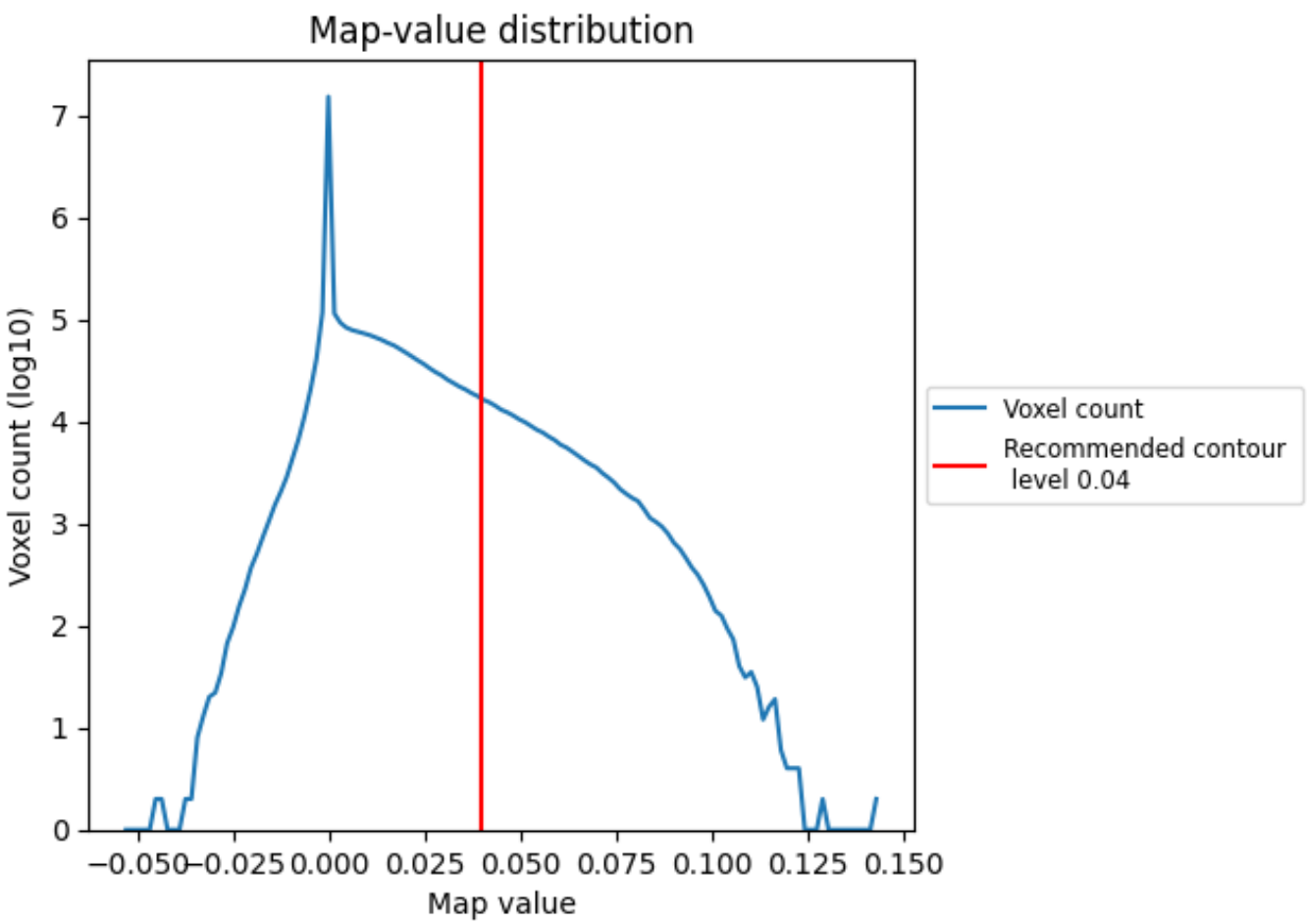
6.6 Mask visualisation (i)

