



Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 03:46 PM EST

PDB ID : 6WGI
EMDB ID : EMD-21666
Title : Atomic model of the mutant OCCM (ORC-Cdc6-Cdt1-Mcm2-7 with Mcm6 WHD truncation) loaded on DNA at 10.5 Å resolution
Authors : Yuan, Z.; Schneider, S.; Dodd, T.; Riera, A.; Bai, L.; Yan, C.; Magdalou, I.; Ivanov, I.; Stillman, B.; Li, H.; Speck, C.
Deposited on : 2020-04-05
Resolution : 10.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
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 : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

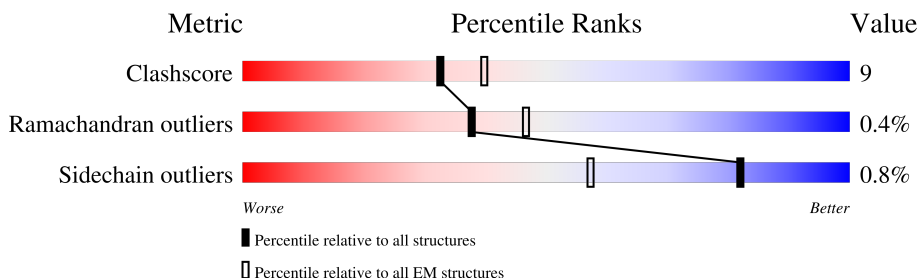
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.00 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	G	34	<div> <div>59%</div> <div>100%</div> </div>
2	H	34	<div> <div>62%</div> <div>76%</div> <div>24%</div> </div>
3	9	513	<div> <div>38%</div> <div>48%</div> <div>24%</div> <div>•</div> <div>27%</div> </div>
4	A	913	<div> <div>19%</div> <div>37%</div> <div>9%</div> <div>54%</div> </div>
5	B	620	<div> <div>32%</div> <div>40%</div> <div>12%</div> <div>48%</div> </div>
6	C	616	<div> <div>42%</div> <div>72%</div> <div>17%</div> <div>12%</div> </div>
7	E	479	<div> <div>33%</div> <div>68%</div> <div>20%</div> <div>12%</div> </div>
8	D	529	<div> <div>25%</div> <div>63%</div> <div>20%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
9	F	435	
10	2	868	
11	3	971	
12	4	933	
13	5	775	
14	L	604	
15	6	1017	
16	7	845	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 52948 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 DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	34	Total	C	N	O	P	0	0
			694	340	101	220	33		

- Molecule 2 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	34	Total	C	N	O	P	0	0
			697	334	143	186	34		

- Molecule 3 is a protein called Cell division control protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	9	373	Total	C	N	O	S	0	0
			2962	1901	493	551	17		

- Molecule 4 is a protein called Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	420	Total	C	N	O	S	0	0
			3323	2125	556	624	18		

- Molecule 5 is a protein called Origin recognition complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	325	Total	C	N	O	S	0	0
			2640	1705	439	480	16		

- Molecule 6 is a protein called Origin recognition complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	544	Total	C	N	O	S	0	0
			4501	2906	742	838	15		

- Molecule 7 is a protein called Origin recognition complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	422	Total	C	N	O	S	0	0
			3418	2220	545	640	13		

- Molecule 8 is a protein called Origin recognition complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	436	Total	C	N	O	S	0	0
			3534	2262	601	658	13		

- Molecule 9 is a protein called Origin recognition complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	157	Total	C	N	O	S	0	0
			1315	846	222	235	12		

- Molecule 10 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	2	573	Total	C	N	O	S	0	0
			4274	2685	754	817	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	3	637	Total	C	N	O	S	0	0
			4773	3025	819	917	12		

- Molecule 12 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	4	650	Total	C	N	O	S	0	0
			4950	3104	846	975	25		

- Molecule 13 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	5	529	Total	C	N	O	S	0	0
			3955	2484	680	772	19		

- Molecule 14 is a protein called Cell division cycle protein CDT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	367	Total	C	N	O	S	0	0
			2898	1860	487	538	13		

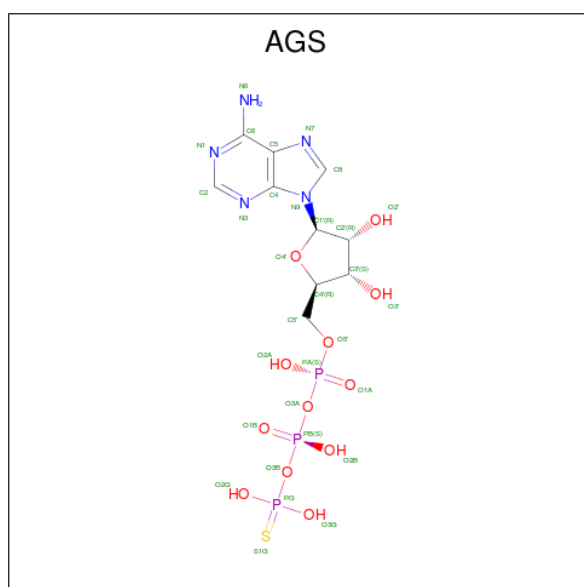
- Molecule 15 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	6	563	Total	C	N	O	S	0	0
			4187	2643	723	799	22		

- Molecule 16 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	7	625	Total	C	N	O	S	0	0
			4701	2966	798	908	29		

- 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).

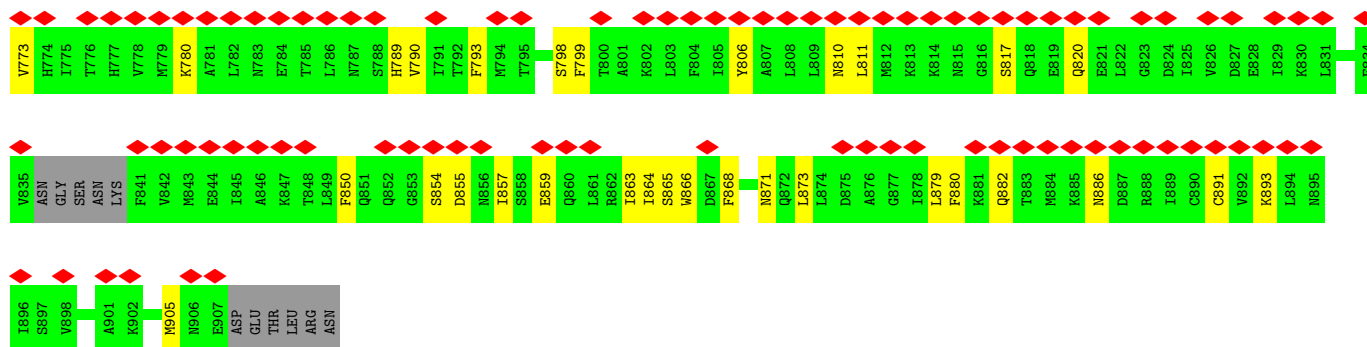


Mol	Chain	Residues	Atoms						AltConf
17	9	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

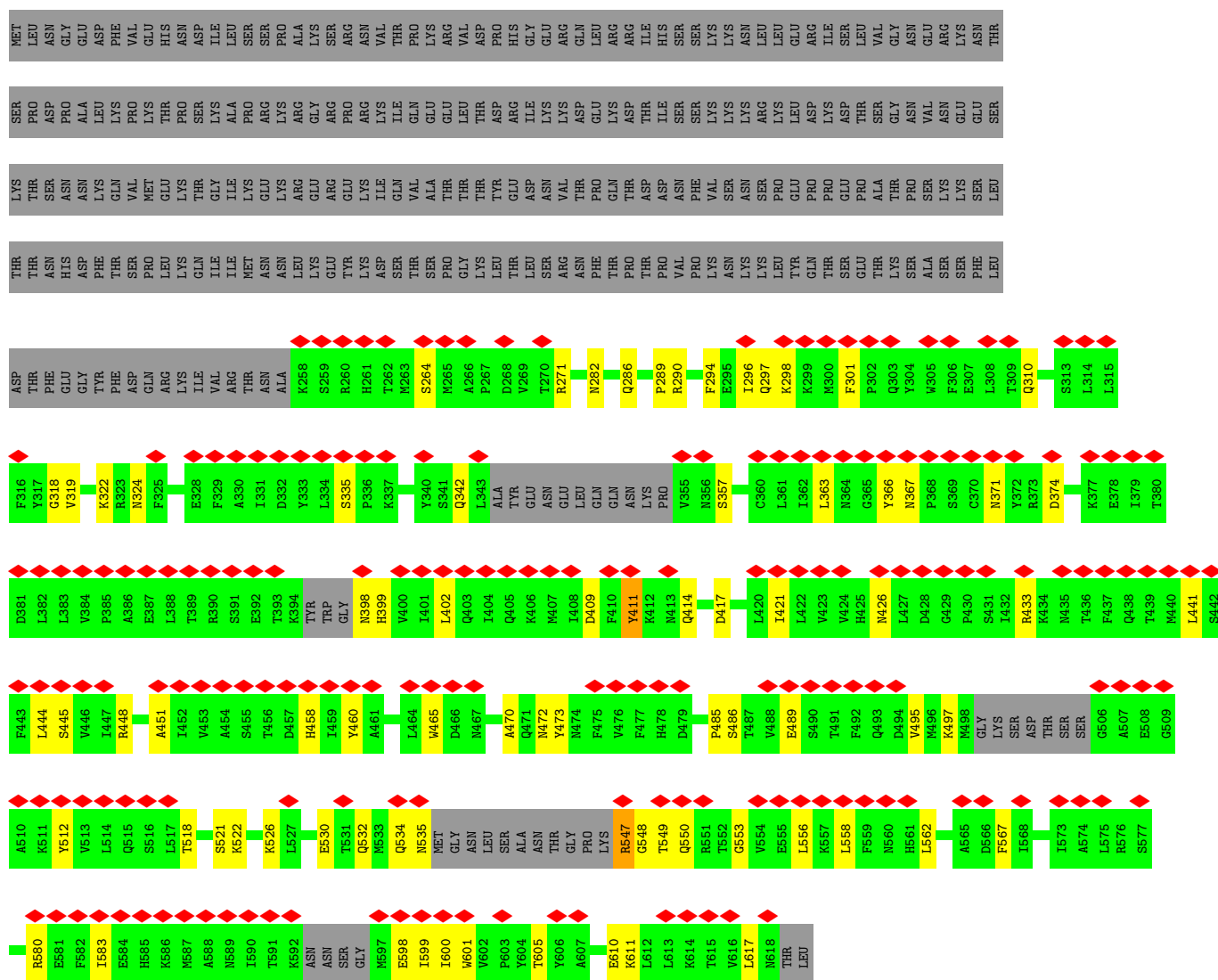
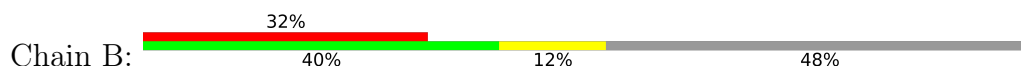
- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total 1	Mg 1	0
18	E	1	Total 1	Mg 1	0



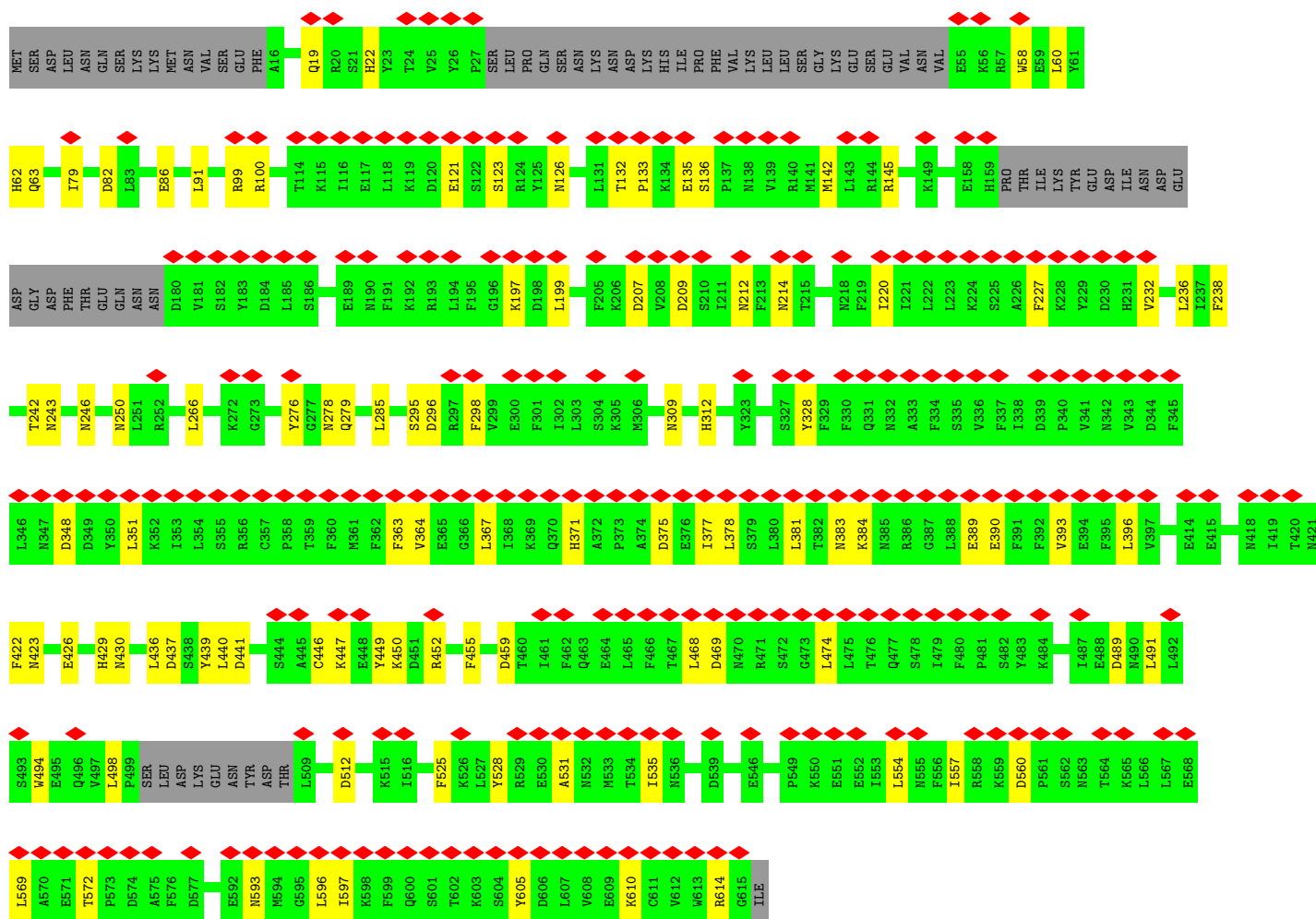


• Molecule 5: Origin recognition complex subunit 2

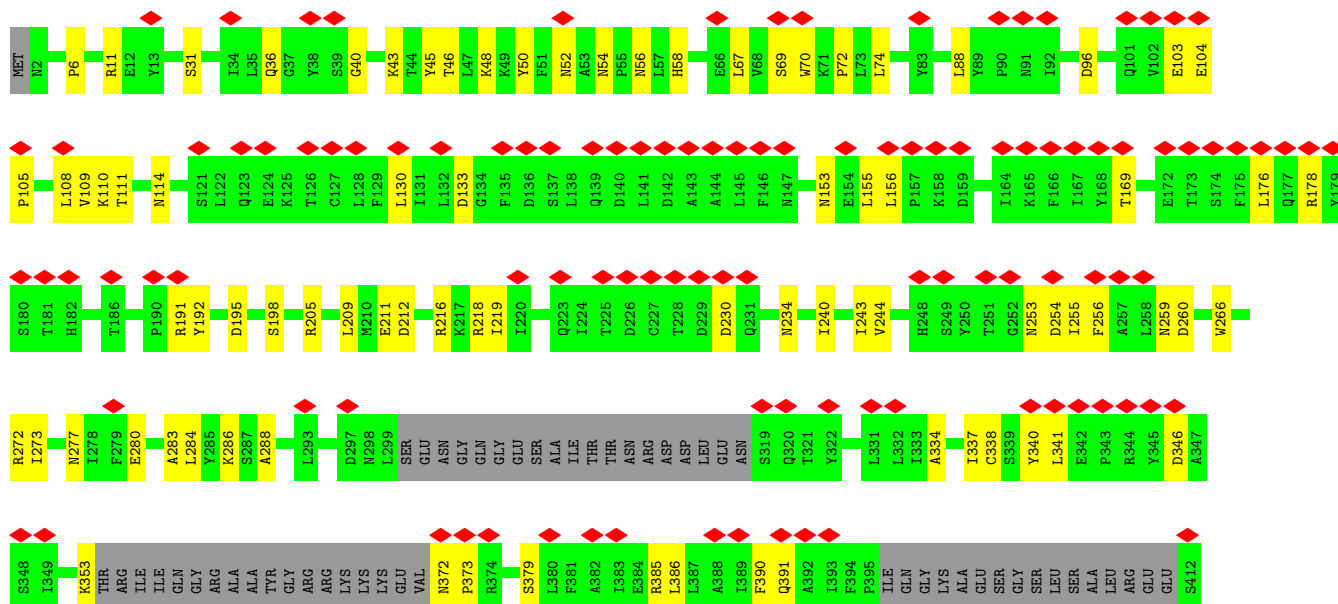


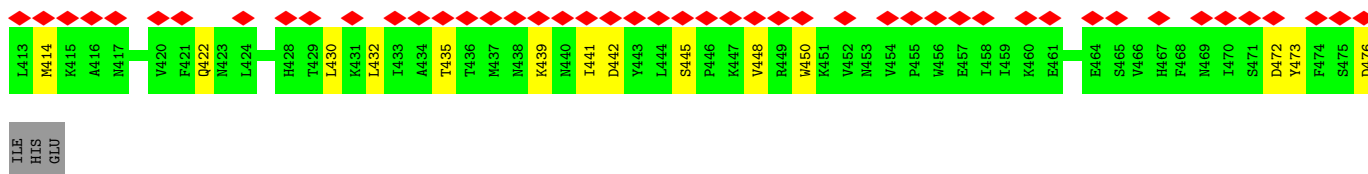
• Molecule 6: Origin recognition complex subunit 3



