Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 01:11 am GMT

PDB ID	:	6RAX
EMDB ID	:	EMD-4786
Title	:	D. melanogaster CMG-DNA, State 1B
Authors	:	Eickhoff, P.; Martino, F.; Costa, A.
Deposited on	:	2019-04-08
Resolution	:	3.99 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:

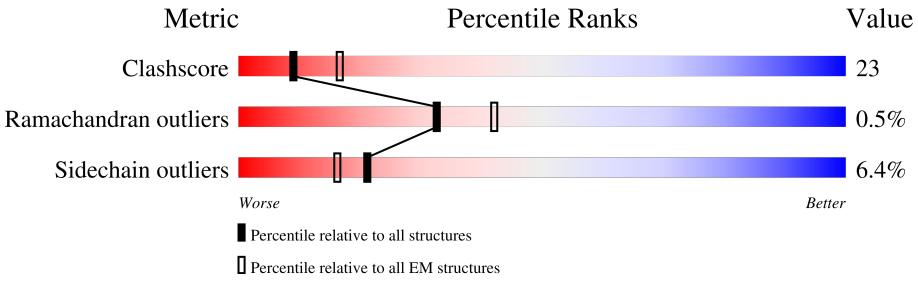
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.99 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	2	887	11% 39% 24% 32%
2	3	819	13% 46% 28% 24%
3	4	866	19% 44% 26% 28%
4	5	733	13% 47% 32% 5% 15%
5	6	817	19% 48% 26% 23%
6	7	720	23% 27% 58% 12%
7	X	21	62% 10% 76% 14%
8	Y	8	62% 25% 75%

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Mol	Chain	Length	Quality of chain
9	A	575	12% 64% 32%
10	H	202	20% 56% 36%
11	L	203	5% 53% 33% 9%
12	M	212	16% 42% 34% 21%
13	N	228	12% 61% 28% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	ATP	3	901	-	-	X	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 40970 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 licensing factor Mcm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	2	605	4788	3023	835	899	31	0	0

- Molecule 2 is a protein called DNA replication licensing factor Mcm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	625	4879	3044	868	939	28	0	0

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	626	5013	3150	886	951	26	0	0

- Molecule 4 is a protein called DNA replication licensing factor Mcm5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	620	4864	3047	869	917	31	0	0

- Molecule 5 is a protein called DNA replication licensing factor Mcm6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	6	628	4986	3121	882	954	29	0	0

- Molecule 6 is a protein called DNA replication licensing factor Mcm7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	7	636	4964	3100	885	945	34	0	1

- Molecule 7 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	21	Total	C	N	O	P	0	0
			424	208	56	139	21		

- Molecule 8 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Y	8	Total	C	N	O	P	0	0
			164	78	30	48	8		

- Molecule 9 is a protein called CDC45L.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	567	Total	C	N	O	S	0	0
			4575	2900	791	862	22		

- Molecule 10 is a protein called IP07275p.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	195	Total	C	N	O	S	0	0
			1583	1007	279	289	8		

- Molecule 11 is a protein called Probable DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	185	Total	C	N	O	S	0	0
			1498	962	252	271	13		

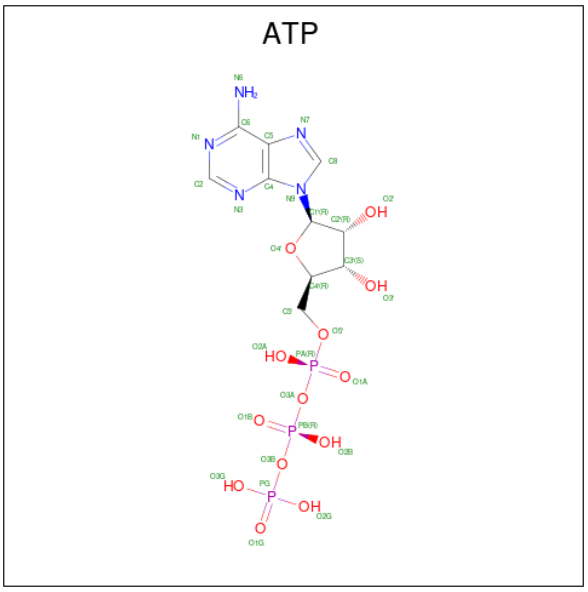
- Molecule 12 is a protein called AT18545p.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	167	Total	C	N	O	S	0	0
			1381	877	245	255	4		

- Molecule 13 is a protein called DNA replication complex GINS protein SLD5.

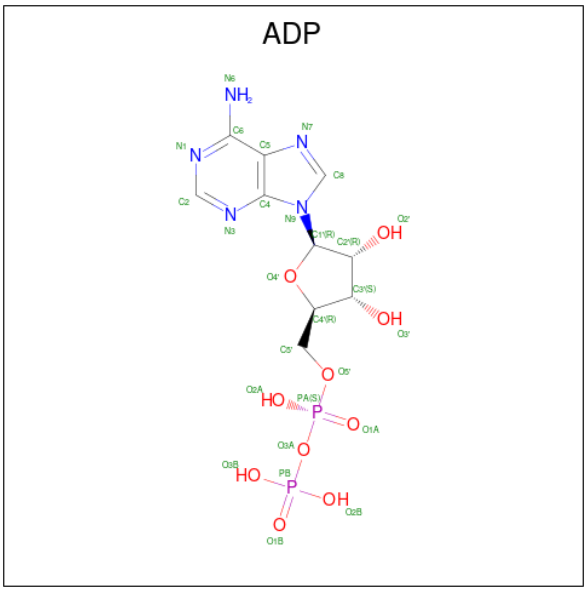
Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	208	Total	C	N	O	S	0	0
			1677	1042	285	337	13		