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

7 Map analysis (i)

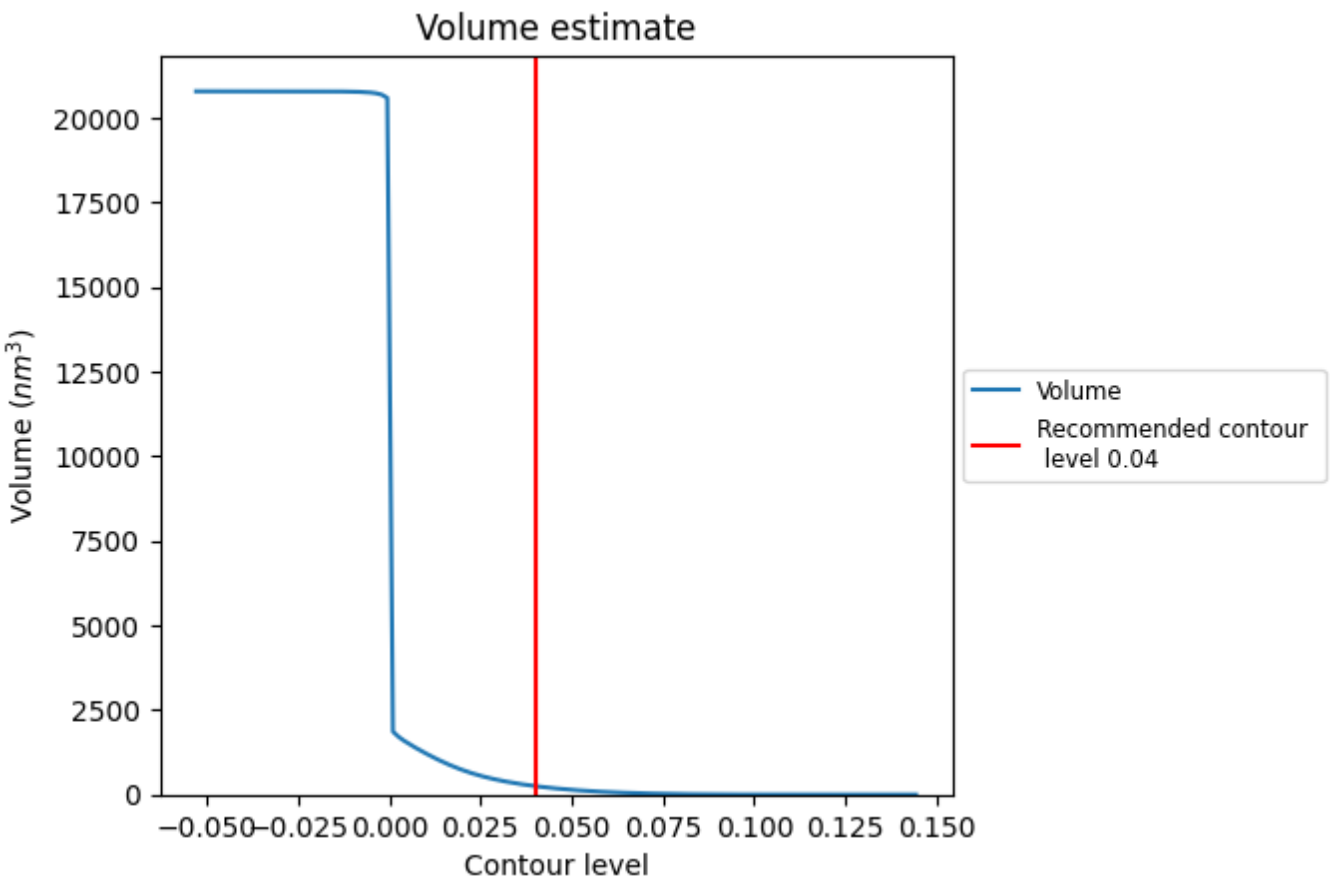
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