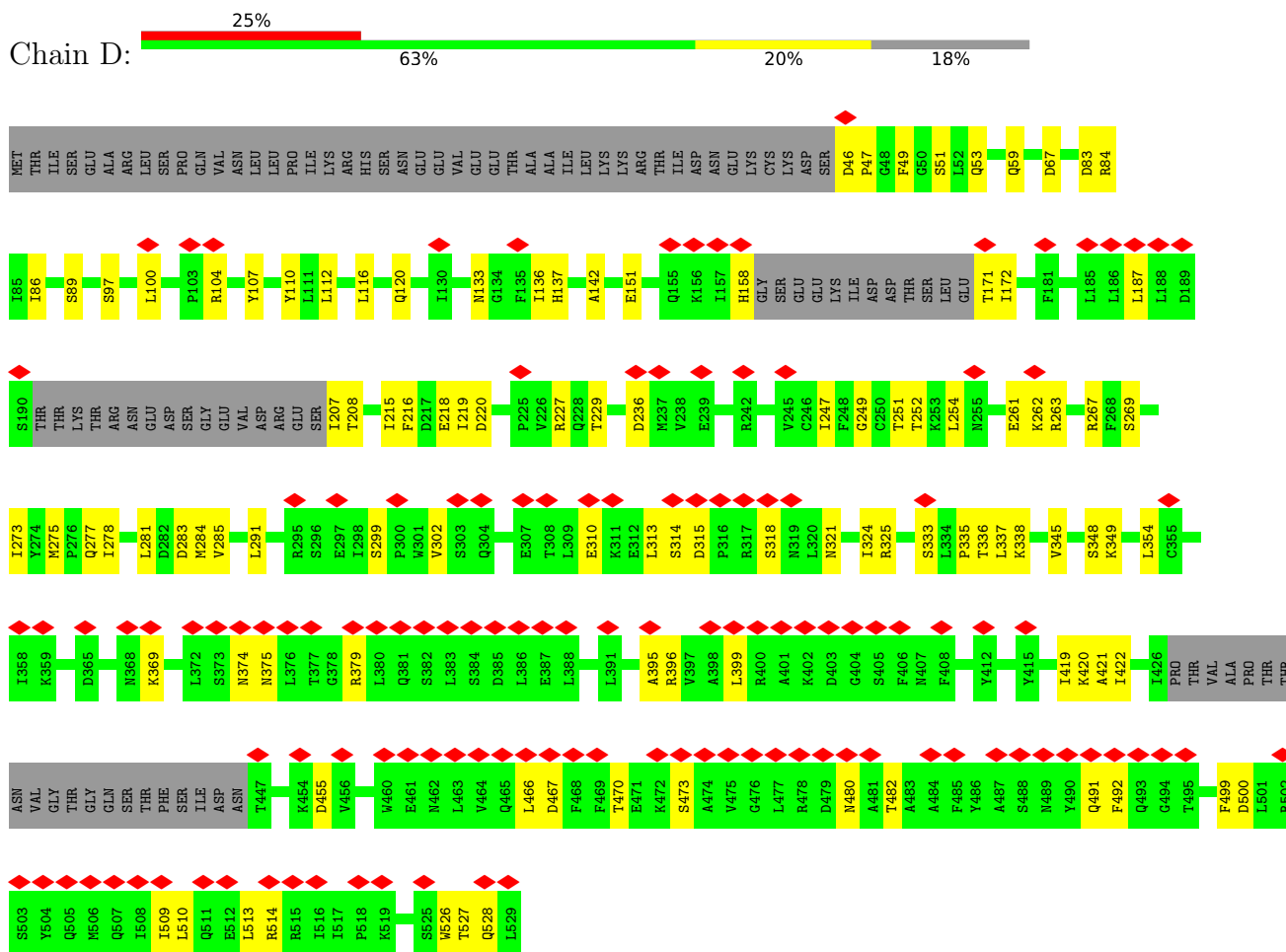


• Molecule 7: Origin recognition complex subunit 5

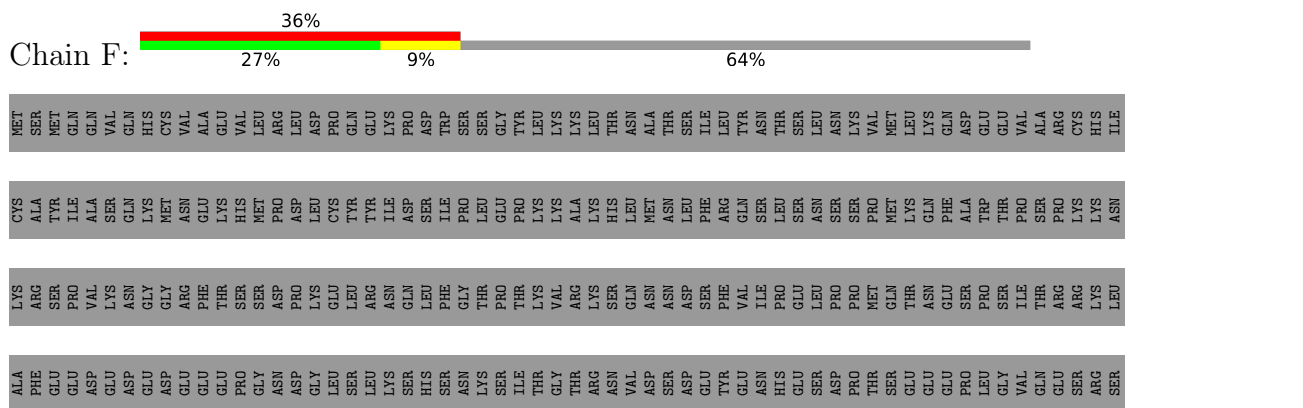




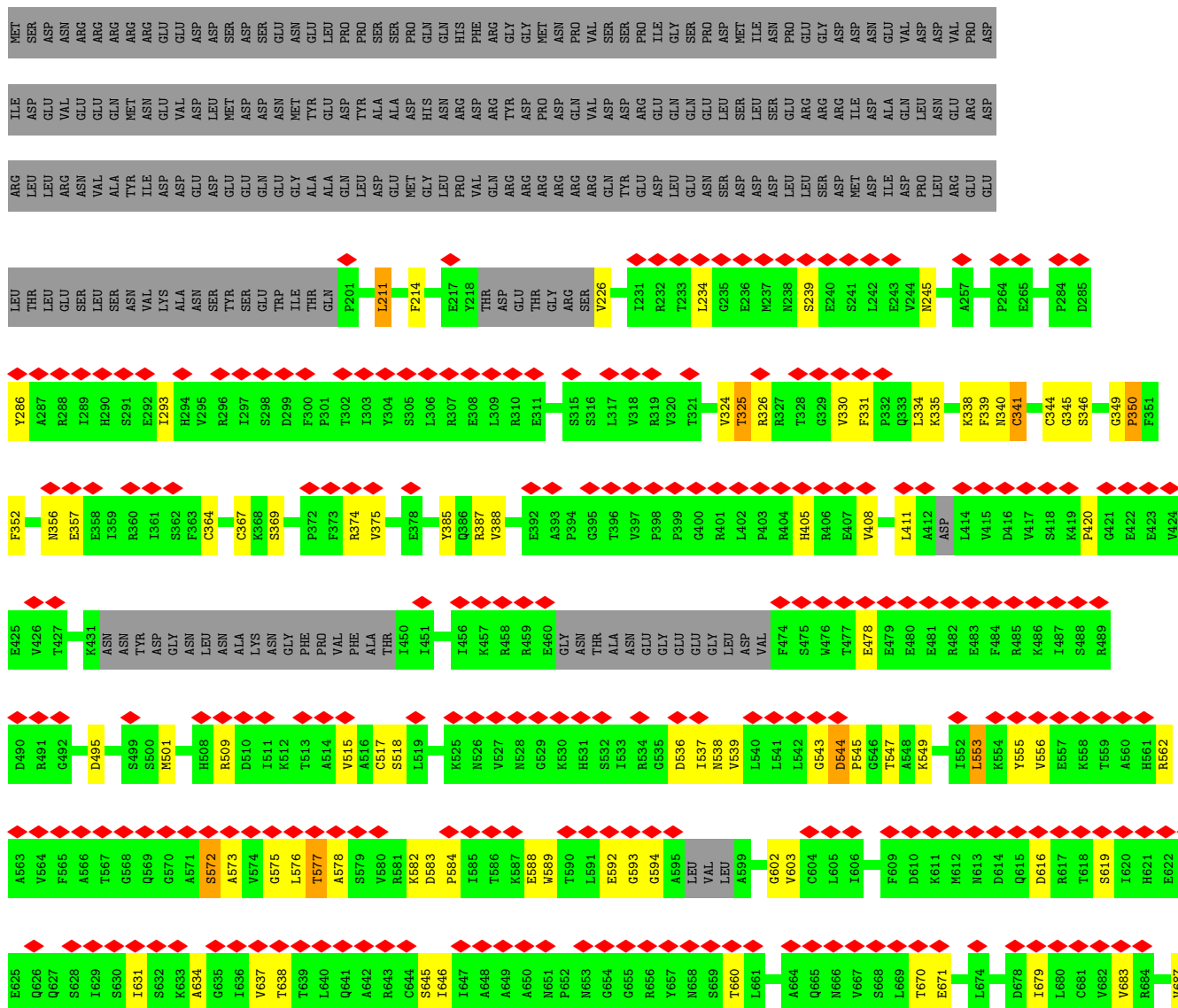
• Molecule 8: Origin recognition complex subunit 4

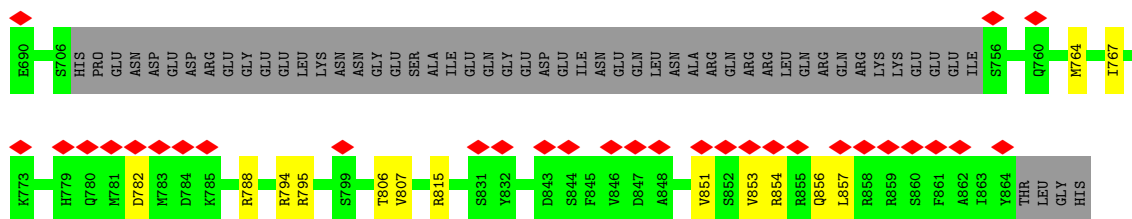


• Molecule 9: Origin recognition complex subunit 6

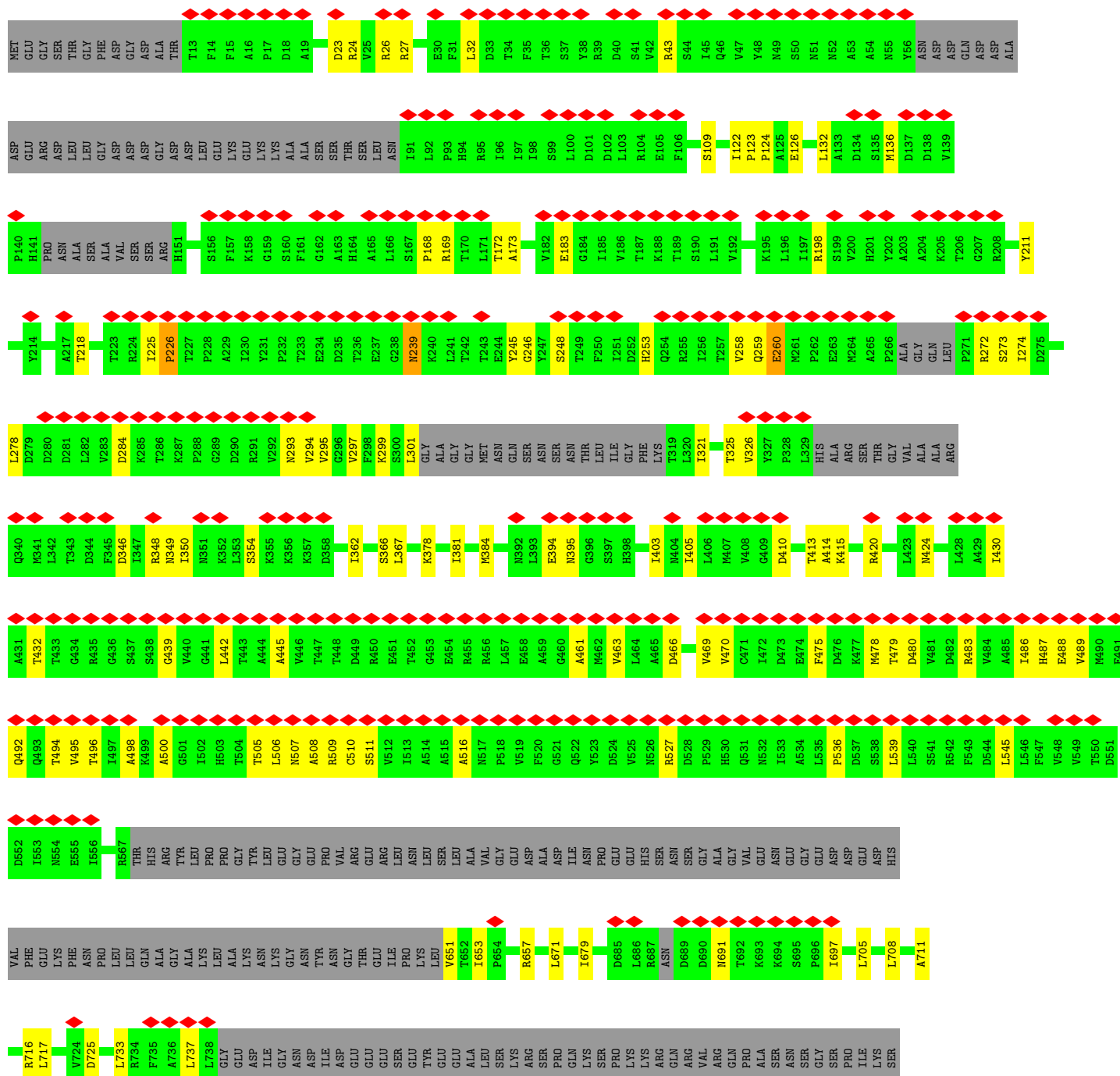


- Molecule 10: DNA replication licensing factor MCM2



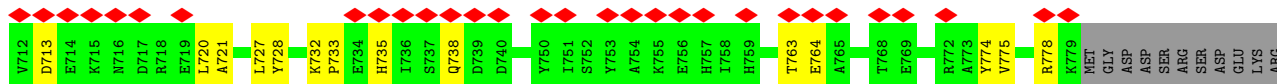
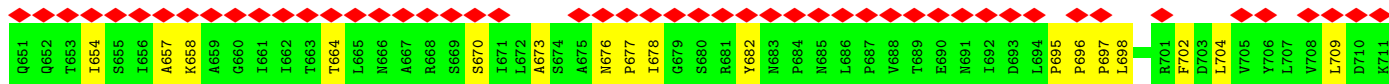
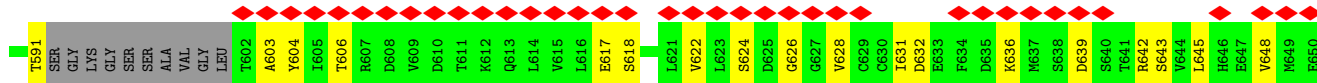
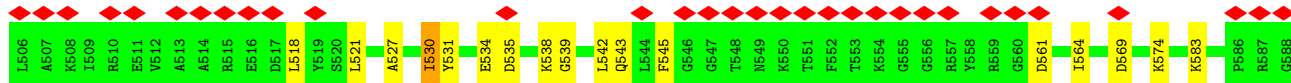
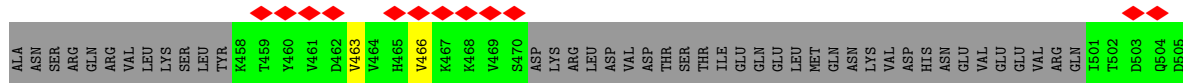
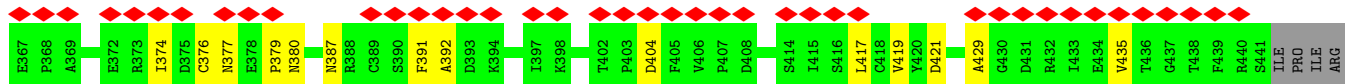
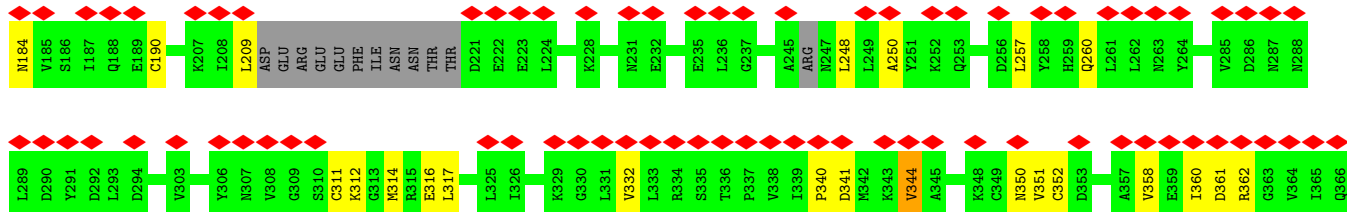
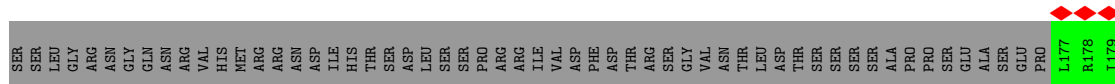


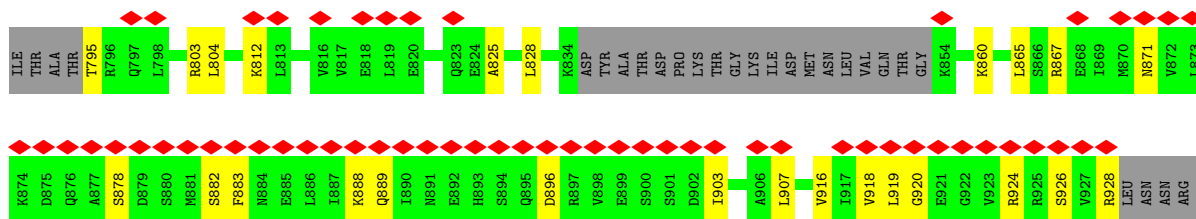
• Molecule 11: DNA replication licensing factor MCM3



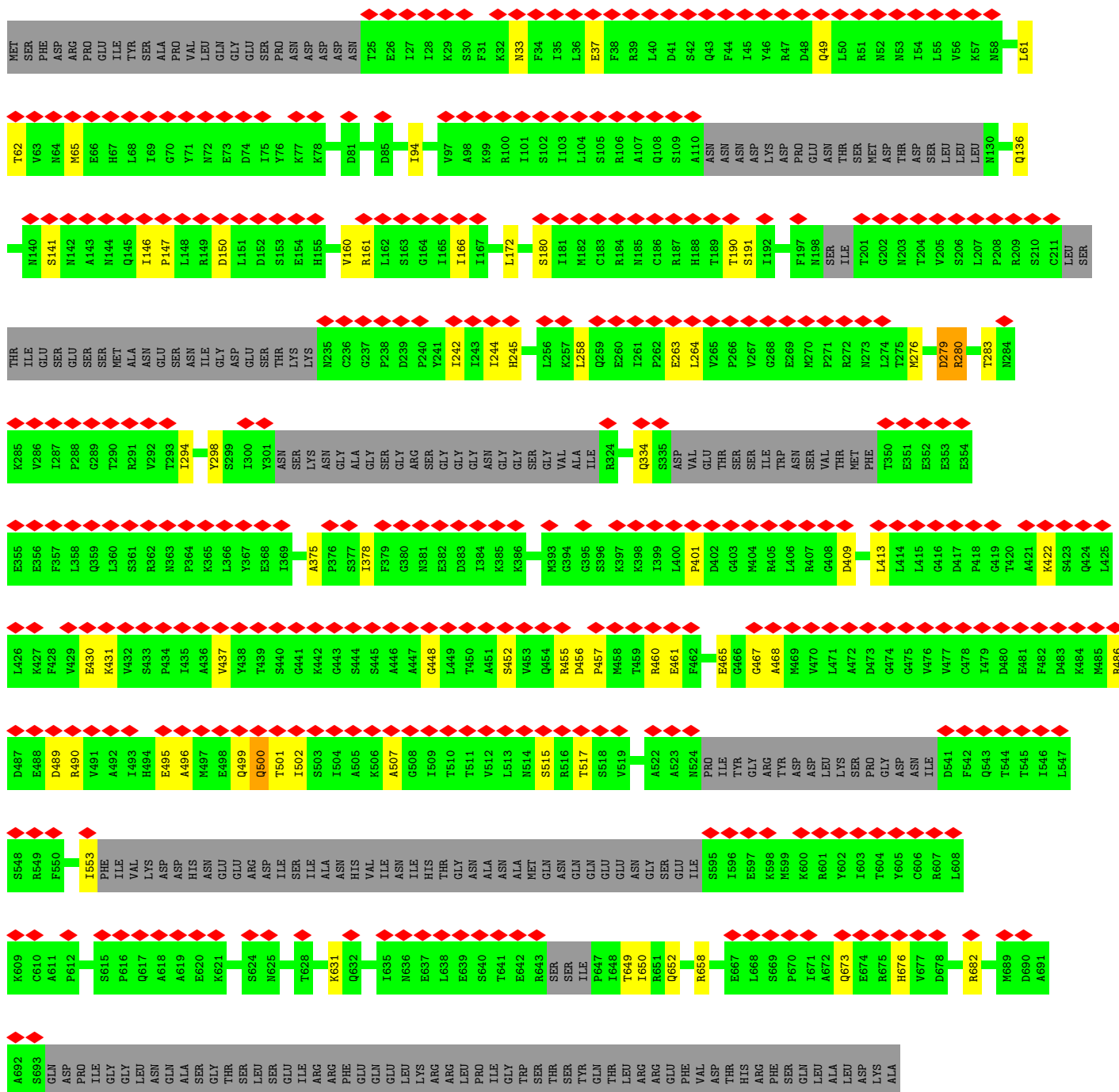


- Molecule 12: DNA replication licensing factor MCM4

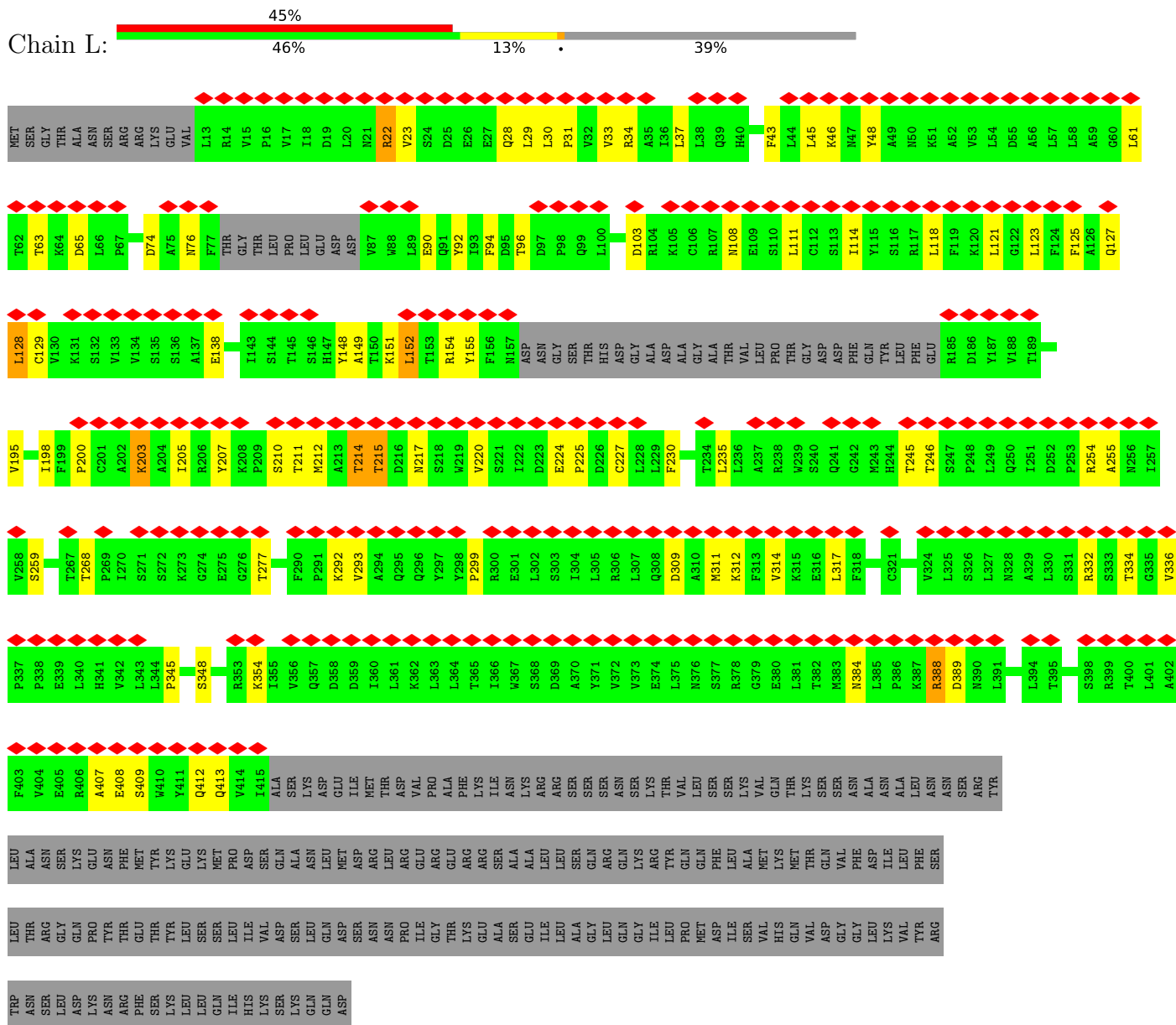




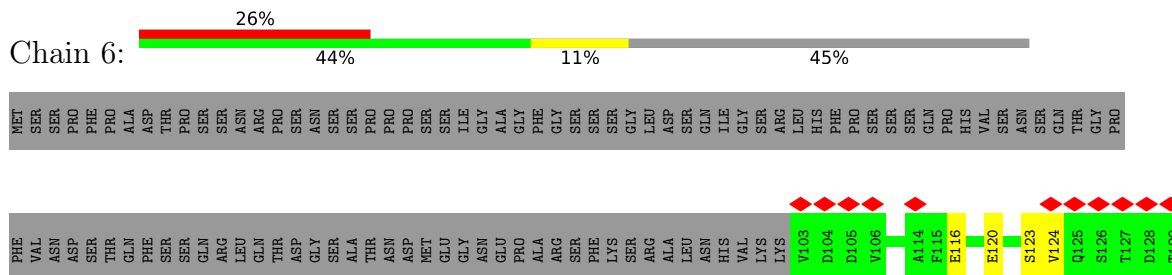
• Molecule 13: Minichromosome maintenance protein 5