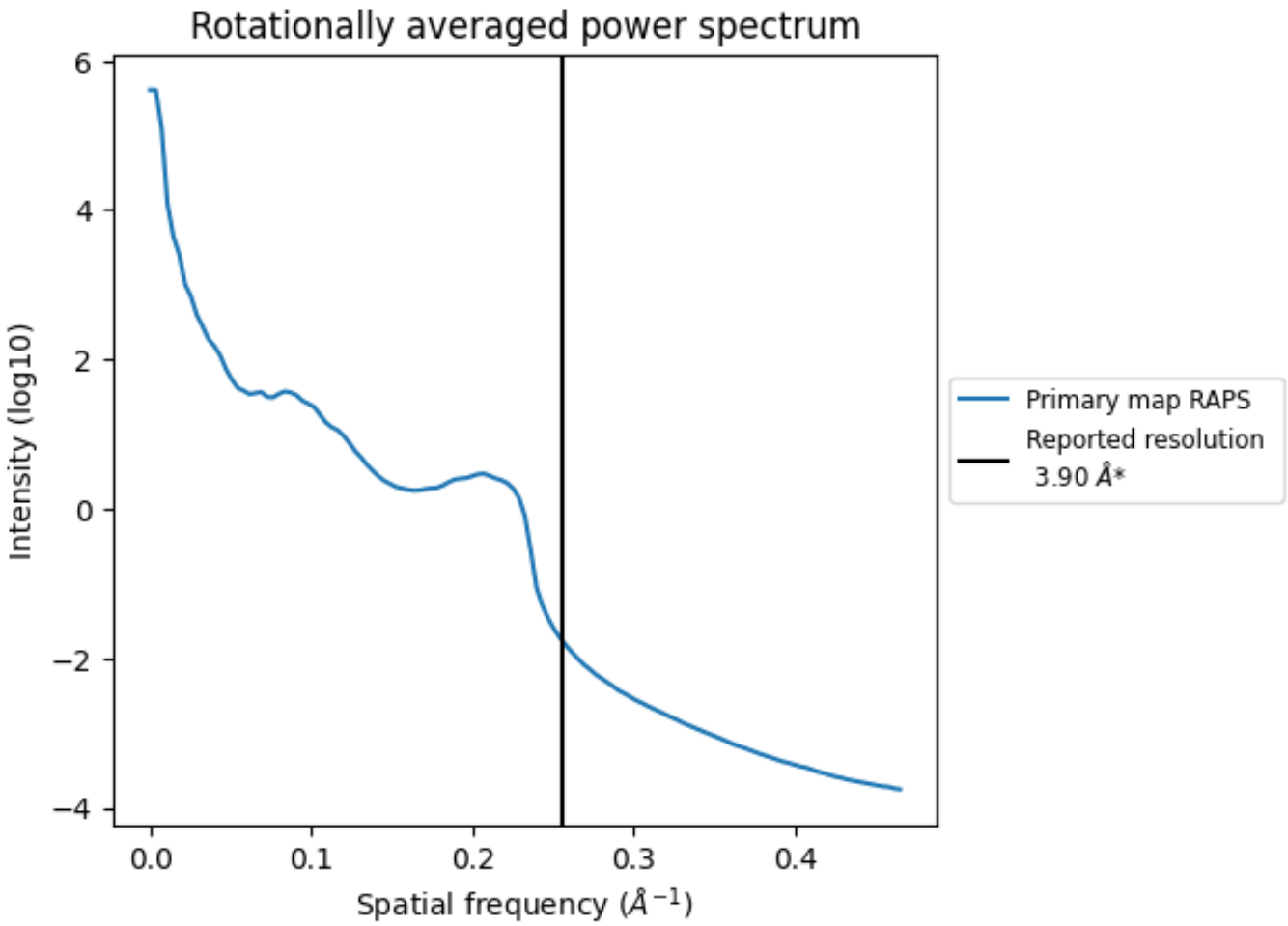
7.2 Volume estimate (i)



The volume at the recommended contour level is 250 nm^3; this corresponds to an approximate mass of 226 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 0.256 Å^{-1}

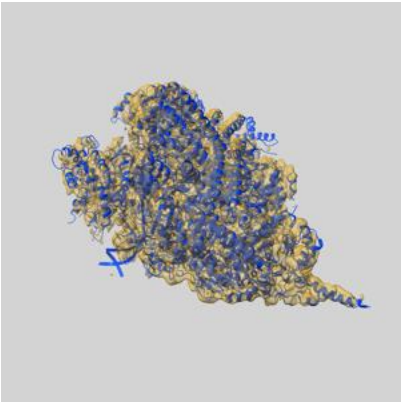
8 Fourier-Shell correlation (i)

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

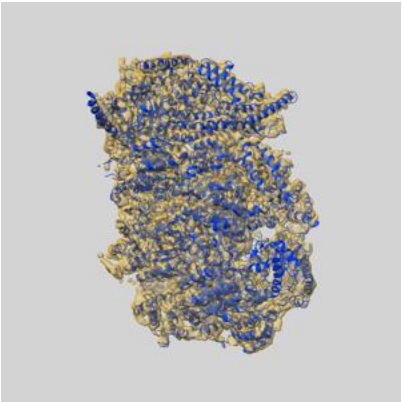
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20607 and PDB model 6U0M. Per-residue inclusion information can be found in section 3 on page 7.