Chain L:



Chain 6:





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27830	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	0.050	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0173	Depositor
Map size (Å)	335.36, 335.36, 335.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	G	0.78	0/772	1.13	0/1193
2	H	0.80	0/787	0.95	0/1209
3	9	0.32	0/3004	0.58	0/4042
4	A	0.34	0/3369	0.54	0/4536
5	B	0.34	0/2692	0.53	0/3629
6	C	0.34	0/4598	0.55	0/6208
7	E	0.38	0/3497	0.55	0/4756
8	D	0.36	0/3595	0.53	0/4859
9	F	0.29	0/1336	0.50	0/1798
10	2	0.39	0/4340	0.66	2/5873 (0.0%)
11	3	0.43	1/4850 (0.0%)	0.69	2/6597 (0.0%)
12	4	0.39	0/5014	0.69	4/6791 (0.1%)
13	5	0.39	0/4001	0.66	0/5423
14	L	0.47	0/2958	0.83	4/4028 (0.1%)
15	6	0.39	0/4256	0.63	0/5771
16	7	0.40	0/4761	0.64	1/6448 (0.0%)
All	All	0.40	1/53830 (0.0%)	0.65	13/73161 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	3	0	1
12	4	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	3	260	GLU	C-N	-10.03	1.10	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	3	717	LEU	CA-CB-CG	6.46	130.15	115.30
11	3	938	TYR	CA-CB-CG	6.45	125.65	113.40
14	L	152	LEU	CA-CB-CG	6.20	129.55	115.30
14	L	37	LEU	CA-CB-CG	5.87	128.80	115.30
10	2	687	VAL	N-CA-C	5.78	126.61	111.00
12	4	804	LEU	CA-CB-CG	5.75	128.53	115.30
14	L	128	LEU	CA-CB-CG	5.62	128.21	115.30
14	L	74	ASP	N-CA-C	-5.57	95.95	111.00
16	7	238	LEU	CA-CB-CG	5.47	127.88	115.30
12	4	896	ASP	N-CA-C	5.31	125.33	111.00
10	2	211	LEU	CA-CB-CG	5.10	127.03	115.30
12	4	907	LEU	CA-CB-CG	5.03	126.86	115.30
12	4	417	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	3	260	GLU	Mainchain
12	4	617	GLU	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	694	0	399	0	0
2	H	697	0	380	14	0
3	9	2962	0	3063	96	0
4	A	3323	0	3366	68	0
5	B	2640	0	2646	51	0
6	C	4501	0	4445	72	0
7	E	3418	0	3394	73	0
8	D	3534	0	3571	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	1315	0	1353	30	0
10	2	4274	0	4110	97	0
11	3	4773	0	4608	114	0
12	4	4950	0	4771	105	0
13	5	3955	0	3878	52	0
14	L	2898	0	2912	54	0
15	6	4187	0	3940	96	0
16	7	4701	0	4581	84	0
17	9	31	0	12	4	0
17	A	31	0	12	7	0
17	D	31	0	12	3	0
17	E	31	0	12	2	0
18	A	1	0	0	0	0
18	E	1	0	0	0	0
All	All	52948	0	51465	971	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 9.

All (971) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:35:DA:OP1	3:9:232:ASN:CB	1.95	1.14
10:2:576:LEU:CB	10:2:619:SER:HB3	1.78	1.13
7:E:340:TYR:CB	7:E:373:PRO:HB2	1.77	1.12
14:L:30:LEU:CD1	14:L:128:LEU:O	2.04	1.06
15:6:608:LEU:O	15:6:628:LEU:CB	2.04	1.05
10:2:584:PRO:HG2	15:6:619:GLY:HA3	1.40	1.02
11:3:494:THR:CB	11:3:507:ASN:OD1	2.09	1.00
14:L:23:VAL:HG21	14:L:29:LEU:HD12	1.39	1.00
2:H:35:DA:P	3:9:232:ASN:CB	2.50	0.98
2:H:39:DC:H3'	6:C:145:ARG:HH12	1.26	0.96
11:3:470:VAL:CG2	11:3:510:CYS:SG	2.58	0.91
12:4:603:ALA:HB2	12:4:618:SER:CB	2.02	0.90
12:4:603:ALA:CB	12:4:618:SER:CB	2.50	0.90
11:3:470:VAL:HG22	11:3:510:CYS:SG	2.13	0.88
14:L:30:LEU:HD13	14:L:128:LEU:O	1.75	0.84
14:L:94:PHE:O	14:L:149:ALA:HA	1.77	0.84
2:H:38:DA:H3'	5:B:398:ASN:N	1.92	0.84
10:2:544:ASP:O	10:2:549:LYS:NZ	2.10	0.83
2:H:39:DC:OP2	5:B:398:ASN:N	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:5:448:GLY:O	13:5:467:GLY:HA3	1.79	0.82
15:6:556:HIS:HB3	15:6:567:GLY:HA3	1.61	0.82
11:3:466:ASP:HA	11:3:508:ALA:HB1	1.60	0.82
11:3:466:ASP:O	11:3:509:ARG:N	2.12	0.81
2:H:39:DC:OP1	6:C:145:ARG:HD2	1.82	0.80
3:9:103:SER:HA	3:9:281:LEU:HD12	1.62	0.80
14:L:30:LEU:HD12	14:L:128:LEU:O	1.82	0.78
7:E:340:TYR:CB	7:E:373:PRO:CB	2.61	0.78
11:3:470:VAL:HG21	11:3:510:CYS:SG	2.24	0.78
11:3:168:PRO:C	11:3:272:ARG:CB	2.53	0.77
10:2:387:ARG:HA	10:2:408:VAL:O	1.84	0.77
2:H:14:DC:OP1	11:3:479:THR:HG21	1.85	0.76
2:H:29:DC:OP1	8:D:473:SER:OG	2.02	0.76
10:2:501:MET:O	10:2:555:TYR:CE2	2.38	0.76
2:H:34:DA:O3'	3:9:232:ASN:CB	2.34	0.76
16:7:738:GLU:HG2	16:7:740:PRO:HD3	1.68	0.76
10:2:576:LEU:CB	10:2:619:SER:CB	2.62	0.75
10:2:544:ASP:OD1	10:2:544:ASP:N	2.20	0.74
3:9:103:SER:HB3	3:9:281:LEU:HA	1.69	0.74
9:F:357:SER:HB2	10:2:788:ARG:HG2	1.70	0.74
10:2:478:GLU:CB	14:L:354:LYS:CB	2.65	0.74
15:6:551:MET:HE2	15:6:755:ILE:HD13	1.70	0.73
11:3:239:ASN:N	11:3:239:ASN:HD22	1.88	0.72
10:2:631:ILE:HD11	10:2:638:THR:HB	1.72	0.72
13:5:448:GLY:O	13:5:467:GLY:CA	2.38	0.71
12:4:721:ALA:HB2	16:7:664:TYR:CD2	2.25	0.71
2:H:39:DC:H3'	6:C:145:ARG:NH1	2.02	0.71
4:A:850:PHE:O	4:A:864:ILE:HD11	1.89	0.71
12:4:603:ALA:HB1	12:4:618:SER:CB	2.19	0.71
10:2:631:ILE:HG12	10:2:638:THR:O	1.90	0.71
12:4:340:PRO:HD3	15:6:452:ILE:HG13	1.72	0.71
12:4:696:PRO:HD2	12:4:697:PRO:HD2	1.73	0.71
16:7:588:ALA:O	16:7:592:SER:HB3	1.91	0.70
13:5:452:SER:HB2	13:5:465:GLU:HB2	1.73	0.70
16:7:251:VAL:HG23	16:7:340:VAL:HG21	1.73	0.70
11:3:123:PRO:HB2	11:3:124:PRO:CD	2.21	0.70
11:3:259:GLN:HA	11:3:272:ARG:O	1.92	0.70
8:D:396:ARG:HH21	15:6:691:ARG:NH2	1.89	0.70
14:L:23:VAL:CG2	14:L:29:LEU:HD12	2.18	0.70
15:6:355:ASP:N	15:6:355:ASP:OD1	2.24	0.70
10:2:326:ARG:H	10:2:592:GLU:CB	2.04	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2:631:ILE:HD11	10:2:638:THR:CB	2.21	0.69
3:9:281:LEU:N	3:9:281:LEU:HD22	2.08	0.69
7:E:435:THR:HG22	7:E:450:TRP:HE1	1.58	0.69
2:H:37:DA:OP2	5:B:371:ASN:CB	2.41	0.69
11:3:169:ARG:HA	11:3:272:ARG:CB	2.22	0.69
12:4:728:TYR:CE1	16:7:697:GLN:NE2	2.61	0.69
16:7:508:LEU:HD13	16:7:508:LEU:C	2.13	0.69
11:3:274:ILE:HD12	11:3:321:ILE:HD13	1.75	0.68
13:5:280:ARG:HD3	13:5:280:ARG:N	2.08	0.68
15:6:298:SER:OG	15:6:358:LYS:O	2.09	0.68
3:9:103:SER:HA	3:9:281:LEU:CD1	2.23	0.68
13:5:486:ARG:O	13:5:489:ASP:OD1	2.11	0.68
10:2:226:VAL:CB	14:L:215:THR:CB	2.71	0.68
11:3:671:LEU:HD12	16:7:621:MET:HB2	1.74	0.68
10:2:584:PRO:HG2	15:6:619:GLY:CA	2.22	0.67
16:7:461:ASP:CB	16:7:462:PRO:HD2	2.24	0.67
10:2:501:MET:SD	10:2:555:TYR:HE2	2.18	0.67
13:5:495:GLU:O	13:5:499:GLN:OE1	2.11	0.67
11:3:420:ARG:HH11	13:5:499:GLN:HG2	1.59	0.67
13:5:500:GLN:O	13:5:515:SER:HB3	1.94	0.67
15:6:394:ARG:HH12	15:6:593:PRO:HB2	1.57	0.67
16:7:506:MET:SD	16:7:553:ILE:CB	2.83	0.67
12:4:696:PRO:CD	12:4:697:PRO:HD2	2.24	0.67
12:4:697:PRO:HA	15:6:577:PRO:HB3	1.77	0.66
12:4:812:LYS:O	12:4:812:LYS:HG2	1.95	0.66
14:L:214:THR:HG21	14:L:220:VAL:HG21	1.77	0.66
5:B:567:PHE:CB	11:3:950:ASN:CB	2.74	0.66
12:4:697:PRO:HA	15:6:577:PRO:CB	2.26	0.66
13:5:457:PRO:HA	13:5:460:ARG:HH21	1.61	0.66
15:6:317:ILE:HG21	15:6:350:ARG:NH2	2.11	0.66
11:3:274:ILE:HD12	11:3:321:ILE:CD1	2.25	0.66
12:4:696:PRO:N	12:4:697:PRO:HD2	2.12	0.66
4:A:857:ILE:HG21	8:D:369:LYS:HA	1.78	0.65
16:7:500:ASP:O	16:7:504:ASP:HA	1.96	0.65
10:2:631:ILE:O	10:2:631:ILE:HG13	1.97	0.65
11:3:274:ILE:CD1	11:3:321:ILE:HD13	2.26	0.65
8:D:324:ILE:HG12	8:D:337:LEU:HD11	1.79	0.65
10:2:331:PHE:O	10:2:385:TYR:CB	2.45	0.65
12:4:583:LYS:HD2	16:7:447:GLY:O	1.96	0.65
11:3:483:ARG:O	11:3:487:HIS:CD2	2.50	0.65
3:9:118:LEU:HA	3:9:121:ILE:HD12	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:333:ASN:HA	9:F:336:ARG:HB2	1.77	0.65
5:B:421:ILE:HG22	5:B:451:ALA:HB3	1.78	0.64
11:3:218:THR:O	11:3:299:LYS:NZ	2.29	0.64
12:4:379:PRO:O	12:4:380:ASN:ND2	2.31	0.64
3:9:245:LEU:HB3	3:9:258:LEU:HD11	1.79	0.64
7:E:338:CYS:SG	7:E:385:ARG:NH1	2.71	0.64
10:2:631:ILE:CD1	10:2:638:THR:HB	2.28	0.64
2:H:14:DC:OP1	11:3:479:THR:CG2	2.45	0.64
6:C:298:PHE:HB2	6:C:469:ASP:HA	1.79	0.64
10:2:631:ILE:HG13	10:2:638:THR:H	1.62	0.64
11:3:169:ARG:N	11:3:272:ARG:CB	2.61	0.64
7:E:337:ILE:O	7:E:341:LEU:HD23	1.98	0.64
10:2:547:THR:O	10:2:549:LYS:NZ	2.24	0.64
13:5:264:LEU:HD22	13:5:431:LYS:HD2	1.79	0.63
11:3:671:LEU:HB2	16:7:621:MET:SD	2.38	0.63
16:7:517:ASP:O	16:7:560:ARG:O	2.16	0.63
4:A:859:GLU:O	4:A:859:GLU:HG2	1.99	0.62
10:2:589:TRP:CB	10:2:634:ALA:HB1	2.30	0.62
12:4:698:LEU:O	12:4:702:PHE:HD2	1.81	0.62
15:6:399:GLY:HA3	15:6:455:LEU:O	1.99	0.62
15:6:551:MET:CE	15:6:755:ILE:HD13	2.29	0.62
3:9:113:GLY:HA2	17:9:2001:AGS:H3'	1.80	0.62
12:4:624:SER:C	12:4:626:GLY:H	2.02	0.62
3:9:505:ILE:HG13	3:9:505:ILE:O	1.99	0.61
6:C:132:THR:O	6:C:135:GLU:N	2.32	0.61
10:2:338:LYS:HD3	10:2:349:GLY:HA3	1.82	0.61
16:7:768:THR:O	16:7:772:ARG:HB3	2.00	0.61
15:6:307:ALA:HA	15:6:351:SER:HB3	1.82	0.61
3:9:315:MET:HA	3:9:318:LYS:HD2	1.82	0.61
11:3:274:ILE:CD1	11:3:321:ILE:CD1	2.78	0.61
3:9:412:ILE:HG21	16:7:745:PHE:CZ	2.35	0.61
5:B:294:PHE:HA	5:B:297:GLN:HE21	1.65	0.61
15:6:555:VAL:HG13	15:6:555:VAL:O	2.00	0.61
15:6:576:ASP:CB	15:6:577:PRO:HD2	2.30	0.61
12:4:341:ASP:O	12:4:392:ALA:N	2.34	0.61
11:3:198:ARG:O	11:3:198:ARG:HG2	2.01	0.60
12:4:340:PRO:HD3	15:6:452:ILE:CG1	2.31	0.60
11:3:122:ILE:N	11:3:123:PRO:CD	2.64	0.60
12:4:643:SER:CB	15:6:601:LYS:CB	2.79	0.60
11:3:442:LEU:HB3	11:3:461:ALA:HB3	1.83	0.60
11:3:169:ARG:CA	11:3:272:ARG:CB	2.79	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:92:TYR:HB2	14:L:152:LEU:HB2	1.84	0.60
5:B:319:VAL:HG21	6:C:491:LEU:HD21	1.82	0.60
15:6:582:SER:O	15:6:585:LEU:HB3	2.01	0.60
3:9:171:ASN:HA	3:9:223:ASP:HB2	1.83	0.60
10:2:330:VAL:HG12	10:2:330:VAL:O	2.01	0.60
6:C:328:TYR:HB2	6:C:468:LEU:HD21	1.84	0.59
3:9:331:LEU:O	3:9:335:PHE:N	2.35	0.59
10:2:341:CYS:O	10:2:345:GLY:HA2	2.03	0.59
15:6:306:LYS:O	15:6:351:SER:HB2	2.02	0.59
4:A:722:MET:HB3	8:D:84:ARG:HH22	1.67	0.59
3:9:240:ARG:NH2	3:9:241:THR:OG1	2.35	0.59
8:D:278:ILE:HG23	8:D:283:ASP:HB2	1.84	0.59
13:5:455:ARG:HA	13:5:461:GLU:O	2.03	0.59
14:L:214:THR:HG23	14:L:214:THR:O	2.03	0.59
11:3:246:GLY:CA	16:7:109:ASN:HA	2.32	0.59
5:B:486:SER:HB2	5:B:489:GLU:HB2	1.85	0.59
12:4:527:ALA:HB3	12:4:530:ILE:HD11	1.84	0.59
12:4:604:TYR:CE1	12:4:606:THR:OG1	2.56	0.59
12:4:698:LEU:O	12:4:702:PHE:CD2	2.56	0.58
5:B:470:ALA:HA	5:B:473:TYR:HB2	1.85	0.58
8:D:379:ARG:HH12	8:D:467:ASP:HB2	1.68	0.58
14:L:293:VAL:HG11	14:L:299:PRO:HB2	1.85	0.58
15:6:560:VAL:HG22	15:6:560:VAL:O	2.02	0.58
3:9:197:LEU:O	3:9:204:HIS:ND1	2.36	0.58
7:E:50:TYR:O	7:E:54:ASN:ND2	2.35	0.58
12:4:591:THR:O	12:4:631:ILE:HA	2.03	0.58
13:5:279:ASP:O	13:5:283:THR:CG2	2.52	0.58
3:9:115:THR:OG1	17:9:2001:AGS:S1G	2.62	0.58
4:A:790:VAL:HG12	8:D:254:LEU:HD13	1.85	0.58
5:B:318:GLY:O	5:B:322:LYS:NZ	2.37	0.58
17:A:2001:AGS:O2G	8:D:267:ARG:NH1	2.37	0.58
8:D:133:ASN:HB3	8:D:136:ILE:HG22	1.85	0.58
10:2:356:ASN:OD1	10:2:357:GLU:N	2.34	0.57
8:D:528:GLN:NE2	15:6:719:CYS:H	2.02	0.57
12:4:728:TYR:HE1	16:7:697:GLN:NE2	2.01	0.57
15:6:307:ALA:HA	15:6:351:SER:CB	2.35	0.57
16:7:436:LEU:CD1	16:7:642:ILE:HD13	2.34	0.57
7:E:353:LYS:O	7:E:353:LYS:HG3	2.02	0.57
4:A:607:ARG:HE	4:A:608:GLN:HE22	1.51	0.57
4:A:806:TYR:O	4:A:810:ASN:ND2	2.37	0.57
15:6:609:THR:CB	15:6:651:ALA:HB1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:4:778:ARG:O	15:6:719:CYS:CB	2.53	0.57
10:2:334:LEU:O	10:2:352:PHE:O	2.22	0.57
15:6:690:ASN:HB2	15:6:692:LYS:HG2	1.86	0.57
8:D:261:GLU:OE2	8:D:263:ARG:NH1	2.38	0.56
12:4:604:TYR:HE1	12:4:606:THR:OG1	1.87	0.56
14:L:336:VAL:HG23	14:L:336:VAL:O	2.04	0.56
7:E:283:ALA:HA	7:E:286:LYS:HD2	1.86	0.56
4:A:560:THR:HG23	4:A:592:LYS:HB3	1.87	0.56
4:A:625:THR:OG1	4:A:626:GLY:N	2.38	0.56
4:A:704:ARG:HG3	17:A:2001:AGS:H5'2	1.88	0.56
4:A:789:HIS:O	4:A:793:PHE:N	2.32	0.56
6:C:309:ASN:ND2	6:C:312:HIS:O	2.38	0.56
10:2:584:PRO:CG	15:6:619:GLY:HA3	2.25	0.56
4:A:421:THR:OG1	4:A:422:ILE:N	2.39	0.56
7:E:435:THR:HG21	7:E:442:ASP:CG	2.26	0.56
10:2:544:ASP:OD1	10:2:683:VAL:HG23	2.06	0.56
11:3:122:ILE:N	11:3:123:PRO:HD2	2.20	0.56
11:3:284:ASP:OD2	16:7:231:LYS:HG2	2.06	0.56
4:A:850:PHE:C	4:A:864:ILE:HD11	2.26	0.56
7:E:216:ARG:HA	7:E:219:ILE:HD12	1.88	0.56
12:4:534:GLU:O	12:4:538:LYS:HB2	2.06	0.56
7:E:103:GLU:HG2	7:E:104:GLU:HG2	1.87	0.56
11:3:246:GLY:HA3	16:7:109:ASN:HA	1.87	0.56
7:E:31:SER:OG	7:E:153:ASN:ND2	2.39	0.56
9:F:328:THR:HA	9:F:331:VAL:HG12	1.88	0.56
10:2:515:VAL:CG1	10:2:556:VAL:HG21	2.35	0.56
11:3:432:THR:HG21	11:3:442:LEU:HD11	1.88	0.56
16:7:722:VAL:HA	16:7:725:GLU:HB2	1.88	0.56
15:6:656:MET:HA	15:6:656:MET:HE3	1.86	0.55
6:C:242:THR:OG1	6:C:243:ASN:N	2.40	0.55
6:C:378:LEU:O	6:C:383:ASN:ND2	2.38	0.55
6:C:528:TYR:O	6:C:610:LYS:NZ	2.38	0.55
13:5:456:ASP:HB3	13:5:461:GLU:HB2	1.88	0.55
16:7:506:MET:SD	16:7:552:GLY:O	2.65	0.55
12:4:721:ALA:HB2	16:7:664:TYR:HD2	1.72	0.55
10:2:631:ILE:HD11	10:2:638:THR:OG1	2.05	0.55
3:9:473:ILE:HG22	3:9:489:ILE:HG22	1.89	0.55
4:A:413:THR:HA	8:D:207:ILE:HD12	1.89	0.55
4:A:704:ARG:NH2	17:A:2001:AGS:O3A	2.39	0.55
7:E:153:ASN:OD1	7:E:153:ASN:N	2.40	0.55
7:E:430:LEU:HB3	7:E:432:LEU:HG	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:30:LEU:N	14:L:31:PRO:HD2	2.22	0.55
3:9:94:LYS:HB3	3:9:99:HIS:HB3	1.88	0.55
8:D:514:ARG:NH2	15:6:720:ASN:OD1	2.39	0.55
13:5:65:MET:SD	13:5:161:ARG:NH2	2.78	0.55
3:9:60:ALA:O	3:9:64:LYS:N	2.40	0.55
3:9:268:LYS:NZ	5:B:512:TYR:OH	2.40	0.55
6:C:209:ASP:OD1	6:C:209:ASP:N	2.37	0.55
7:E:6:PRO:HG3	7:E:50:TYR:HA	1.89	0.55
3:9:234:SER:OG	3:9:235:GLU:N	2.40	0.55
3:9:464:ILE:HG12	4:A:699:VAL:HA	1.89	0.55
12:4:340:PRO:HG3	15:6:452:ILE:HG12	1.89	0.55
10:2:573:ALA:HB3	15:6:664:ALA:O	2.06	0.55
10:2:764:MET:HA	10:2:767:ILE:HD12	1.89	0.55
7:E:218:ARG:NH2	7:E:273:ILE:O	2.40	0.54
11:3:246:GLY:HA3	16:7:109:ASN:CB	2.36	0.54
12:4:654:ILE:O	12:4:664:THR:HA	2.07	0.54
3:9:412:ILE:HG21	16:7:745:PHE:HZ	1.71	0.54
13:5:264:LEU:HD22	13:5:431:LYS:CE	2.37	0.54
16:7:260:TYR:HB3	16:7:298:LEU:HD12	1.88	0.54
4:A:857:ILE:HG23	4:A:857:ILE:O	2.07	0.54
5:B:282:ASN:HB3	5:B:485:PRO:HG3	1.90	0.54
12:4:645:LEU:HA	12:4:648:VAL:HG22	1.88	0.54
4:A:404:SER:OG	4:A:405:ARG:N	2.40	0.54
8:D:313:LEU:O	8:D:321:ASN:ND2	2.41	0.54
11:3:168:PRO:O	11:3:272:ARG:CB	2.55	0.54
11:3:405:ILE:HG12	11:3:545:LEU:HB2	1.89	0.54
6:C:375:ASP:N	6:C:375:ASP:OD1	2.40	0.54
12:4:561:ASP:H	12:4:803:ARG:HD2	1.73	0.54
15:6:635:ILE:HG12	15:6:677:SER:OG	2.08	0.54
3:9:292:THR:OG1	3:9:293:ALA:N	2.38	0.54
7:E:230:ASP:O	7:E:234:ASN:ND2	2.41	0.54
11:3:123:PRO:HB2	11:3:124:PRO:HD3	1.89	0.54
17:A:2001:AGS:O2A	17:A:2001:AGS:O1B	2.25	0.54
11:3:495:VAL:HG22	11:3:496:THR:N	2.23	0.54
7:E:56:ASN:OD1	7:E:56:ASN:N	2.41	0.53
8:D:47:PRO:O	8:D:51:SER:N	2.40	0.53
12:4:344:VAL:HG12	12:4:358:VAL:O	2.07	0.53
6:C:199:LEU:HB3	6:C:232:VAL:HG12	1.88	0.53
8:D:375:ASN:O	8:D:379:ARG:NE	2.40	0.53
7:E:442:ASP:HA	7:E:448:VAL:HG21	1.91	0.53
10:2:286:TYR:HE2	10:2:293:ILE:HD11	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:4:583:LYS:HD3	16:7:447:GLY:HA2	1.91	0.53
3:9:491:VAL:HG22	3:9:493:LEU:H	1.73	0.53
12:4:429:ALA:O	15:6:371:GLY:O	2.27	0.53
6:C:381:LEU:HD21	9:F:422:LYS:HE3	1.90	0.53
8:D:97:SER:HB2	8:D:247:ILE:HB	1.91	0.53
11:3:469:VAL:HG12	11:3:511:SER:HB3	1.91	0.53
14:L:123:LEU:O	14:L:127:GLN:NE2	2.42	0.53
11:3:733:LEU:O	11:3:737:LEU:HB2	2.08	0.53
13:5:489:ASP:OD1	13:5:490:ARG:N	2.42	0.53
16:7:118:CYS:SG	16:7:198:ARG:NH2	2.82	0.53
2:H:39:DC:O5'	6:C:145:ARG:NH1	2.41	0.53
3:9:283:PRO:O	3:9:285:THR:N	2.42	0.53
5:B:547:ARG:NH1	5:B:548:GLY:O	2.42	0.53
9:F:329:PHE:O	9:F:336:ARG:NH2	2.42	0.53
12:4:543:GLN:NE2	12:4:670:SER:OG	2.42	0.53
8:D:53:GLN:NE2	8:D:345:VAL:O	2.42	0.52
9:F:291:ASP:OD1	9:F:291:ASP:N	2.38	0.52
11:3:915:PRO:HA	11:3:958:VAL:HA	1.90	0.52
5:B:363:LEU:HD13	6:C:22:HIS:HB3	1.91	0.52
14:L:34:ARG:HD2	14:L:34:ARG:O	2.09	0.52
15:6:167:ALA:O	15:6:171:SER:HB3	2.09	0.52
15:6:304:LEU:HD11	15:6:307:ALA:HB2	1.91	0.52
3:9:475:LYS:HB3	3:9:485:PHE:HB3	1.90	0.52
11:3:691:ASN:HD21	11:3:697:ILE:H	1.56	0.52
3:9:494:ASP:OD1	3:9:494:ASP:N	2.41	0.52
9:F:376:GLU:O	9:F:380:ARG:NH2	2.40	0.52
13:5:136:GLN:HB2	13:5:280:ARG:HH21	1.73	0.52
5:B:526:LYS:NZ	5:B:530:GLU:OE2	2.40	0.52
10:2:411:LEU:C	10:2:411:LEU:HD12	2.30	0.52
17:9:2001:AGS:S1G	17:9:2001:AGS:O2B	2.68	0.52
8:D:251:THR:OG1	8:D:252:THR:N	2.43	0.52
3:9:226:ASP:HA	3:9:229:LEU:HB2	1.91	0.52
3:9:495:MET:SD	3:9:495:MET:N	2.82	0.52
7:E:439:LYS:NZ	8:D:491:GLN:OE1	2.41	0.52
10:2:341:CYS:O	10:2:345:GLY:CA	2.58	0.52
10:2:854:ARG:HA	10:2:857:LEU:HD13	1.92	0.52
15:6:734:LEU:HD13	15:6:742:ILE:HG21	1.91	0.52
8:D:528:GLN:NE2	15:6:719:CYS:N	2.58	0.52
3:9:61:LEU:HA	3:9:64:LYS:HB2	1.92	0.52
5:B:342:GLN:NE2	5:B:417:ASP:OD1	2.43	0.52
7:E:96:ASP:OD1	7:E:96:ASP:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:3:466:ASP:O	11:3:509:ARG:CB	2.58	0.52
13:5:264:LEU:HD22	13:5:431:LYS:CD	2.40	0.52
14:L:33:VAL:HG21	14:L:128:LEU:HD12	1.92	0.52
14:L:96:THR:HB	14:L:148:TYR:H	1.74	0.52
3:9:330:ASP:OD1	3:9:330:ASP:N	2.41	0.52
4:A:543:MET:HA	4:A:546:LEU:HB2	1.91	0.52
5:B:367:ASN:ND2	6:C:19:GLN:O	2.43	0.52
6:C:278:ASN:ND2	6:C:422:PHE:O	2.36	0.52
7:E:341:LEU:N	7:E:341:LEU:HD22	2.25	0.52
14:L:108:ASN:HB2	14:L:111:LEU:HB3	1.92	0.52
7:E:192:TYR:O	7:E:253:ASN:ND2	2.44	0.51
8:D:236:ASP:OD2	8:D:267:ARG:NE	2.39	0.51
14:L:151:LYS:HB2	14:L:259:SER:HB3	1.92	0.51
3:9:226:ASP:OD2	4:A:612:LYS:NZ	2.43	0.51
3:9:345:TYR:OH	3:9:388:ASN:ND2	2.42	0.51
11:3:32:LEU:HD13	11:3:132:LEU:HD22	1.90	0.51
12:4:564:ILE:HG22	12:4:704:LEU:HB3	1.91	0.51
16:7:766:VAL:HG12	16:7:779:LEU:HD21	1.91	0.51
4:A:481:PRO:O	8:D:262:LYS:NZ	2.43	0.51
7:E:133:ASP:HA	7:E:169:THR:HB	1.93	0.51
9:F:305:GLU:O	9:F:309:ASN:ND2	2.43	0.51
10:2:806:THR:OG1	10:2:807:VAL:N	2.43	0.51
13:5:280:ARG:N	13:5:280:ARG:CD	2.73	0.51
6:C:554:LEU:HA	6:C:557:ILE:HG22	1.93	0.51
12:4:795:THR:HG22	15:6:727:LEU:HD21	1.91	0.51
9:F:306:TYR:O	9:F:310:ALA:N	2.43	0.51
13:5:190:THR:OG1	13:5:191:SER:N	2.43	0.51
5:B:556:LEU:CD2	5:B:600:ILE:HG23	2.41	0.51
7:E:195:ASP:N	7:E:195:ASP:OD1	2.40	0.51
8:D:491:GLN:NE2	8:D:492:PHE:O	2.43	0.51
10:2:575:GLY:HA3	10:2:616:ASP:HA	1.91	0.51
11:3:27:ARG:NH2	11:3:109:SER:OG	2.43	0.51
11:3:466:ASP:O	11:3:509:ARG:CA	2.59	0.51
12:4:603:ALA:HB2	12:4:622:VAL:CB	2.41	0.51
13:5:649:THR:HG23	13:5:652:GLN:H	1.76	0.51
11:3:488:GLU:O	11:3:492:GLN:CB	2.59	0.51
3:9:88:VAL:HG22	3:9:92:LEU:HD23	1.93	0.51
6:C:512:ASP:OD1	6:C:512:ASP:N	2.44	0.51
8:D:171:THR:HG23	8:D:172:ILE:HG13	1.92	0.51
8:D:107:TYR:HB3	8:D:110:TYR:HD2	1.75	0.51
8:D:399:LEU:HD22	8:D:510:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:3:394:GLU:OE1	11:3:394:GLU:HA	2.09	0.51
7:E:338:CYS:O	7:E:379:SER:OG	2.29	0.50
7:E:111:THR:HA	7:E:114:ASN:HD22	1.74	0.50
13:5:649:THR:OG1	13:5:650:ILE:N	2.44	0.50
4:A:620:THR:OG1	4:A:621:ARG:N	2.43	0.50
8:D:83:ASP:HA	8:D:86:ILE:HG22	1.93	0.50
10:2:545:PRO:HG3	15:6:703:ALA:HB1	1.92	0.50
11:3:43:ARG:NH1	11:3:136:MET:O	2.45	0.50
12:4:387:ASN:CB	15:6:175:TYR:CE2	2.94	0.50
14:L:90:GLU:HG3	14:L:154:ARG:HB2	1.92	0.50
4:A:526:GLU:HG3	4:A:537:LEU:O	2.12	0.50
5:B:534:GLN:OE1	5:B:535:ASN:ND2	2.44	0.50
6:C:426:GLU:HA	6:C:429:HIS:HB3	1.93	0.50
10:2:286:TYR:CE2	10:2:293:ILE:HD11	2.46	0.50
6:C:447:LYS:HA	6:C:450:LYS:HD3	1.93	0.50
6:C:489:ASP:OD2	6:C:614:ARG:NH1	2.45	0.50
8:D:112:LEU:HD13	8:D:215:ILE:HD12	1.93	0.50
9:F:357:SER:CB	10:2:788:ARG:HG2	2.40	0.50
12:4:351:VAL:CG1	15:6:332:PHE:CE1	2.95	0.50
12:4:374:ILE:O	12:4:377:ASN:ND2	2.42	0.50
3:9:107:THR:OG1	3:9:108:GLY:N	2.45	0.50
3:9:227:ARG:NH2	4:A:577:ASP:OD1	2.41	0.50
4:A:857:ILE:HG21	8:D:369:LYS:CA	2.42	0.50
6:C:449:TYR:HD1	6:C:452:ARG:HD3	1.77	0.50
8:D:500:ASP:OD1	8:D:500:ASP:N	2.36	0.50
11:3:226:PRO:HG2	13:5:242:ILE:HG22	1.94	0.50
11:3:483:ARG:O	11:3:487:HIS:HD2	1.94	0.50
12:4:657:ALA:HB2	15:6:598:THR:OG1	2.12	0.50
14:L:34:ARG:HD2	14:L:34:ARG:C	2.32	0.50
16:7:122:ASP:OD2	16:7:198:ARG:NH2	2.44	0.50
3:9:423:GLN:NE2	3:9:512:LEU:O	2.44	0.50
4:A:811:LEU:HB3	4:A:820:GLN:HG3	1.93	0.50
5:B:433:ARG:HH21	7:E:441:ILE:HD11	1.76	0.50
6:C:393:VAL:HA	6:C:396:LEU:HB2	1.93	0.50
7:E:58:HIS:CD2	7:E:88:LEU:HD21	2.46	0.50
7:E:212:ASP:N	7:E:212:ASP:OD1	2.45	0.50
7:E:472:ASP:OD1	7:E:472:ASP:N	2.44	0.50
10:2:405:HIS:NE2	15:6:299:GLU:OE1	2.44	0.50
13:5:258:LEU:HD22	13:5:294:ILE:HD12	1.93	0.50
16:7:648:LYS:HB2	16:7:701:LYS:HG2	1.92	0.50
7:E:205:ARG:NH1	7:E:259:ASN:OD1	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:6:275:ARG:NH1	15:6:367:GLU:O	2.45	0.50
3:9:226:ASP:OD1	3:9:226:ASP:N	2.43	0.50
3:9:234:SER:OG	3:9:235:GLU:OE1	2.28	0.50
3:9:248:LEU:CD1	3:9:281:LEU:HD21	2.42	0.50
7:E:11:ARG:NH2	7:E:192:TYR:OH	2.42	0.50
8:D:59:GLN:NE2	8:D:291:LEU:O	2.45	0.50
8:D:379:ARG:NH1	8:D:466:LEU:O	2.45	0.50
11:3:679:ILE:HD11	11:3:705:LEU:HD12	1.94	0.50
15:6:317:ILE:HG21	15:6:350:ARG:HH21	1.75	0.50
3:9:399:ASN:O	3:9:404:ARG:NH1	2.45	0.49
10:2:364:CYS:HB3	10:2:367:CYS:HB2	1.94	0.49
7:E:58:HIS:CE1	7:E:88:LEU:HD11	2.48	0.49
14:L:61:LEU:HD13	14:L:154:ARG:HH12	1.77	0.49
3:9:281:LEU:N	3:9:281:LEU:CD2	2.75	0.49
3:9:311:ILE:HG13	3:9:311:ILE:O	2.12	0.49
7:E:69:SER:OG	7:E:70:TRP:N	2.45	0.49
11:3:172:THR:OG1	11:3:173:ALA:N	2.44	0.49
3:9:332:ARG:O	3:9:336:ASP:N	2.45	0.49
5:B:399:HIS:HB2	5:B:402:LEU:HD22	1.95	0.49
14:L:245:THR:OG1	14:L:246:THR:N	2.44	0.49
16:7:436:LEU:HD13	16:7:642:ILE:HD13	1.94	0.49
3:9:331:LEU:HA	3:9:334:LEU:HB2	1.93	0.49
4:A:486:THR:OG1	17:A:2001:AGS:O2B	2.30	0.49
4:A:873:LEU:HB3	4:A:879:LEU:HD23	1.93	0.49
5:B:599:ILE:HG22	5:B:601:TRP:HD1	1.77	0.49
11:3:258:VAL:O	11:3:273:SER:HA	2.13	0.49
11:3:478:MET:O	11:3:483:ARG:NH2	2.45	0.49
11:3:671:LEU:HB2	16:7:621:MET:CG	2.43	0.49
16:7:539:GLU:O	16:7:543:GLN:O	2.30	0.49
3:9:237:GLN:HA	3:9:240:ARG:HE	1.77	0.49
6:C:296:ASP:OD1	6:C:296:ASP:N	2.44	0.49
16:7:436:LEU:CD1	16:7:642:ILE:CD1	2.91	0.49
4:A:637:ASP:OD1	4:A:637:ASP:N	2.43	0.49
7:E:473:TYR:HE1	10:2:851:VAL:CG2	2.25	0.49
8:D:86:ILE:O	8:D:89:SER:OG	2.29	0.49
16:7:73:ARG:NH2	16:7:130:LYS:O	2.46	0.49
16:7:208:SER:OG	16:7:209:GLN:N	2.46	0.49
3:9:88:VAL:O	3:9:92:LEU:N	2.44	0.49
4:A:708:LYS:HD3	8:D:269:SER:HA	1.94	0.49
7:E:109:VAL:HG23	7:E:156:LEU:HD22	1.94	0.49
9:F:365:CYS:SG	10:2:795:ARG:NH2	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:151:GLU:HB3	8:D:172:ILE:HD12	1.94	0.49
10:2:411:LEU:HD12	10:2:411:LEU:O	2.13	0.49
10:2:853:VAL:O	10:2:856:GLN:HB2	2.13	0.49
12:4:920:GLY:O	12:4:924:ARG:NH1	2.46	0.49
4:A:817:SER:OG	4:A:820:GLN:OE1	2.31	0.49
15:6:308:SER:O	15:6:347:ASN:HB3	2.12	0.49
4:A:871:ASN:ND2	7:E:178:ARG:O	2.46	0.48
4:A:880:PHE:HD2	4:A:893:LYS:HB3	1.78	0.48
7:E:67:LEU:HD23	7:E:72:PRO:HB2	1.95	0.48
10:2:603:VAL:HG22	10:2:645:SER:HB3	1.95	0.48
14:L:118:LEU:HD23	14:L:121:LEU:HD13	1.94	0.48
16:7:653:SER:OG	16:7:654:GLU:N	2.46	0.48
7:E:272:ARG:HH21	7:E:288:ALA:HA	1.77	0.48
11:3:253:HIS:HA	11:3:278:LEU:O	2.13	0.48
11:3:367:LEU:HD21	11:3:378:LYS:HB2	1.96	0.48
6:C:371:HIS:HB2	6:C:377:ILE:HD11	1.94	0.48
8:D:116:LEU:O	8:D:120:GLN:N	2.46	0.48
15:6:123:SER:O	15:6:133:GLU:HG2	2.13	0.48
4:A:486:THR:OG1	17:A:2001:AGS:O3G	2.31	0.48
4:A:865:SER:HB2	4:A:868:PHE:HB3	1.96	0.48
10:2:594:GLY:HA2	15:6:667:GLY:O	2.14	0.48
10:2:670:THR:OG1	10:2:671:GLU:N	2.46	0.48
15:6:387:GLU:O	15:6:387:GLU:HG2	2.14	0.48
15:6:570:ASN:ND2	15:6:708:ARG:O	2.46	0.48
16:7:775:THR:OG1	16:7:776:MET:N	2.47	0.48
3:9:395:SER:HA	3:9:398:VAL:HG22	1.94	0.48
4:A:412:THR:HG23	8:D:208:THR:HG23	1.95	0.48
5:B:286:GLN:H	5:B:290:ARG:HH21	1.61	0.48
8:D:299:SER:HB3	8:D:302:VAL:HG23	1.95	0.48
15:6:656:MET:HA	15:6:656:MET:CE	2.41	0.48
16:7:436:LEU:HD23	16:7:473:ILE:HD12	1.94	0.48
7:E:476:ASP:N	7:E:476:ASP:OD1	2.46	0.48
10:2:631:ILE:CG1	10:2:638:THR:H	2.26	0.48
11:3:294:VAL:HG12	11:3:326:VAL:HG22	1.96	0.48
12:4:184:ASN:O	12:4:260:GLN:NE2	2.46	0.48
13:5:61:LEU:HD21	13:5:94:ILE:HD13	1.95	0.48
3:9:500:ASP:OD1	3:9:500:ASP:N	2.45	0.48
10:2:536:ASP:O	10:2:815:ARG:NH1	2.47	0.48
11:3:123:PRO:O	11:3:126:GLU:HG2	2.13	0.48
14:L:409:SER:O	14:L:413:GLN:NE2	2.47	0.48
4:A:514:ASN:HB3	4:A:517:LYS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:296:ILE:HD13	9:F:398:ILE:HD12	1.95	0.48
5:B:445:SER:OG	5:B:472:ASN:O	2.31	0.48
6:C:441:ASP:OD1	6:C:441:ASP:N	2.46	0.48
11:3:348:ARG:NH2	11:3:349:ASN:OD1	2.47	0.48
14:L:22:ARG:HH12	14:L:29:LEU:HD11	1.79	0.48
4:A:432:SER:O	17:A:2001:AGS:O2'	2.32	0.48
4:A:882:GLN:NE2	4:A:891:CYS:SG	2.86	0.48
7:E:40:GLY:N	17:E:2001:AGS:O1B	2.42	0.48
7:E:74:LEU:HD23	7:E:108:LEU:HB2	1.96	0.48
10:2:515:VAL:HG13	10:2:556:VAL:HG21	1.96	0.48
12:4:311:CYS:SG	12:4:312:LYS:N	2.87	0.48
12:4:543:GLN:HE22	12:4:628:VAL:HG12	1.78	0.48
12:4:713:ASP:OD1	12:4:713:ASP:N	2.47	0.48
15:6:610:ALA:HA	15:6:624:GLU:O	2.14	0.48
3:9:282:LEU:N	3:9:283:PRO:CD	2.76	0.48
3:9:506:SER:O	3:9:506:SER:OG	2.31	0.48
12:4:341:ASP:O	12:4:391:PHE:CA	2.61	0.48
12:4:344:VAL:CG1	12:4:358:VAL:O	2.62	0.48
15:6:703:ALA:HB3	15:6:704:PRO:HD3	1.95	0.48
16:7:20:GLU:OE1	16:7:92:LYS:NZ	2.47	0.48
3:9:92:LEU:HD12	3:9:95:ALA:HB2	1.95	0.47
8:D:104:ARG:NH2	8:D:218:GLU:OE2	2.46	0.47
12:4:631:ILE:O	12:4:673:ALA:HA	2.13	0.47
16:7:436:LEU:HD11	16:7:642:ILE:HD11	1.95	0.47
4:A:857:ILE:HG21	8:D:369:LYS:HB2	1.97	0.47