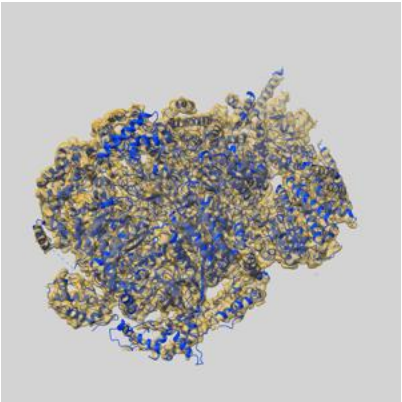
9.1 Map-model overlay (i)



X



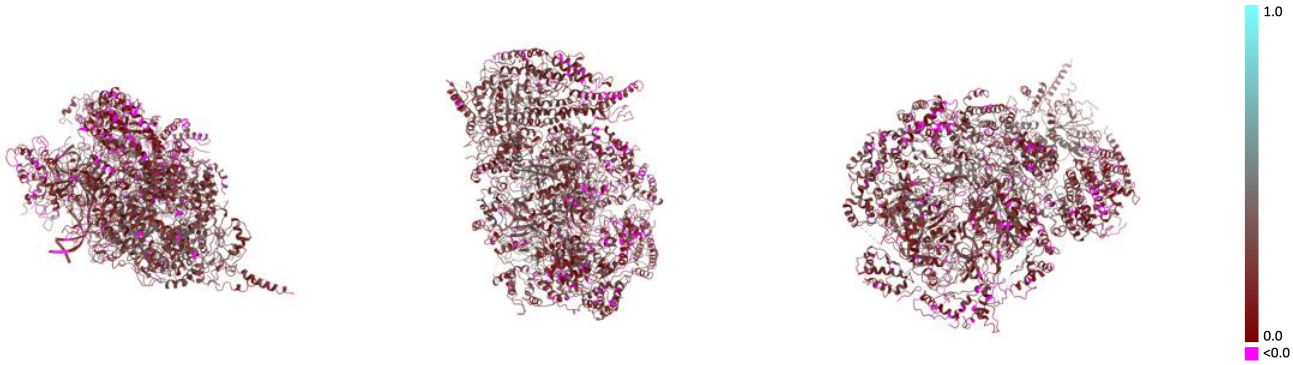
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

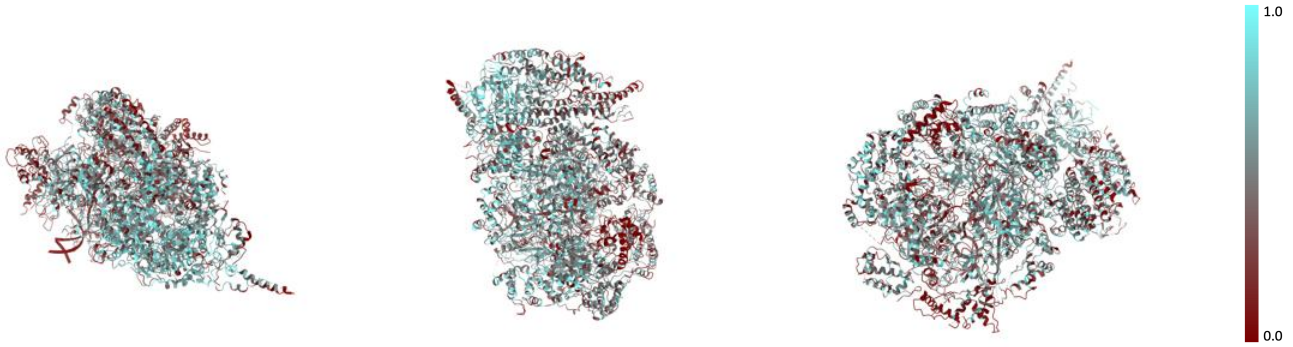
9.2 Q-score mapped to coordinate model (i)



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.