8:D:275:MET:O	8:D:277:GLN:NE2	2.47	0.47
12:4:350:ASN:N	12:4:350:ASN:OD1	2.47	0.47
7:E:110:LYS:O	7:E:114:ASN:ND2	2.48	0.47
12:4:419:VAL:HG12	12:4:463:VAL:HG11	1.97	0.47
3:9:338:LEU:O	3:9:342:ILE:HG13	2.15	0.47
6:C:390:GLU:HA	6:C:393:VAL:HG22	1.97	0.47
7:E:254:ASP:OD2	7:E:255:ILE:N	2.48	0.47
8:D:315:ASP:O	8:D:318:SER:OG	2.32	0.47
11:3:486:ILE:HA	11:3:489:VAL:CB	2.45	0.47
12:4:632:ASP:OD1	12:4:632:ASP:N	2.47	0.47
12:4:795:THR:CG2	15:6:727:LEU:HD21	2.43	0.47
14:L:210:SER:OG	14:L:211:THR:N	2.46	0.47
3:9:343:GLU:O	3:9:347:LEU:N	2.40	0.47
7:E:43:LYS:HA	7:E:46:THR:HG22	1.97	0.47
7:E:473:TYR:CE1	10:2:851:VAL:HG21	2.49	0.47
10:2:324:VAL:HG23	10:2:420:PRO:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:4:735:HIS:O	12:4:738:GLN:NE2	2.48	0.47
13:5:409:ASP:O	13:5:658:ARG:NH1	2.47	0.47
14:L:309:ASP:O	14:L:312:LYS:NZ	2.48	0.47
16:7:677:SER:OG	16:7:678:LYS:N	2.46	0.47
3:9:217:THR:HA	3:9:254:VAL:HG12	1.97	0.47
3:9:316:ALA:HA	3:9:319:PHE:HB3	1.97	0.47
3:9:495:MET:HA	3:9:498:PHE:HB2	1.96	0.47
3:9:504:LYS:HG3	3:9:505:ILE:HG23	1.97	0.47
5:B:289:PRO:HB2	6:C:498:LEU:HD12	1.96	0.47
7:E:211:GLU:O	7:E:216:ARG:NH2	2.47	0.47
8:D:333:SER:O	8:D:336:THR:OG1	2.31	0.47
10:2:326:ARG:N	10:2:592:GLU:CB	2.76	0.47
10:2:515:VAL:HG11	10:2:556:VAL:HG21	1.96	0.47
11:3:957:LYS:HD2	11:3:958:VAL:HG13	1.97	0.47
14:L:111:LEU:HA	14:L:114:ILE:HG12	1.97	0.47
15:6:623:ILE:HD12	15:6:663:ILE:CB	2.44	0.47
15:6:734:LEU:HD13	15:6:742:ILE:CG2	2.44	0.47
3:9:277:LEU:O	3:9:279:ARG:NH1	2.43	0.47
5:B:409:ASP:N	5:B:409:ASP:OD1	2.46	0.47
8:D:220:ASP:OD1	8:D:220:ASP:N	2.47	0.47
8:D:281:LEU:HD21	8:D:325:ARG:HH21	1.79	0.47
8:D:338:LYS:NZ	17:D:2001:AGS:O3'	2.48	0.47
9:F:396:GLU:O	9:F:400:ARG:N	2.47	0.47
10:2:387:ARG:CA	10:2:408:VAL:O	2.59	0.47
10:2:501:MET:O	10:2:555:TYR:CZ	2.67	0.47
15:6:612:VAL:HG22	15:6:623:ILE:HD13	1.96	0.47
5:B:264:SER:HB2	5:B:605:THR:HG21	1.97	0.47
17:D:2001:AGS:O1B	17:D:2001:AGS:O3G	2.31	0.47
10:2:562:ARG:O	10:2:602:GLY:HA3	2.15	0.47
10:2:577:THR:O	10:2:593:GLY:C	2.53	0.47
11:3:708:LEU:O	11:3:711:ALA:HB3	2.15	0.47
12:4:763:THR:OG1	12:4:764:GLU:N	2.48	0.47
12:4:775:VAL:HA	12:4:778:ARG:HB2	1.97	0.47
12:4:867:ARG:O	12:4:871:ASN:ND2	2.48	0.47
16:7:656:VAL:HG23	16:7:710:ILE:HD12	1.95	0.47
2:H:8:DA:H5'	12:4:658:LYS:CB	2.45	0.47
5:B:310:GLN:O	5:B:448:ARG:NH1	2.43	0.47
4:A:886:ASN:HA	8:D:470:THR:HG21	1.97	0.47
6:C:423:ASN:O	6:C:439:TYR:OH	2.32	0.47
15:6:453:SER:OG	15:6:454:PHE:N	2.48	0.47
3:9:409:LYS:O	3:9:415:LYS:NZ	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:333:ASN:HD21	9:F:388:ASP:HB3	1.80	0.46
9:F:381:ASP:O	9:F:385:ARG:N	2.44	0.46
12:4:435:VAL:HG23	12:4:466:VAL:HG12	1.97	0.46
12:4:639:ASP:OD1	12:4:642:ARG:NH1	2.48	0.46
12:4:825:ALA:O	12:4:828:LEU:HB3	2.15	0.46
15:6:811:ALA:HB2	15:6:819:ILE:HD13	1.97	0.46
12:4:542:LEU:HA	12:4:545:PHE:HB2	1.97	0.46
4:A:708:LYS:NZ	8:D:267:ARG:O	2.47	0.46
7:E:109:VAL:HG21	7:E:155:LEU:HB3	1.97	0.46
8:D:527:THR:OG1	8:D:528:GLN:N	2.48	0.46
11:3:480:ASP:OD1	11:3:480:ASP:N	2.48	0.46
13:5:500:GLN:HA	13:5:500:GLN:OE1	2.15	0.46
16:7:400:ARG:NH1	16:7:636:SER:OG	2.48	0.46
17:9:2001:AGS:O2A	17:9:2001:AGS:O1B	2.31	0.46
5:B:271:ARG:NH2	5:B:497:LYS:O	2.49	0.46
7:E:277:ASN:HA	7:E:280:GLU:HB2	1.98	0.46
12:4:535:ASP:OD1	12:4:535:ASP:N	2.48	0.46
16:7:350:ASP:HB2	16:7:382:ARG:HG2	1.97	0.46
3:9:84:GLU:HB3	3:9:288:PHE:HE1	1.81	0.46
3:9:388:ASN:O	3:9:392:LYS:NZ	2.41	0.46
3:9:430:ASP:HA	3:9:488:LYS:HD3	1.97	0.46
5:B:335:SER:O	5:B:357:SER:OG	2.34	0.46
14:L:203:LYS:NZ	14:L:205:ILE:O	2.44	0.46
15:6:150:THR:HG21	15:6:384:ASP:HB2	1.98	0.46
16:7:451:ARG:NH2	16:7:453:ASP:O	2.48	0.46
3:9:439:HIS:HA	3:9:442:LYS:HG2	1.97	0.46
5:B:580:ARG:HA	5:B:583:ILE:HB	1.97	0.46
7:E:212:ASP:OD2	7:E:266:TRP:NE1	2.47	0.46
8:D:335:PRO:HA	8:D:338:LYS:HB3	1.98	0.46
4:A:460:TYR:O	4:A:464:TYR:N	2.44	0.46
10:2:234:LEU:HA	10:2:239:SER:HB3	1.98	0.46
11:3:378:LYS:HA	11:3:381:ILE:HB	1.97	0.46
13:5:515:SER:OG	13:5:517:THR:OG1	2.17	0.46
7:E:74:LEU:HD21	7:E:105:PRO:HA	1.96	0.46
10:2:334:LEU:HB3	10:2:352:PHE:HD2	1.81	0.46
10:2:335:LYS:HA	10:2:352:PHE:O	2.16	0.46
10:2:495:ASP:OD1	10:2:509:ARG:NH1	2.46	0.46
12:4:676:ASN:HA	12:4:677:PRO:HD3	1.68	0.46
14:L:103:ASP:N	14:L:103:ASP:OD1	2.47	0.46
16:7:591:LEU:HA	16:7:594:PHE:HB2	1.98	0.46
16:7:769:VAL:HG21	16:7:779:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:9:219:VAL:HG13	3:9:257:VAL:HB	1.97	0.46
6:C:123:SER:HA	6:C:197:LYS:HD3	1.97	0.46
6:C:596:LEU:HB3	6:C:597:ILE:HD12	1.98	0.46
11:3:297:VAL:O	11:3:321:ILE:HA	2.16	0.46
12:4:421:ASP:N	12:4:421:ASP:OD1	2.46	0.46
12:4:583:LYS:HD3	16:7:447:GLY:CA	2.44	0.46
12:4:636:LYS:HD3	16:7:535:THR:HG22	1.98	0.46
14:L:314:VAL:O	14:L:317:LEU:HB3	2.15	0.46
15:6:710:ASP:CB	15:6:802:SER:CB	2.94	0.46
3:9:400:ASN:ND2	3:9:404:ARG:O	2.49	0.46
4:A:422:ILE:HG22	4:A:682:LEU:HD22	1.98	0.46
5:B:518:THR:HG23	5:B:521:SER:H	1.81	0.46
6:C:58:TRP:O	6:C:62:HIS:ND1	2.49	0.46
9:F:369:VAL:HA	9:F:372:LEU:HD12	1.97	0.46
12:4:209:LEU:HD12	12:4:250:ALA:HB2	1.97	0.46
14:L:311:MET:HG2	14:L:407:ALA:HB1	1.98	0.46
3:9:198:GLN:HA	3:9:204:HIS:HB3	1.98	0.45
3:9:282:LEU:N	3:9:283:PRO:HD2	2.32	0.45
3:9:387:LEU:HD22	3:9:390:ILE:HG13	1.98	0.45
4:A:633:LYS:HD3	4:A:690:GLU:HG2	1.97	0.45
8:D:100:LEU:N	8:D:249:GLY:O	2.43	0.45
9:F:363:ILE:HA	9:F:366:VAL:HG12	1.98	0.45
11:3:906:THR:OG1	11:3:907:GLU:N	2.49	0.45
13:5:160:VAL:HG11	13:5:298:TYR:HB2	1.98	0.45
14:L:43:PHE:HB3	14:L:230:PHE:HB3	1.98	0.45
16:7:715:GLU:OE2	16:7:718:ARG:NH1	2.46	0.45
4:A:605:PRO:HA	4:A:609:LEU:HB2	1.97	0.45
10:2:631:ILE:O	10:2:637:VAL:HA	2.16	0.45
12:4:696:PRO:HD2	12:4:697:PRO:CD	2.45	0.45
3:9:399:ASN:HB3	3:9:404:ARG:HD3	1.97	0.45
11:3:301:LEU:HA	13:5:245:HIS:ND1	2.31	0.45
11:3:384:MET:SD	11:3:511:SER:OG	2.72	0.45
14:L:345:PRO:HA	14:L:348:SER:HB2	1.99	0.45
16:7:597:LEU:O	16:7:723:SER:OG	2.34	0.45
3:9:170:ILE:HG12	3:9:184:LYS:HG3	1.97	0.45
7:E:45:TYR:HB2	17:E:2001:AGS:H3'	1.98	0.45
8:D:46:ASP:OD2	8:D:49:PHE:N	2.45	0.45
8:D:455:ASP:OD1	8:D:455:ASP:N	2.38	0.45
14:L:45:LEU:HB3	14:L:48:TYR:HE2	1.81	0.45
15:6:298:SER:HG	15:6:358:LYS:C	2.16	0.45
6:C:348:ASP:HA	6:C:351:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:569:LEU:O	6:C:572:THR:OG1	2.31	0.45
7:E:254:ASP:OD2	7:E:256:PHE:N	2.50	0.45
11:3:239:ASN:N	11:3:239:ASN:ND2	2.59	0.45
4:A:772:THR:OG1	4:A:773:VAL:N	2.50	0.45
8:D:284:MET:HB2	8:D:284:MET:HE3	1.75	0.45
11:3:496:THR:HG21	16:7:482:TYR:CG	2.32	0.45
3:9:201:ASN:HB3	3:9:204:HIS:CG	2.52	0.45
5:B:374:ASP:OD1	5:B:374:ASP:N	2.48	0.45
5:B:549:THR:OG1	5:B:550:GLN:N	2.48	0.45
6:C:60:LEU:HA	6:C:63:GLN:HE21	1.82	0.45
7:E:240:ILE:HA	7:E:243:ILE:HG22	1.99	0.45
11:3:466:ASP:C	11:3:509:ARG:O	2.55	0.45
12:4:531:TYR:HE1	12:4:720:LEU:HA	1.80	0.45
13:5:166:ILE:HD11	13:5:294:ILE:HD11	1.99	0.45
10:2:583:ASP:HA	10:2:584:PRO:HD3	1.81	0.45
11:3:430:ILE:HB	11:3:470:VAL:HG12	1.99	0.45
15:6:652:ILE:O	15:6:656:MET:HG2	2.16	0.45
3:9:106:ILE:HD12	3:9:118:LEU:HD21	1.99	0.45
5:B:495:VAL:HG13	5:B:497:LYS:H	1.82	0.45
11:3:226:PRO:HG2	13:5:242:ILE:CG2	2.47	0.45
11:3:246:GLY:HA3	16:7:109:ASN:CA	2.47	0.45
11:3:716:ARG:NH2	11:3:725:ASP:OD1	2.49	0.45
5:B:556:LEU:HD21	5:B:600:ILE:HG23	1.99	0.45
6:C:351:LEU:HD21	6:C:389:GLU:HB3	1.97	0.45
10:2:501:MET:SD	10:2:555:TYR:CE2	3.06	0.45
11:3:245:TYR:HA	11:3:248:SER:OG	2.17	0.45
12:4:604:TYR:CD1	12:4:604:TYR:O	2.70	0.45
15:6:317:ILE:CG2	15:6:350:ARG:NH2	2.78	0.45
7:E:473:TYR:HE1	10:2:851:VAL:HB	1.83	0.44
11:3:705:LEU:HD21	11:3:733:LEU:HD11	1.99	0.44
13:5:146:ILE:HD11	13:5:160:VAL:HG23	2.00	0.44
14:L:408:GLU:HG3	14:L:412:GLN:HE22	1.83	0.44
15:6:303:GLU:N	15:6:354:LEU:O	2.47	0.44
8:D:67:ASP:OD1	8:D:67:ASP:N	2.48	0.44
10:2:331:PHE:CE2	10:2:588:GLU:HG2	2.53	0.44
11:3:506:LEU:CD1	16:7:325:GLY:HA2	2.47	0.44
11:3:536:PRO:HD2	11:3:539:LEU:HD12	2.00	0.44
6:C:593:ASN:N	6:C:593:ASN:OD1	2.50	0.44
7:E:334:ALA:HA	7:E:337:ILE:HD12	1.99	0.44
11:3:413:THR:HB	11:3:414:ALA:H	1.66	0.44
12:4:696:PRO:N	12:4:697:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:425:LYS:HD2	4:A:425:LYS:HA	1.82	0.44
6:C:276:TYR:HA	6:C:279:GLN:HB3	2.00	0.44
11:3:942:LEU:HD22	11:3:951:LEU:HD22	2.00	0.44
16:7:418:ILE:HG13	16:7:429:LYS:HD3	1.97	0.44
3:9:319:PHE:CZ	11:3:960:ARG:HB3	2.52	0.44
11:3:424:ASN:O	11:3:657:ARG:NH1	2.44	0.44
12:4:527:ALA:CB	12:4:530:ILE:HD11	2.48	0.44
13:5:180:SER:OG	13:5:244:ILE:HB	2.17	0.44
15:6:356:TRP:CE3	15:6:356:TRP:O	2.70	0.44
4:A:583:PHE:O	4:A:586:THR:OG1	2.34	0.44
5:B:600:ILE:O	5:B:600:ILE:HG13	2.16	0.44
10:2:543:GLY:HA3	10:2:683:VAL:HG22	2.00	0.44
11:3:350:ILE:O	11:3:354:SER:OG	2.35	0.44
12:4:518:LEU:HA	12:4:521:LEU:HB3	1.99	0.44
12:4:604:TYR:CE2	16:7:551:ALA:HB1	2.53	0.44
12:4:697:PRO:CA	15:6:577:PRO:HB3	2.46	0.44
12:4:882:SER:OG	12:4:883:PHE:N	2.51	0.44
13:5:141:SER:O	13:5:334:GLN:NE2	2.51	0.44
16:7:431:ALA:HB2	16:7:719:LEU:HD11	1.99	0.44
7:E:198:SER:HB3	7:E:244:VAL:HG21	2.00	0.44
10:2:515:VAL:HG11	10:2:556:VAL:CG2	2.48	0.44
11:3:346:ASP:HA	11:3:349:ASN:HD22	1.83	0.44
14:L:28:GLN:NE2	14:L:29:LEU:HG	2.33	0.44
6:C:363:PHE:O	6:C:367:LEU:N	2.51	0.44
9:F:336:ARG:NE	9:F:343:ASP:OD1	2.38	0.44
9:F:422:LYS:HB3	9:F:423:LYS:HZ2	1.82	0.44
10:2:339:PHE:CE2	10:2:375:VAL:HG22	2.52	0.44
11:3:410:ASP:O	11:3:415:LYS:NZ	2.40	0.44
13:5:413:LEU:HD23	13:5:553:ILE:HG12	2.00	0.44
15:6:551:MET:CE	15:6:755:ILE:CD1	2.95	0.44
15:6:718:ASP:OD1	15:6:718:ASP:N	2.51	0.44
4:A:481:PRO:HD2	8:D:262:LYS:HD2	2.00	0.44
6:C:246:ASN:O	6:C:250:ASN:ND2	2.47	0.44
9:F:358:LYS:HG2	10:2:788:ARG:HD3	2.00	0.44
12:4:604:TYR:HE2	16:7:551:ALA:HB1	1.83	0.44
14:L:121:LEU:HD22	14:L:198:ILE:HG12	1.99	0.44
4:A:411:LYS:HD2	4:A:411:LYS:HA	1.81	0.43
4:A:640:LEU:HD22	4:A:643:LEU:HD11	2.00	0.43
5:B:610:GLU:OE2	5:B:611:LYS:NZ	2.36	0.43
9:F:429:LEU:HD12	9:F:429:LEU:HA	1.89	0.43
10:2:344:CYS:SG	10:2:367:CYS:SG	3.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2:553:LEU:HD12	10:2:553:LEU:C	2.38	0.43
11:3:475:PHE:HB3	11:3:516:ALA:HB2	1.99	0.43
16:7:436:LEU:HD11	16:7:642:ILE:CD1	2.48	0.43
3:9:236:THR:OG1	3:9:237:GLN:N	2.51	0.43
6:C:236:LEU:HD23	6:C:238:PHE:HE2	1.83	0.43
6:C:560:ASP:OD1	6:C:560:ASP:N	2.42	0.43
10:2:582:LYS:HA	10:2:588:GLU:O	2.18	0.43
12:4:248:LEU:HD11	12:4:257:LEU:HD23	1.99	0.43
14:L:332:ARG:C	14:L:334:THR:H	2.21	0.43
3:9:335:PHE:O	3:9:339:ARG:N	2.49	0.43
7:E:218:ARG:HD2	7:E:218:ARG:HA	1.72	0.43
10:2:854:ARG:O	10:2:857:LEU:HB2	2.17	0.43
11:3:211:TYR:O	11:3:211:TYR:CG	2.72	0.43
3:9:107:THR:HG21	3:9:265:LEU:HD11	2.01	0.43
4:A:561:ILE:HG22	4:A:563:VAL:HG23	1.99	0.43
5:B:550:GLN:HA	5:B:601:TRP:CG	2.54	0.43
10:2:539:VAL:HG12	10:2:679:ILE:HB	1.99	0.43
13:5:279:ASP:O	13:5:283:THR:HG23	2.18	0.43
13:5:496:ALA:HB2	13:5:502:ILE:HG12	2.00	0.43
6:C:437:ASP:OD1	6:C:437:ASP:N	2.52	0.43
12:4:812:LYS:O	12:4:812:LYS:CG	2.64	0.43
14:L:76:ASN:OD1	14:L:76:ASN:N	2.51	0.43
14:L:138:GLU:OE2	14:L:268:THR:OG1	2.37	0.43
4:A:632:LEU:HD23	4:A:632:LEU:HA	1.88	0.43
6:C:100:ARG:NH2	6:C:227:PHE:O	2.47	0.43
6:C:426:GLU:O	6:C:430:ASN:ND2	2.34	0.43
10:2:573:ALA:CB	15:6:664:ALA:O	2.67	0.43
10:2:782:ASP:OD1	10:2:782:ASP:N	2.49	0.43
11:3:496:THR:HG22	11:3:505:THR:CB	2.48	0.43
12:4:312:LYS:HB2	12:4:316:GLU:HB2	2.00	0.43
14:L:125:PHE:HA	14:L:128:LEU:HG	2.00	0.43
4:A:863:ILE:HG12	4:A:866:TRP:HB2	2.01	0.43
5:B:522:LYS:HG2	5:B:617:LEU:HD23	1.99	0.43
6:C:557:ILE:HD12	6:C:557:ILE:HA	1.90	0.43
7:E:273:ILE:HA	7:E:284:LEU:HD11	2.01	0.43
8:D:419:ILE:C	8:D:421:ALA:H	2.22	0.43
11:3:496:THR:HG21	16:7:482:TYR:CB	2.49	0.43
12:4:404:ASP:OD1	12:4:404:ASP:N	2.47	0.43
16:7:245:ILE:HD13	16:7:343:LEU:HD12	2.01	0.43
16:7:547:SER:CB	16:7:556:THR:HG22	2.49	0.43
5:B:298:LYS:HE2	5:B:301:PHE:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:48:LYS:HD2	7:E:52:ASN:HD21	1.84	0.43
10:2:572:SER:HB3	10:2:616:ASP:OD2	2.19	0.43
16:7:354:ILE:HG22	16:7:377:GLU:HB3	2.00	0.43
6:C:220:ILE:HD12	6:C:220:ILE:HA	1.90	0.43
8:D:480:ASN:HD21	8:D:482:THR:HG22	1.82	0.43
14:L:155:TYR:HB2	14:L:255:ALA:HB1	2.00	0.43
16:7:685:THR:O	16:7:688:THR:OG1	2.35	0.43
4:A:409:LYS:HB3	8:D:158:HIS:HE1	1.84	0.43
6:C:79:ILE:HA	6:C:82:ASP:HB3	2.00	0.43
11:3:295:VAL:HB	11:3:325:THR:HB	2.01	0.43
11:3:366:SER:OG	11:3:651:VAL:O	2.37	0.43
12:4:569:ASP:H	12:4:709:LEU:HA	1.84	0.43
15:6:330:PRO:HG2	15:6:344:TRP:CD2	2.54	0.43
15:6:381:LEU:HG	15:6:386:VAL:HG12	2.01	0.43
15:6:594:ARG:HG2	15:6:632:ASP:O	2.17	0.43
16:7:500:ASP:O	16:7:504:ASP:CA	2.66	0.43
6:C:86:GLU:HG3	6:C:266:LEU:HD21	2.00	0.42
7:E:346:ASP:N	7:E:346:ASP:OD1	2.51	0.42
17:D:2001:AGS:O1A	17:D:2001:AGS:O2B	2.34	0.42
9:F:276:LYS:HD2	9:F:318:GLN:HE22	1.83	0.42
10:2:515:VAL:CG1	10:2:556:VAL:CG2	2.97	0.42
12:4:624:SER:C	12:4:626:GLY:N	2.69	0.42
13:5:499:GLN:C	13:5:501:THR:H	2.22	0.42
13:5:673:GLN:H	13:5:676:HIS:HD2	1.66	0.42
15:6:576:ASP:CB	15:6:577:PRO:CD	2.96	0.42
16:7:275:SER:OG	16:7:277:THR:O	2.37	0.42
4:A:430:LEU:HD12	4:A:430:LEU:HA	1.86	0.42
8:D:514:ARG:NH1	8:D:527:THR:OG1	2.44	0.42
10:2:374:ARG:HA	10:2:374:ARG:HD3	1.77	0.42
12:4:539:GLY:O	12:4:543:GLN:HB2	2.19	0.42
14:L:200:PRO:O	14:L:254:ARG:NH1	2.52	0.42
5:B:366:TYR:HB3	5:B:426:ASN:HD22	1.85	0.42
9:F:418:TYR:O	9:F:422:LYS:N	2.50	0.42
11:3:395:ASN:HB2	16:7:635:PRO:HD3	2.01	0.42
14:L:65:ASP:N	14:L:65:ASP:OD2	2.52	0.42
14:L:388:ARG:HH11	14:L:389:ASP:HB2	1.84	0.42
3:9:170:ILE:HD12	3:9:170:ILE:HA	1.88	0.42
4:A:511:VAL:CG2	4:A:563:VAL:HG22	2.50	0.42
5:B:465:TRP:O	7:E:422:GLN:NE2	2.52	0.42
6:C:364:VAL:HA	6:C:367:LEU:HD12	2.01	0.42
6:C:384:LYS:HA	6:C:384:LYS:HD3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2:349:GLY:HA2	10:2:350:PRO:HD3	1.72	0.42
12:4:360:ILE:HG13	12:4:361:ASP:N	2.34	0.42
13:5:631:LYS:HD2	13:5:631:LYS:HA	1.89	0.42
15:6:309:PHE:CD2	15:6:330:PRO:HD3	2.55	0.42
16:7:318:LEU:HD23	16:7:320:GLN:H	1.85	0.42
16:7:330:SER:OG	16:7:331:LEU:N	2.52	0.42
3:9:228:LEU:HD11	3:9:241:THR:HG21	2.02	0.42
5:B:441:LEU:HD13	5:B:444:LEU:HD12	2.02	0.42
6:C:214:ASN:N	6:C:214:ASN:OD1	2.53	0.42
8:D:310:GLU:O	8:D:314:SER:N	2.42	0.42
12:4:657:ALA:CB	15:6:598:THR:OG1	2.67	0.42
3:9:411:ASN:HB3	3:9:414:GLN:HB2	2.01	0.42
11:3:463:VAL:HG12	11:3:463:VAL:O	2.19	0.42
16:7:124:ASN:OD1	16:7:124:ASN:N	2.51	0.42
3:9:125:LYS:HG2	3:9:129:LEU:HD13	2.01	0.42
7:E:386:LEU:O	7:E:390:PHE:N	2.48	0.42
8:D:227:ARG:HB3	8:D:229:THR:HG23	2.02	0.42
9:F:361:ASP:OD1	9:F:361:ASP:N	2.50	0.42
11:3:430:ILE:O	11:3:470:VAL:HA	2.19	0.42
13:5:49:GLN:NE2	13:5:62:THR:OG1	2.47	0.42
13:5:375:ALA:HB1	13:5:378:ILE:HB	2.02	0.42
4:A:780:LYS:HZ3	4:A:780:LYS:HG2	1.64	0.42
7:E:341:LEU:N	7:E:341:LEU:CD2	2.83	0.42
8:D:349:LYS:HD3	8:D:349:LYS:HA	1.82	0.42
10:2:325:THR:HG21	10:2:594:GLY:O	2.20	0.42
15:6:116:GLU:OE2	15:6:187:ARG:NH1	2.52	0.42
3:9:248:LEU:HD11	3:9:281:LEU:HD21	2.02	0.42
3:9:389:TYR:HA	3:9:392:LYS:HG2	2.02	0.42
11:3:23:ASP:HA	11:3:26:ARG:HE	1.85	0.42
11:3:679:ILE:HD12	11:3:679:ILE:HA	1.92	0.42
12:4:695:PRO:HA	12:4:696:PRO:HD3	1.72	0.42
13:5:456:ASP:HA	13:5:457:PRO:HD3	1.89	0.42
15:6:298:SER:O	15:6:357:GLN:CG	2.68	0.42
3:9:332:ARG:HA	3:9:335:PHE:HB3	2.02	0.42
3:9:496:ARG:O	3:9:496:ARG:NH1	2.53	0.42
5:B:411:TYR:HA	5:B:414:GLN:HG2	2.01	0.42
6:C:212:ASN:OD1	6:C:212:ASN:N	2.53	0.42
7:E:209:LEU:HD12	7:E:266:TRP:CE2	2.55	0.42
10:2:578:ALA:HA	10:2:593:GLY:HA2	2.02	0.42
11:3:653:ILE:CB	13:5:401:PRO:O	2.68	0.42
11:3:900:ILE:O	11:3:904:MET:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:4:732:LYS:HA	12:4:733:PRO:HD3	1.92	0.42
13:5:448:GLY:O	13:5:467:GLY:HA2	2.15	0.42
6:C:367:LEU:HB3	6:C:377:ILE:HD13	2.01	0.41
7:E:391:GLN:NE2	7:E:414:MET:SD	2.93	0.41
9:F:272:LEU:HG	9:F:355:LEU:HB2	2.00	0.41
11:3:463:VAL:HG22	11:3:506:LEU:HD23	2.02	0.41
14:L:207:TYR:HE1	14:L:212:MET:HB2	1.85	0.41
3:9:421:ILE:HG22	3:9:422:ILE:HD13	2.02	0.41
4:A:905:MET:HE3	4:A:905:MET:HB3	2.00	0.41
5:B:324:ASN:OD1	5:B:324:ASN:N	2.51	0.41
6:C:99:ARG:O	6:C:100:ARG:NE	2.53	0.41
6:C:459:ASP:OD1	6:C:459:ASP:N	2.49	0.41
7:E:36:GLN:HG3	7:E:176:LEU:HD22	2.02	0.41
11:3:183:GLU:HA	11:3:293:ASN:HA	2.02	0.41
11:3:284:ASP:O	16:7:228:ARG:NH2	2.53	0.41
12:4:916:VAL:HA	12:4:926:SER:HA	2.02	0.41
16:7:333:ILE:HD13	16:7:351:VAL:HG11	2.02	0.41
6:C:295:SER:OG	6:C:296:ASP:N	2.53	0.41
6:C:531:ALA:HB1	6:C:535:ILE:HG21	2.01	0.41
7:E:260:ASP:OD1	7:E:260:ASP:N	2.42	0.41
8:D:137:HIS:HB3	8:D:142:ALA:HB2	2.01	0.41
8:D:285:VAL:HG13	8:D:313:LEU:HD11	2.02	0.41
10:2:518:SER:HA	10:2:537:ILE:HB	2.02	0.41
15:6:309:PHE:HD1	15:6:346:LEU:HA	1.86	0.41
15:6:463:GLY:HA3	15:6:594:ARG:HE	1.66	0.41
16:7:290:SER:OG	16:7:291:GLN:OE1	2.36	0.41
16:7:549:SER:HA	16:7:554:ASN:HA	2.02	0.41
16:7:769:VAL:HG11	16:7:779:LEU:HB2	2.01	0.41
5:B:558:LEU:O	5:B:562:LEU:N	2.46	0.41
10:2:211:LEU:HA	10:2:214:PHE:HB3	2.02	0.41
12:4:341:ASP:O	12:4:391:PHE:CB	2.68	0.41
14:L:224:GLU:HA	14:L:225:PRO:HD3	1.87	0.41
16:7:703:ARG:NH1	16:7:712:ASP:OD1	2.47	0.41
5:B:556:LEU:HD23	5:B:598:GLU:HG2	2.02	0.41
6:C:133:PRO:HG3	6:C:207:ASP:HB3	2.03	0.41
6:C:446:CYS:O	6:C:450:LYS:N	2.53	0.41
8:D:509:ILE:HD12	8:D:509:ILE:HA	1.93	0.41
9:F:298:VAL:HA	9:F:301:LYS:HB2	2.03	0.41
9:F:335:ARG:O	9:F:339:ASP:N	2.53	0.41
12:4:362:ARG:NE	16:7:299:PHE:CD2	2.86	0.41
14:L:195:VAL:HG12	14:L:235:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:6:152:TYR:OH	15:6:388:ARG:NH1	2.52	0.41
16:7:652:MET:HA	16:7:708:VAL:HB	2.03	0.41
3:9:63:GLN:O	3:9:66:SER:OG	2.33	0.41
3:9:411:ASN:HD21	3:9:413:GLN:HB3	1.86	0.41
6:C:285:LEU:HD12	6:C:285:LEU:HA	1.92	0.41
6:C:525:PHE:HA	6:C:528:TYR:HB3	2.02	0.41
7:E:191:ARG:HH21	7:E:253:ASN:HB2	1.85	0.41
8:D:422:ILE:HD11	8:D:526:TRP:HE1	1.86	0.41
11:3:172:THR:HA	13:5:172:LEU:HD21	2.02	0.41
15:6:124:VAL:HG23	15:6:124:VAL:O	2.20	0.41
15:6:270:LEU:HD12	15:6:289:SER:HB3	2.02	0.41
6:C:136:SER:HA	6:C:142:MET:HG3	2.02	0.41
6:C:494:TRP:HZ2	9:F:380:ARG:HH11	1.68	0.41
11:3:366:SER:OG	11:3:366:SER:O	2.38	0.41
15:6:570:ASN:HB2	15:6:709:PHE:HA	2.02	0.41
15:6:573:VAL:HG12	15:6:713:PHE:HB2	2.03	0.41
7:E:130:LEU:HD12	7:E:130:LEU:HA	1.86	0.41
8:D:348:SER:HB3	8:D:354:LEU:HD12	2.03	0.41
10:2:660:THR:O	10:2:660:THR:OG1	2.38	0.41
11:3:362:ILE:HD12	11:3:362:ILE:HA	1.99	0.41
11:3:403:ILE:O	11:3:511:SER:OG	2.39	0.41
12:4:538:LYS:HE3	12:4:828:LEU:HD12	2.02	0.41
13:5:279:ASP:HB3	13:5:280:ARG:H	1.59	0.41
14:L:46:LYS:HG3	14:L:227:CYS:HB3	2.02	0.41
15:6:116:GLU:O	15:6:120:GLU:HB2	2.21	0.41
15:6:526:TYR:HB2	15:6:814:ASN:OD1	2.20	0.41
16:7:81:ASP:OD1	16:7:81:ASP:N	2.50	0.41
3:9:94:LYS:HB2	3:9:101:SER:HA	2.02	0.41
3:9:414:GLN:HA	3:9:417:ILE:HG22	2.03	0.41
3:9:487:ASP:OD1	3:9:487:ASP:N	2.43	0.41
6:C:440:LEU:HD13	6:C:446:CYS:HB3	2.03	0.41
7:E:209:LEU:HD13	7:E:209:LEU:HA	1.93	0.41
8:D:100:LEU:HD23	8:D:273:ILE:HG23	2.03	0.41
8:D:510:LEU:HD12	8:D:513:LEU:HD12	2.03	0.41
10:2:340:ASN:HA	10:2:346:SER:O	2.20	0.41
11:3:274:ILE:HD11	11:3:321:ILE:CD1	2.49	0.41
12:4:352:CYS:CB	12:4:376:CYS:HB3	2.51	0.41
12:4:735:HIS:HB3	12:4:738:GLN:HE22	1.85	0.41
15:6:542:ALA:HA	15:6:545:LYS:HE3	2.02	0.41
15:6:620:ASP:OD1	15:6:621:TYR:N	2.54	0.41
15:6:661:ILE:O	15:6:671:THR:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:855:ASP:OD1	4:A:855:ASP:N	2.54	0.41
6:C:121:GLU:HB3	6:C:126:ASN:HD21	1.86	0.41
11:3:488:GLU:CB	16:7:482:TYR:OH	2.69	0.41
11:3:498:ALA:CB	16:7:512:ALA:HB2	2.51	0.41
12:4:878:SER:O	12:4:878:SER:OG	2.38	0.41
13:5:147:PRO:HG2	13:5:150:ASP:HB2	2.03	0.41
13:5:263:GLU:HA	13:5:430:GLU:OE1	2.21	0.41
13:5:437:VAL:HG13	13:5:468:ALA:HB1	2.03	0.41
15:6:600:GLY:HA3	15:6:639:ASP:O	2.21	0.41
4:A:565:LEU:HD12	4:A:565:LEU:HA	1.84	0.40
4:A:632:LEU:HD12	4:A:697:ALA:HB2	2.03	0.40
5:B:458:HIS:CE1	5:B:460:TYR:HB2	2.55	0.40
12:4:314:MET:HA	12:4:317:LEU:HD12	2.03	0.40
13:5:33:ASN:O	13:5:37:GLU:CB	2.70	0.40
3:9:86:GLU:O	3:9:90:ASN:ND2	2.54	0.40
4:A:691:ILE:HD12	4:A:691:ILE:HA	1.93	0.40
7:E:372:ASN:HD22	7:E:476:ASP:HB3	1.86	0.40
8:D:374:ASN:OD1	8:D:374:ASN:N	2.55	0.40
12:4:332:VAL:HG23	12:4:429:ALA:HA	2.02	0.40
12:4:518:LEU:HD12	12:4:521:LEU:HD23	2.02	0.40
15:6:516:LEU:HA	15:6:519:MET:HG2	2.04	0.40
3:9:83:ALA:H	3:9:295:GLN:NE2	2.19	0.40
6:C:91:LEU:HD12	6:C:91:LEU:HA	1.95	0.40
9:F:279:LYS:HA	9:F:279:LYS:HD3	1.86	0.40
10:2:245:ASN:HD21	14:L:217:ASN:HD21	1.68	0.40
10:2:388:VAL:O	10:2:408:VAL:HG12	2.21	0.40
10:2:538:ASN:HA	10:2:646:ILE:O	2.20	0.40
10:2:549:LYS:HE2	10:2:549:LYS:HB2	1.87	0.40
11:3:415:LYS:HE2	11:3:415:LYS:HB2	1.94	0.40
12:4:865:LEU:HD21	12:4:903:ILE:HA	2.04	0.40
4:A:406:PHE:HB2	8:D:187:LEU:HD22	2.03	0.40
4:A:798:SER:OG	4:A:799:PHE:N	2.55	0.40
8:D:269:SER:O	8:D:269:SER:OG	2.34	0.40
8:D:395:ALA:HB1	8:D:510:LEU:HB2	2.04	0.40
10:2:367:CYS:HB3	10:2:369:SER:OG	2.22	0.40
11:3:439:GLY:HA3	11:3:445:ALA:HB2	2.04	0.40
12:4:860:LYS:HD3	12:4:860:LYS:HA	1.88	0.40
14:L:384:ASN:N	14:L:384:ASN:OD1	2.55	0.40
15:6:528:LYS:O	15:6:532:SER:HB3	2.22	0.40
4:A:687:ASP:N	4:A:687:ASP:OD1	2.52	0.40
4:A:857:ILE:HG21	8:D:369:LYS:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:532:GLN:HG2	5:B:553:GLY:HA2	2.03	0.40
6:C:436:LEU:HD11	6:C:455:PHE:H	1.87	0.40
6:C:474:LEU:HD11	9:F:405:MET:HA	2.03	0.40
8:D:216:PHE:HD2	8:D:219:ILE:HG13	1.86	0.40
11:3:225:ILE:HA	11:3:226:PRO:HD3	1.81	0.40
12:4:574:LYS:HE2	12:4:574:LYS:HB2	1.94	0.40
12:4:774:TYR:HH	12:4:795:THR:N	2.19	0.40
15:6:303:GLU:CB	15:6:354:LEU:O	2.70	0.40
16:7:768:THR:HA	16:7:771:LEU:HG	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	
3	9	363/513 (71%)	320 (88%)	41 (11%)	2 (1%)	25	66
4	A	406/913 (44%)	374 (92%)	31 (8%)	1 (0%)	47	81
5	B	313/620 (50%)	290 (93%)	23 (7%)	0	100	100
6	C	536/616 (87%)	506 (94%)	29 (5%)	1 (0%)	47	81
7	E	414/479 (86%)	386 (93%)	27 (6%)	1 (0%)	47	81
8	D	428/529 (81%)	402 (94%)	25 (6%)	1 (0%)	47	81
9	F	153/435 (35%)	146 (95%)	7 (5%)	0	100	100
10	2	559/868 (64%)	533 (95%)	23 (4%)	3 (0%)	29	69
11	3	619/971 (64%)	574 (93%)	43 (7%)	2 (0%)	41	77
12	4	634/933 (68%)	594 (94%)	37 (6%)	3 (0%)	29	69
13	5	511/775 (66%)	493 (96%)	15 (3%)	3 (1%)	25	66
14	L	361/604 (60%)	328 (91%)	32 (9%)	1 (0%)	41	77
15	6	551/1017 (54%)	519 (94%)	26 (5%)	6 (1%)	14	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	7	605/845 (72%)	578 (96%)	26 (4%)	1 (0%)	47	81
All	All	6453/10118 (64%)	6043 (94%)	385 (6%)	25 (0%)	38	72

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	9	284	GLN
6	C	605	TYR
7	E	445	SER
10	2	350	PRO
10	2	572	SER
13	5	507	ALA
15	6	557	LYS
10	2	577	THR
11	3	500	ALA
14	L	215	THR
15	6	305	TYR
3	9	283	PRO
16	7	231	LYS
4	A	854	SER
8	D	420	LYS
11	3	226	PRO
12	4	678	ILE
12	4	682	TYR
13	5	279	ASP
13	5	500	GLN
15	6	555	VAL
15	6	817	ASP
15	6	560	VAL
15	6	562	GLY
12	4	530	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	9	335/470 (71%)	330 (98%)	5 (2%)	65	80
4	A	362/812 (45%)	362 (100%)	0	100	100
5	B	294/573 (51%)	292 (99%)	2 (1%)	84	90
6	C	504/576 (88%)	504 (100%)	0	100	100
7	E	386/440 (88%)	386 (100%)	0	100	100
8	D	397/488 (81%)	396 (100%)	1 (0%)	92	95
9	F	151/406 (37%)	151 (100%)	0	100	100
10	2	438/770 (57%)	432 (99%)	6 (1%)	67	80
11	3	493/835 (59%)	488 (99%)	5 (1%)	76	86
12	4	528/848 (62%)	520 (98%)	8 (2%)	65	80
13	5	424/688 (62%)	420 (99%)	4 (1%)	78	87
14	L	325/545 (60%)	317 (98%)	8 (2%)	47	68
15	6	416/886 (47%)	413 (99%)	3 (1%)	84	90
16	7	498/753 (66%)	495 (99%)	3 (1%)	86	92
All	All	5551/9090 (61%)	5506 (99%)	45 (1%)	82	89