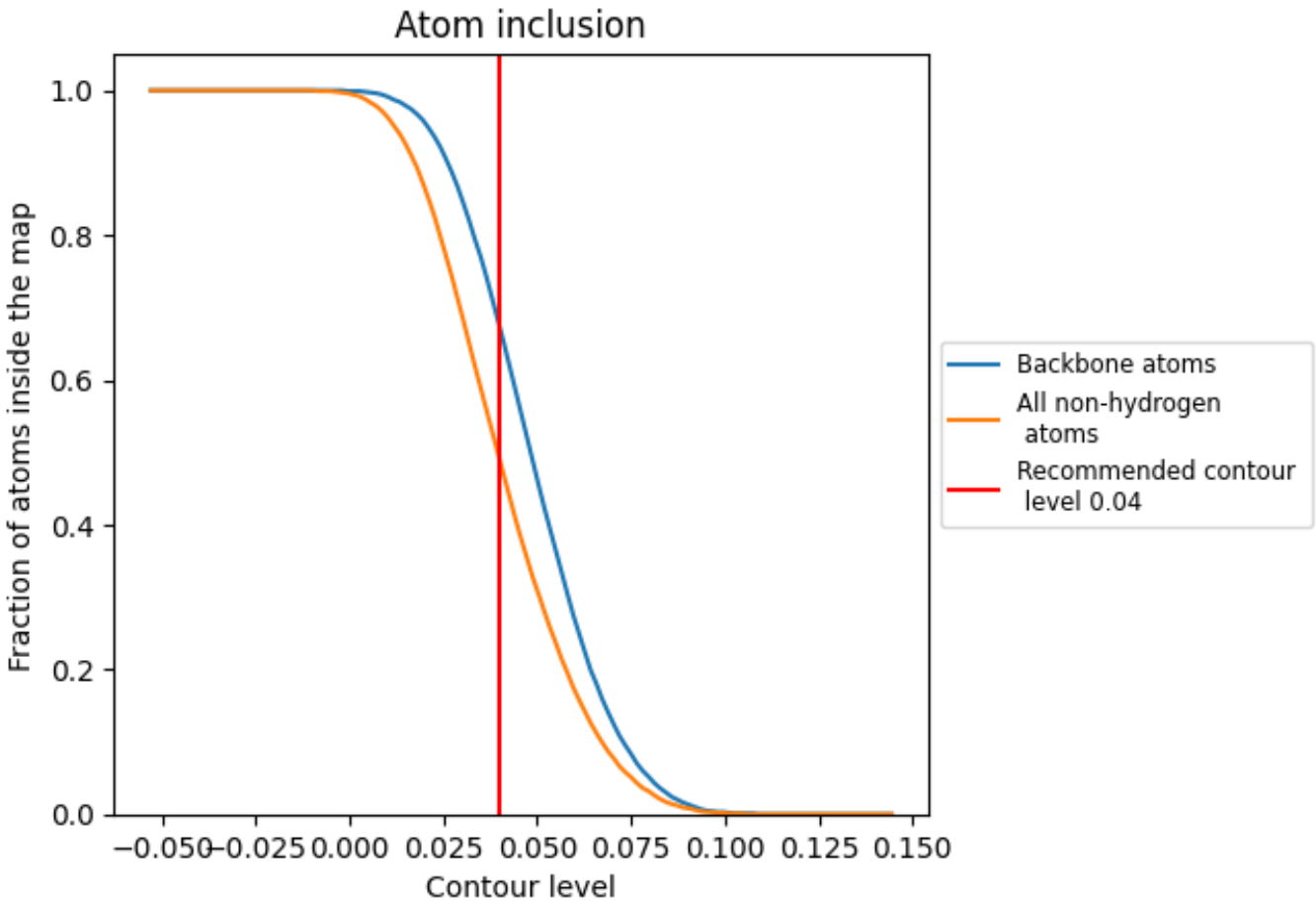
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 49% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4890	0.2190
2	0.5470	0.2500
3	0.4910	0.1950
4	0.4090	0.2100
5	0.5520	0.2620
6	0.5170	0.2280
7	0.3390	0.1700
A	0.4450	0.1840
B	0.6010	0.2500
C	0.5070	0.1650
D	0.5430	0.1750
E	0.5850	0.2660
F	0.3050	0.1880
G	0.1470	0.0990