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	9	297	TYR
3	9	335	PHE
3	9	406	ARG
3	9	477	LYS
3	9	495	MET
5	B	411	TYR
5	B	547	ARG
8	D	499	PHE
10	2	325	THR
10	2	341	CYS
10	2	517	CYS
10	2	544	ASP
10	2	553	LEU
10	2	794	ARG
11	3	24	ARG
11	3	239	ASN
11	3	527	ARG
11	3	953	VAL
11	3	957	LYS

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Mol	Chain	Res	Type
12	4	190	CYS
12	4	344	VAL
12	4	727	LEU
12	4	888	LYS
12	4	889	GLN
12	4	918	VAL
12	4	919	LEU
12	4	928	ARG
13	5	276	MET
13	5	280	ARG
13	5	422	LYS
13	5	682	ARG
14	L	22	ARG
14	L	63	THR
14	L	129	CYS
14	L	203	LYS
14	L	214	THR
14	L	277	THR
14	L	292	LYS
14	L	388	ARG
15	6	355	ASP
15	6	555	VAL
15	6	633	ASN
16	7	73	ARG
16	7	638	MET
16	7	754	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
3	9	90	ASN
3	9	295	GLN
3	9	388	ASN
4	A	530	ASN
4	A	882	GLN
4	A	906	ASN
5	B	279	ASN
5	B	282	ASN
5	B	297	GLN
5	B	310	GLN
5	B	364	ASN
5	B	426	ASN

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Mol	Chain	Res	Type
5	B	458	HIS
5	B	535	ASN
5	B	585	HIS
6	C	63	GLN
6	C	65	HIS
6	C	69	HIS
6	C	78	ASN
6	C	243	ASN
6	C	253	GLN
6	C	486	ASN
7	E	52	ASN
7	E	58	HIS
7	E	114	ASN
7	E	253	ASN
7	E	320	GLN
7	E	422	GLN
7	E	453	ASN
8	D	80	GLN
8	D	105	GLN
8	D	158	HIS
8	D	277	GLN
8	D	321	ASN
8	D	327	ASN
8	D	409	ASN
8	D	511	GLN
9	F	318	GLN
9	F	326	ASN
9	F	407	GLN
10	2	245	ASN
10	2	248	HIS
10	2	384	ASN
11	3	210	HIS
11	3	239	ASN
11	3	351	ASN
11	3	395	ASN
11	3	487	HIS
11	3	691	ASN
12	4	247	ASN
12	4	380	ASN
12	4	543	GLN
13	5	49	GLN
13	5	145	GLN

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Mol	Chain	Res	Type
13	5	203	ASN
13	5	411	ASN
13	5	676	HIS
14	L	99	GLN
14	L	127	GLN
14	L	217	ASN
14	L	412	GLN
14	L	413	GLN
15	6	570	ASN
16	7	108	GLN
16	7	425	ASN
16	7	585	ASN

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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	A	2001	-	26,33,33	0.72	1 (3%)	26,52,52	1.08	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	AGS	D	2001	-	26,33,33	0.75	0	26,52,52	1.40	2 (7%)
17	AGS	E	2001	18	26,33,33	0.67	0	26,52,52	1.32	2 (7%)
17	AGS	9	2001	-	26,33,33	0.73	1 (3%)	26,52,52	1.30	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	A	2001	-	-	7/17/38/38	0/3/3/3
17	AGS	D	2001	-	-	2/17/38/38	0/3/3/3
17	AGS	E	2001	18	-	7/17/38/38	0/3/3/3
17	AGS	9	2001	-	-	7/17/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	2001	AGS	C8-N7	-2.04	1.31	1.34
17	A	2001	AGS	C8-N7	-2.01	1.31	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	2001	AGS	PA-O3A-PB	-5.96	112.36	132.83
17	9	2001	AGS	PA-O3A-PB	-5.45	114.11	132.83
17	E	2001	AGS	PA-O3A-PB	-5.19	115.00	132.83
17	A	2001	AGS	PA-O3A-PB	-3.85	119.63	132.83
17	A	2001	AGS	C5-C6-N6	2.25	123.78	120.35
17	D	2001	AGS	C5-C6-N6	2.24	123.76	120.35
17	E	2001	AGS	C5-C6-N6	2.19	123.68	120.35
17	9	2001	AGS	C5-C6-N6	2.16	123.64	120.35

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	9	2001	AGS	C5'-O5'-PA-O2A
17	9	2001	AGS	C5'-O5'-PA-O3A
17	A	2001	AGS	C5'-O5'-PA-O1A

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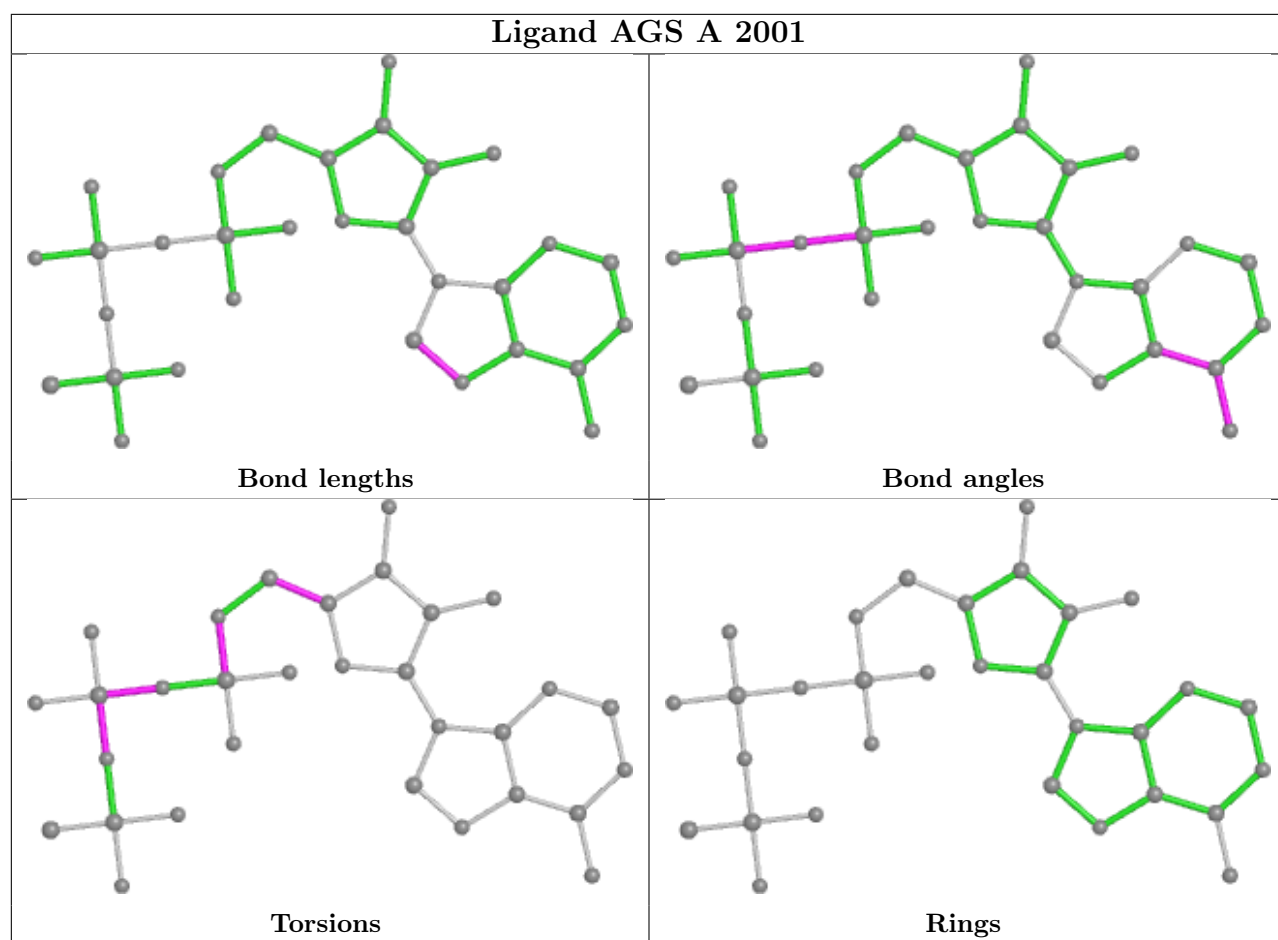
Mol	Chain	Res	Type	Atoms
17	A	2001	AGS	C5'-O5'-PA-O2A
17	A	2001	AGS	O4'-C4'-C5'-O5'
17	E	2001	AGS	C5'-O5'-PA-O1A
17	E	2001	AGS	C5'-O5'-PA-O2A
17	E	2001	AGS	C5'-O5'-PA-O3A
17	9	2001	AGS	O4'-C4'-C5'-O5'
17	E	2001	AGS	O4'-C4'-C5'-O5'
17	9	2001	AGS	C3'-C4'-C5'-O5'
17	E	2001	AGS	C3'-C4'-C5'-O5'
17	9	2001	AGS	PB-O3A-PA-O1A
17	A	2001	AGS	PG-O3B-PB-O1B
17	9	2001	AGS	C4'-C5'-O5'-PA
17	D	2001	AGS	C4'-C5'-O5'-PA
17	E	2001	AGS	PG-O3B-PB-O2B
17	D	2001	AGS	C3'-C4'-C5'-O5'
17	A	2001	AGS	PA-O3A-PB-O1B
17	A	2001	AGS	C5'-O5'-PA-O3A
17	9	2001	AGS	PB-O3A-PA-O2A
17	E	2001	AGS	PA-O3A-PB-O1B
17	A	2001	AGS	C3'-C4'-C5'-O5'

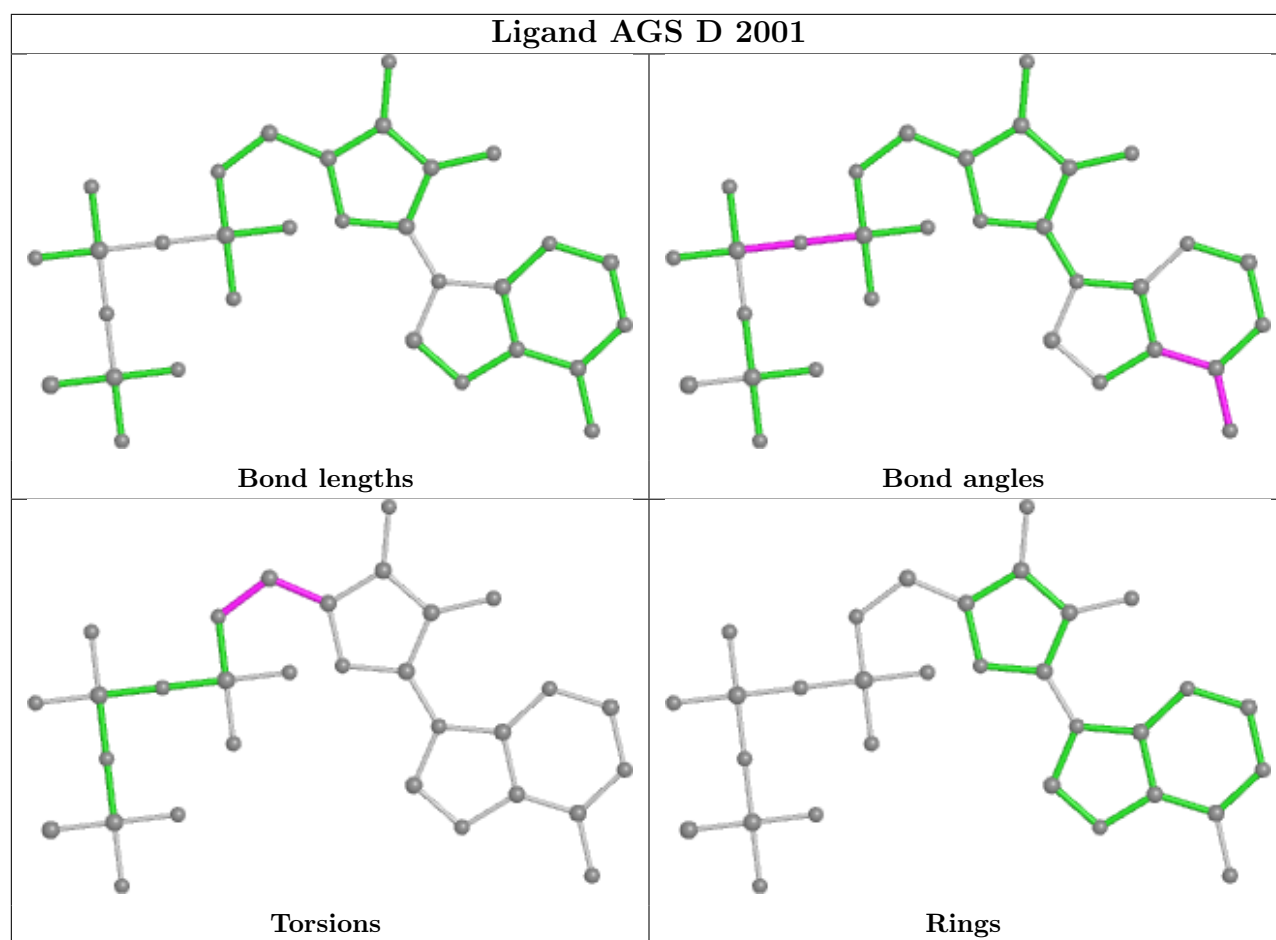
There are no ring outliers.

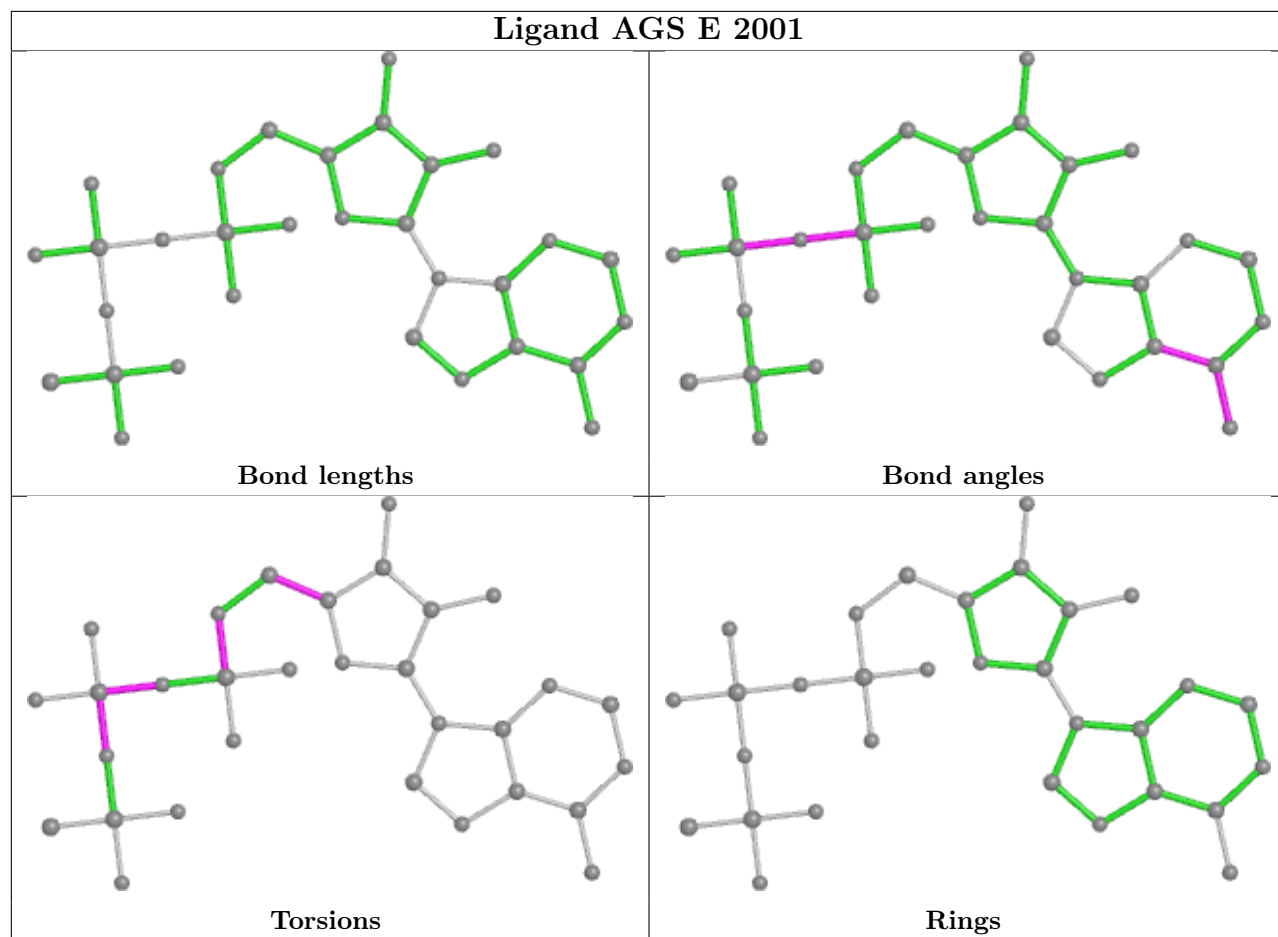
4 monomers are involved in 16 short contacts:

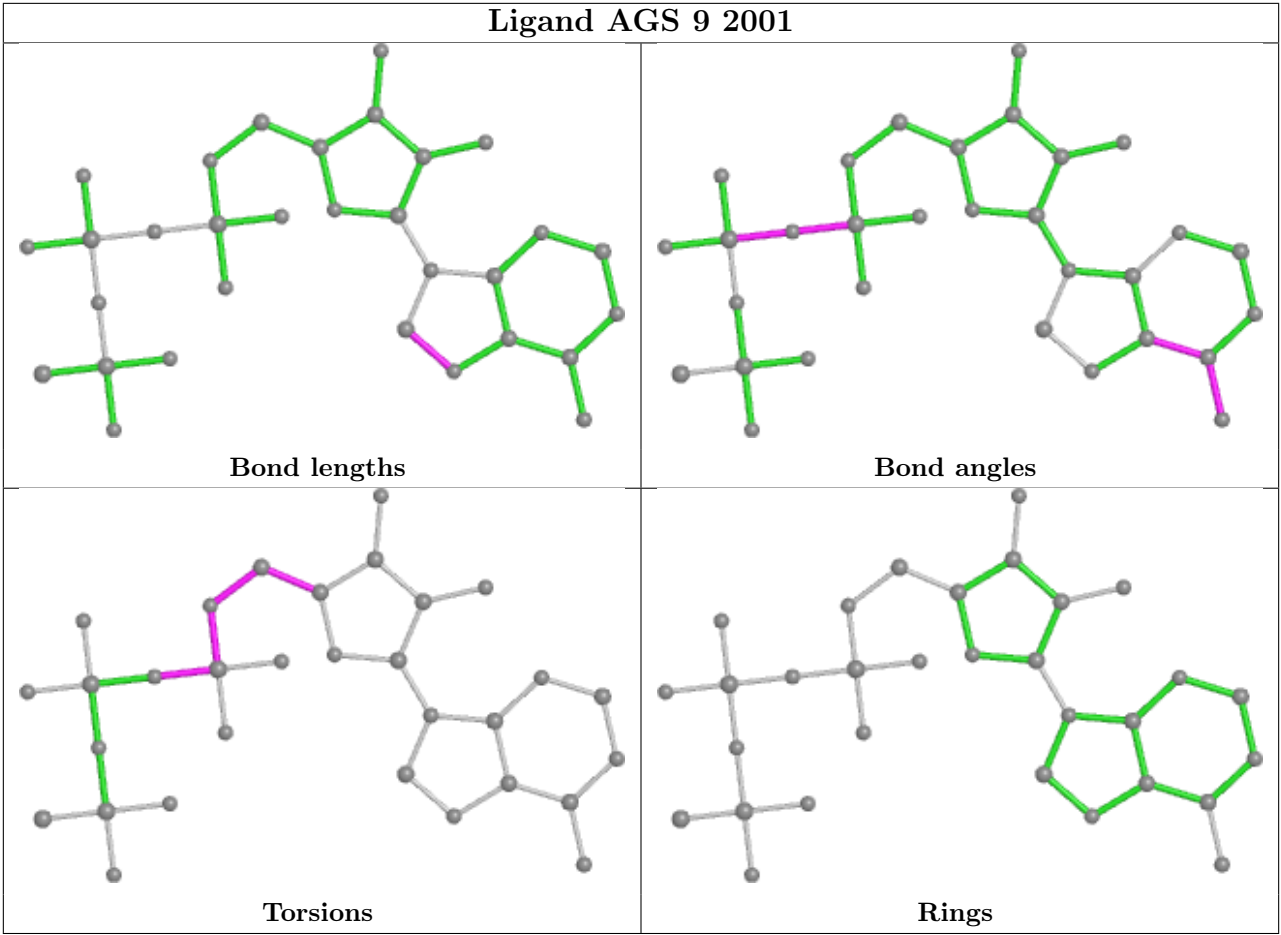
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	2001	AGS	7	0
17	D	2001	AGS	3	0
17	E	2001	AGS	2	0
17	9	2001	AGS	4	0

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









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	9	1
11	3	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	9	399:ASN	C	400:ASN	N	3.97
1	3	260:GLU	C	261:MET	N	1.11

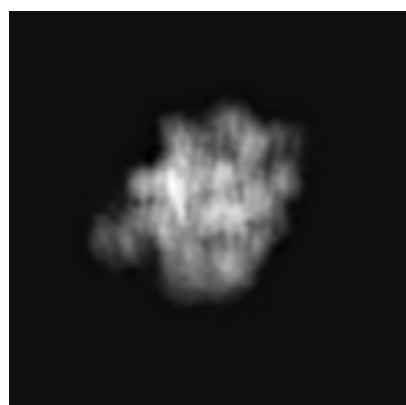
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21666. These allow visual inspection of the internal detail of the map and identification of artifacts.

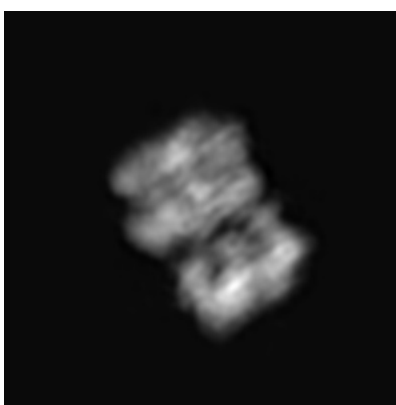
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

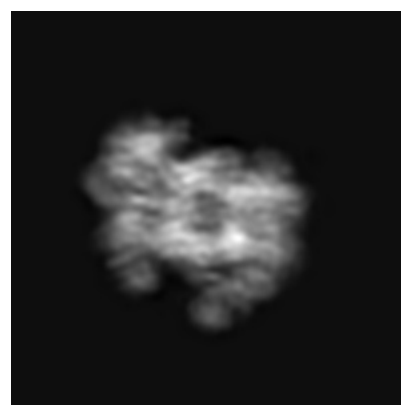
6.1.1 Primary map



X



Y

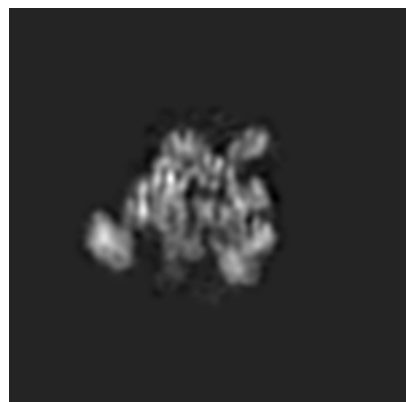


Z

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

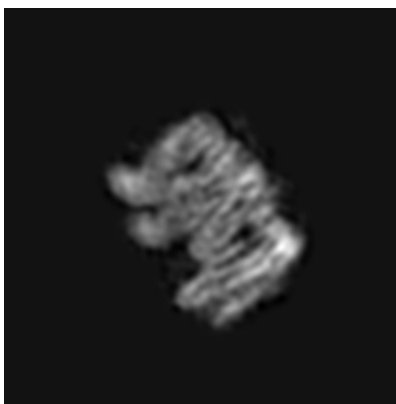
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 85



Y Index: 109

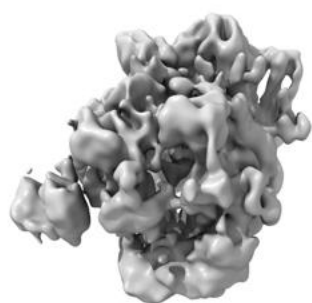


Z Index: 145

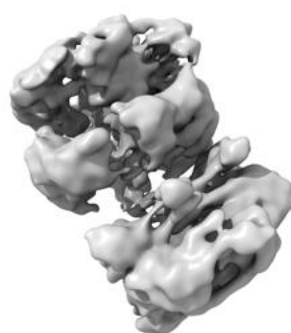
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

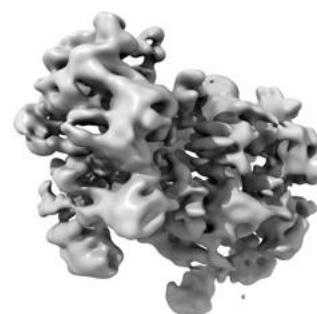
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0173. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

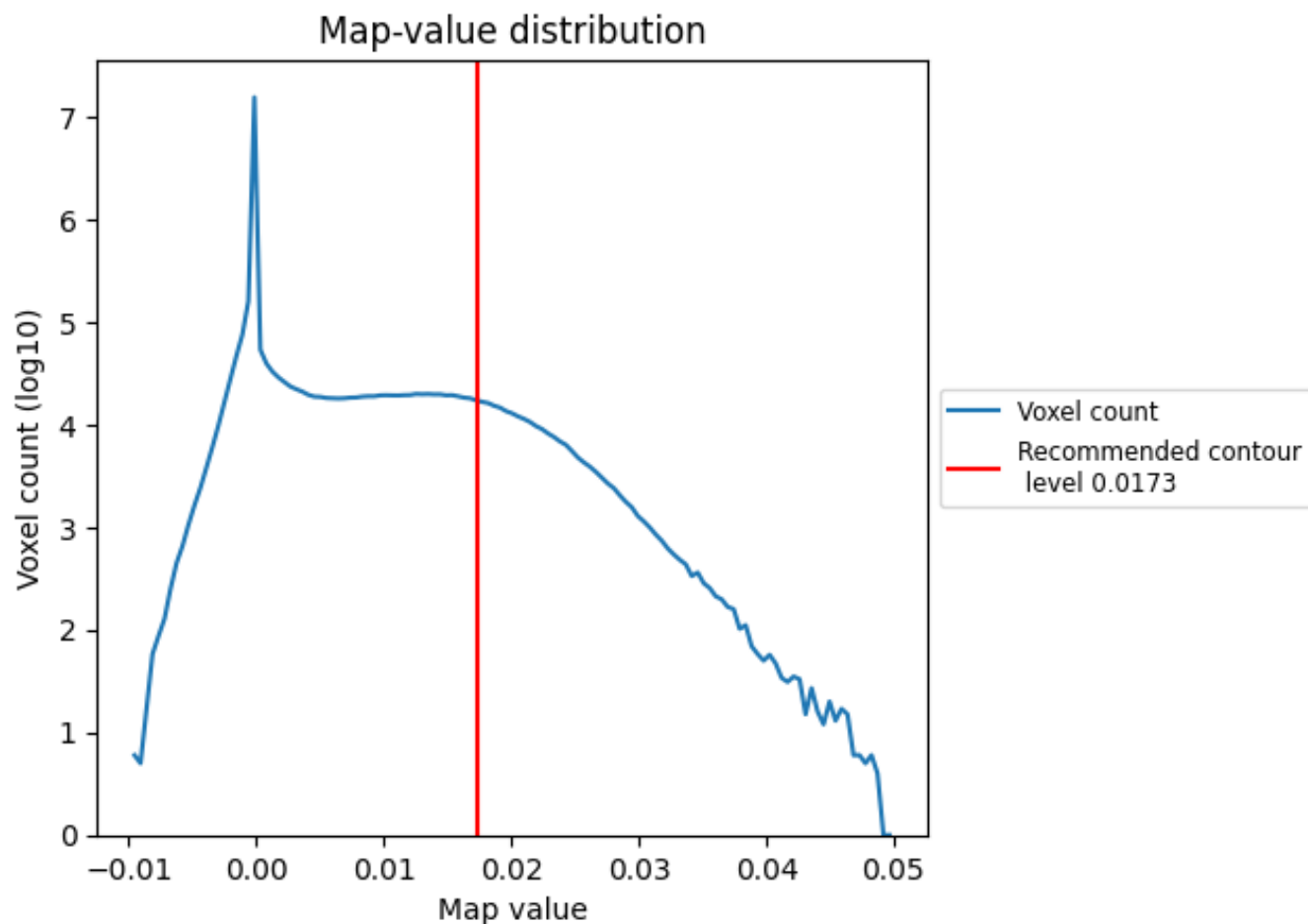
6.5 Mask visualisation

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

7 Map analysis [i](#)

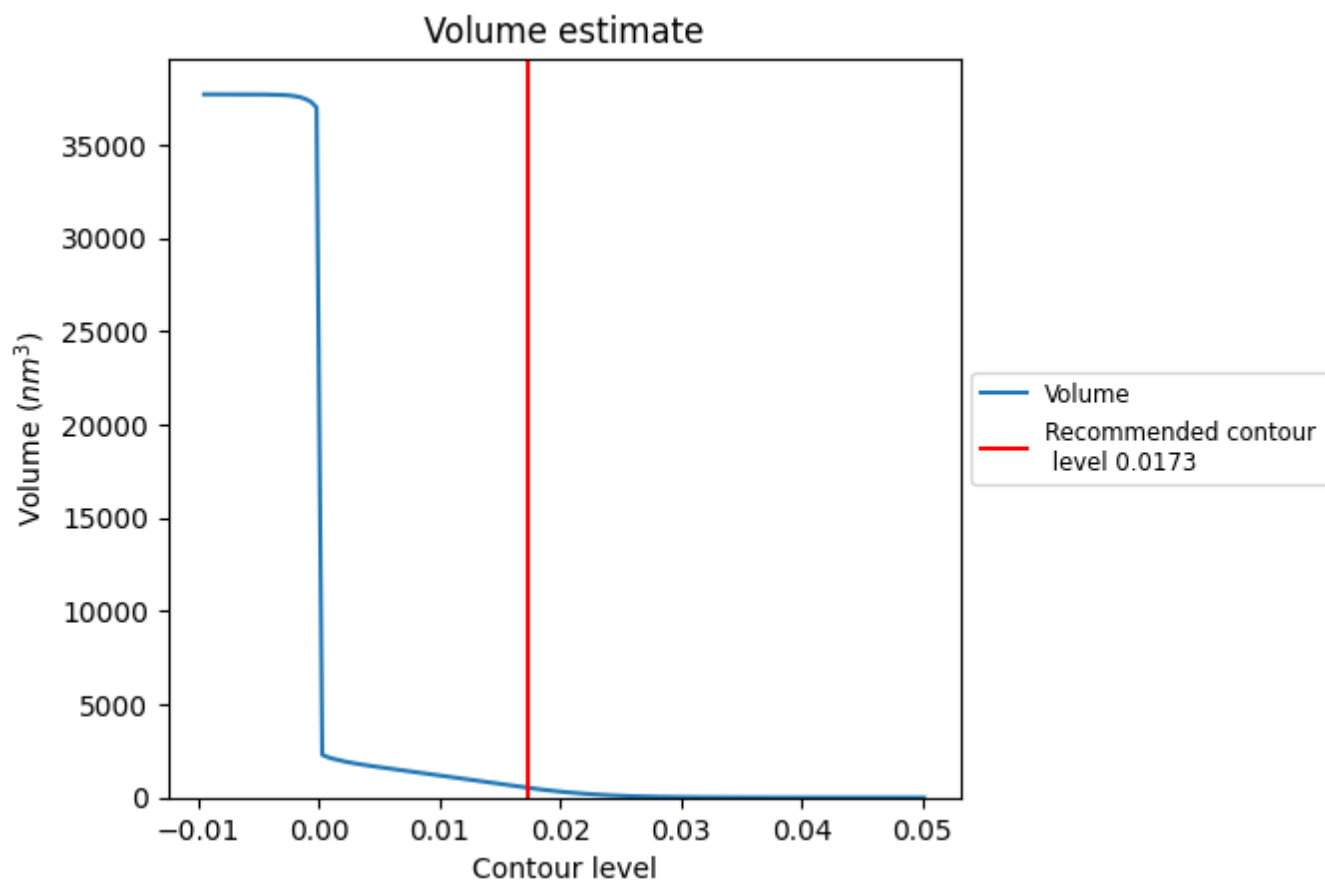
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

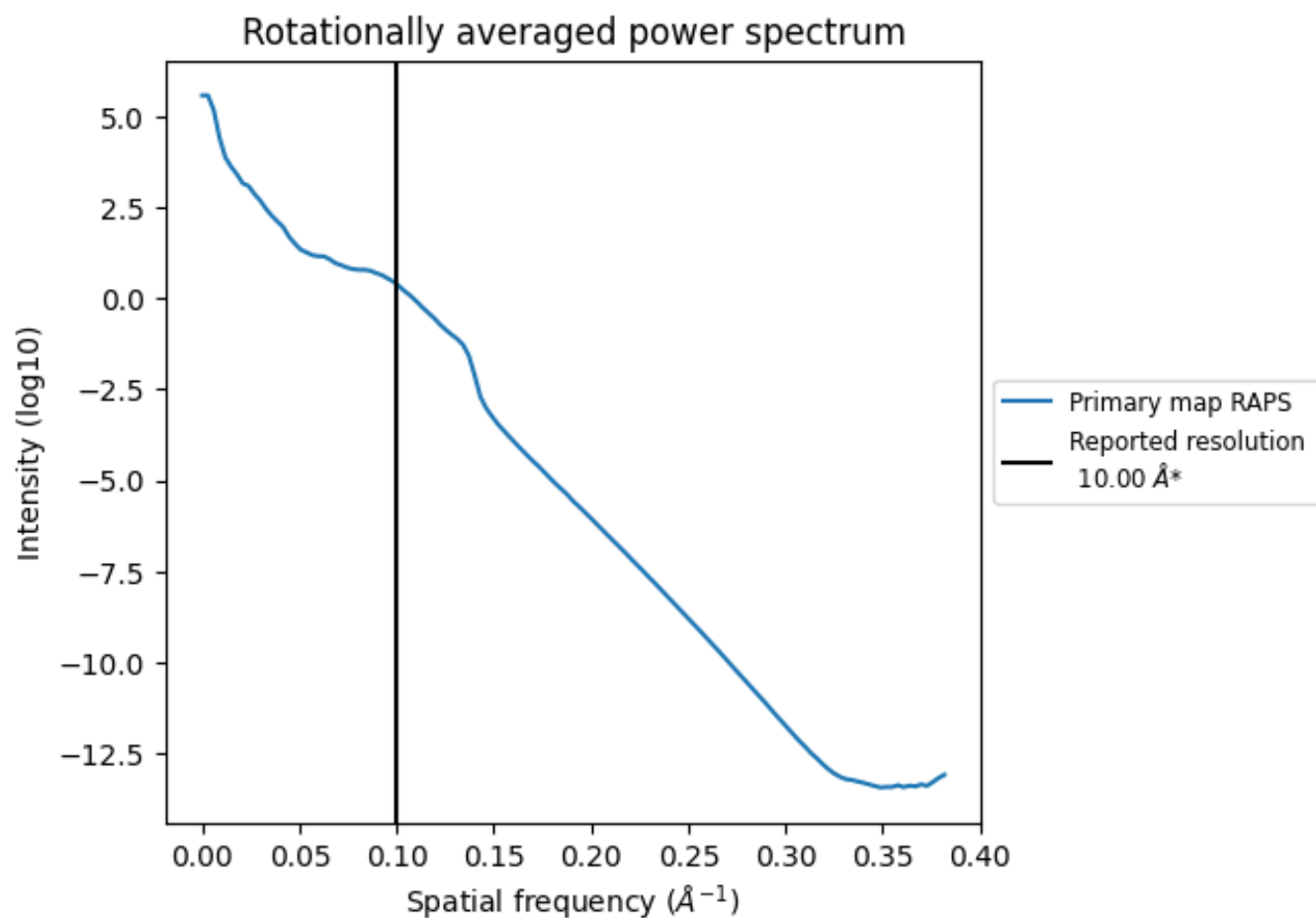
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 519 nm³; this corresponds to an approximate mass of 469 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.100 Å⁻¹

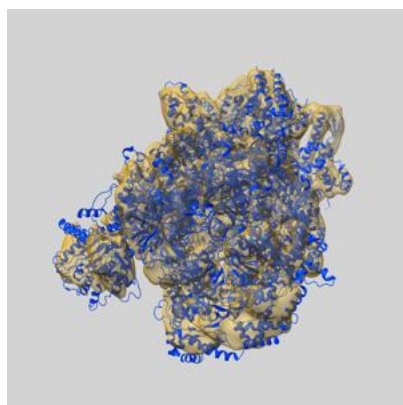
8 Fourier-Shell correlation ⓘ

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

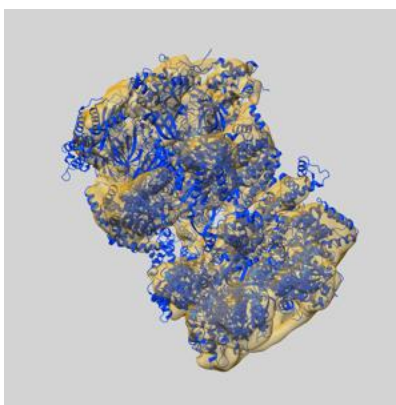
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21666 and PDB model 6WGI. Per-residue inclusion information can be found in section [3](#) on page [8](#).

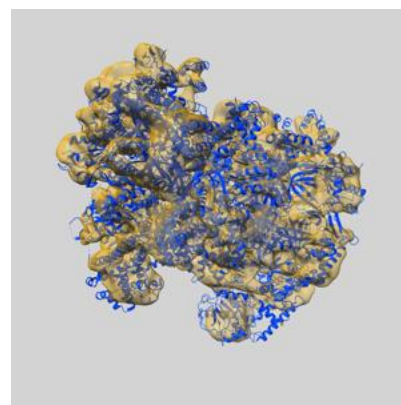
9.1 Map-model overlay [i](#)



X



Y



Z

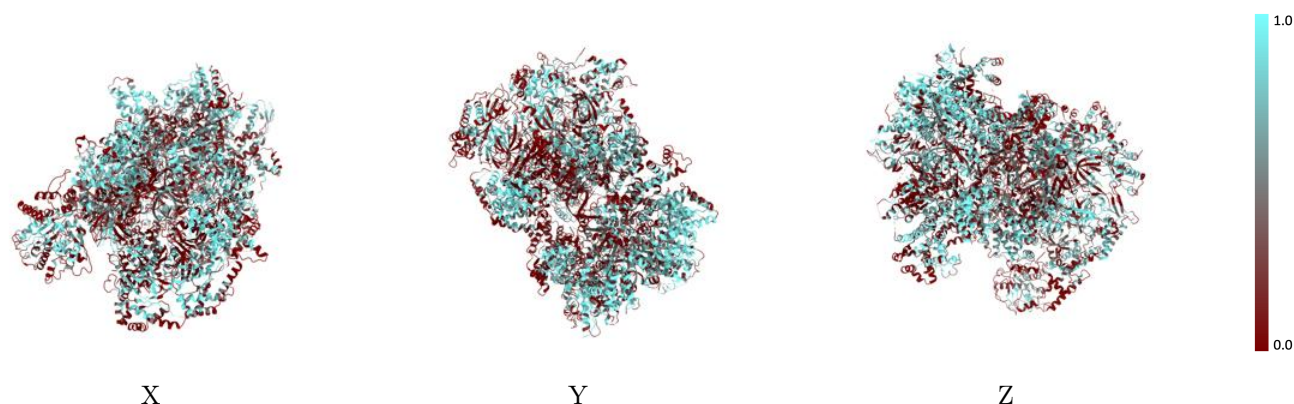
The images above show the 3D surface view of the map at the recommended contour level 0.0173 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



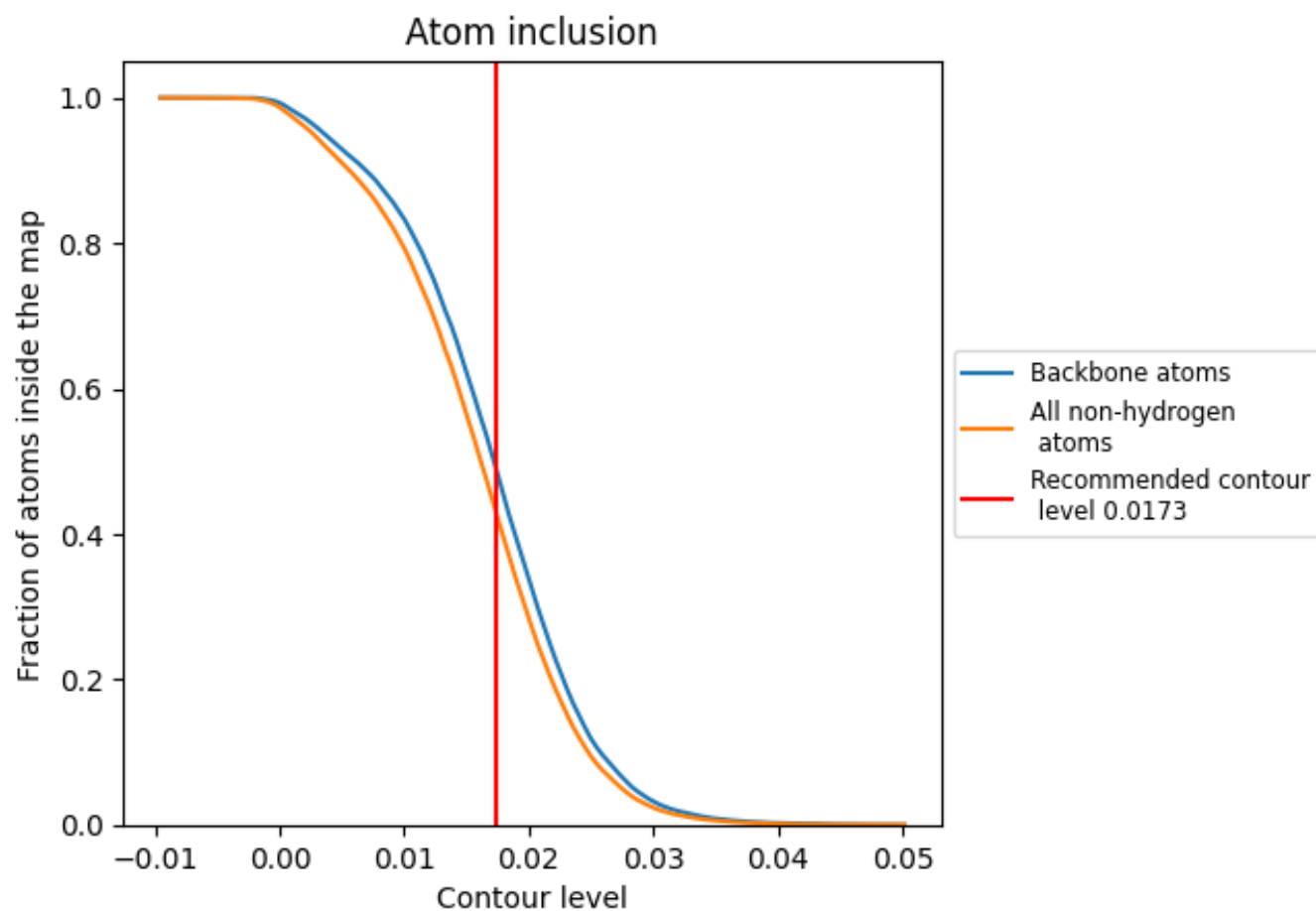
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0173).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 49% of all backbone atoms, 43% 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 (0.0173) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4336	 0.0860
2	 0.4522	 0.0970
3	 0.4413	 0.0710
4	 0.4213	 0.0990
5	 0.2949	 0.0450
6	 0.4895	 0.0900
7	 0.4524	 0.0890
9	 0.4553	 0.0710
A	 0.5077	 0.0980
B	 0.3499	 0.0900
C	 0.4872	 0.0980
D	 0.6173	 0.1050
E	 0.5632	 0.1060
F	 0.0062	 0.0330
G	 0.3127	 0.0950
H	 0.3529	 0.1190
L	 0.2382	 0.0700