- 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	

- Molecule 15 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



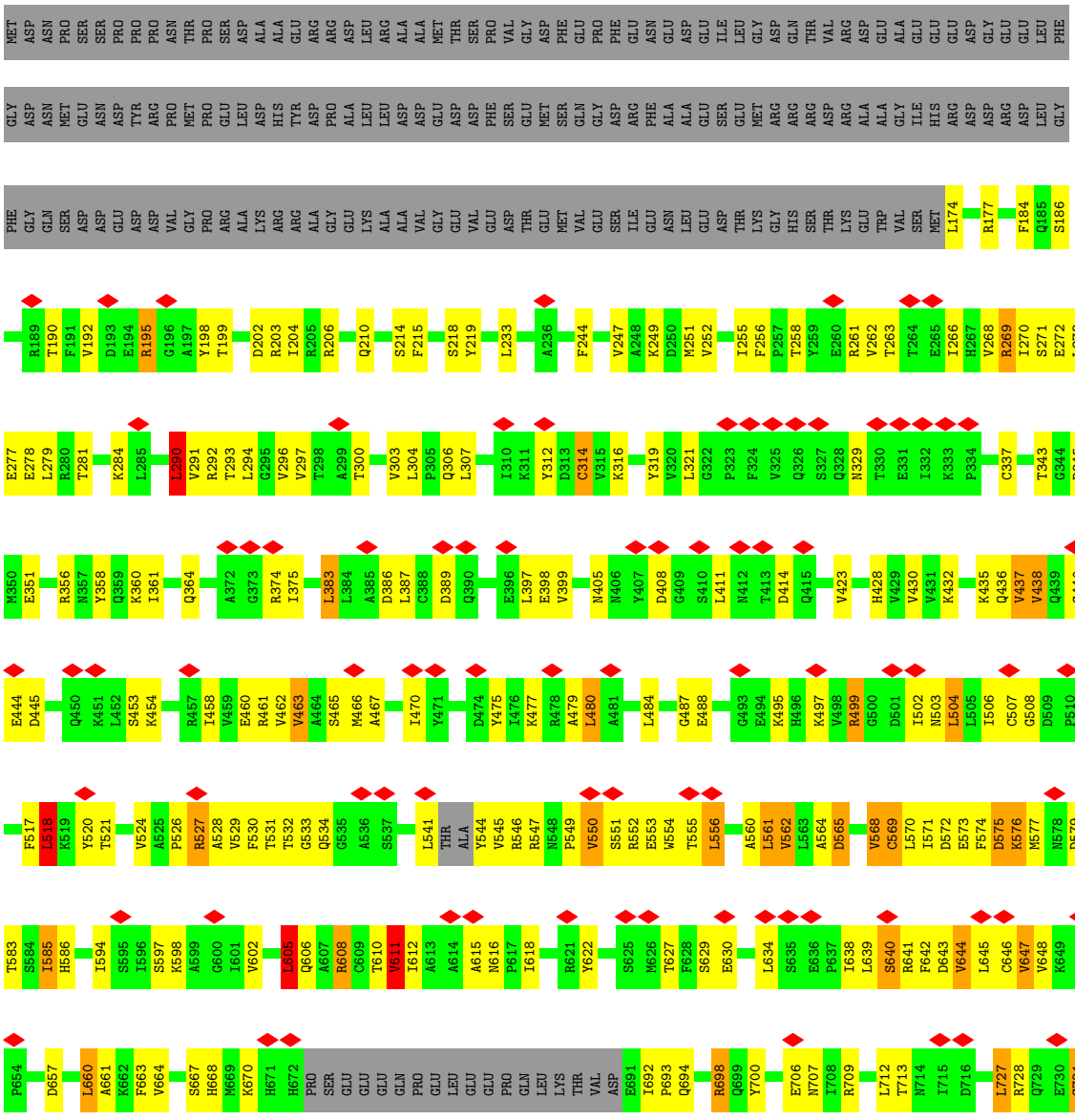
Mol	Chain	Residues	Atoms					AltConf
15	4	1	Total	C	N	O	P	0
			27	10	5	10	2	
15	6	1	Total	C	N	O	P	0
			27	10	5	10	2	
15	7	1	Total	C	N	O	P	0
			27	10	5	10	2	

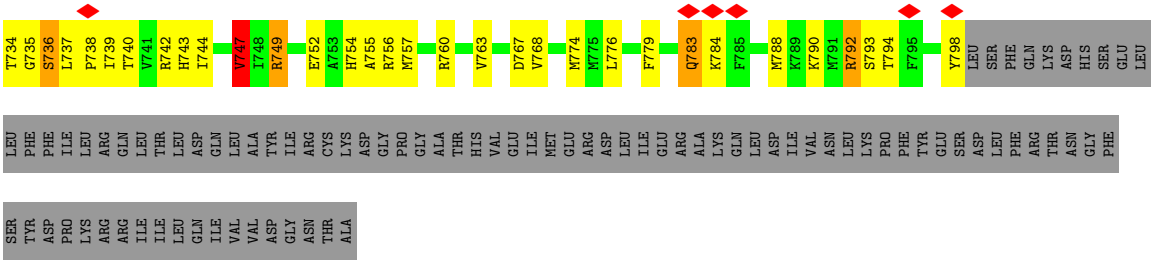
3 Residue-property plots (i)

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 licensing factor Mcm2

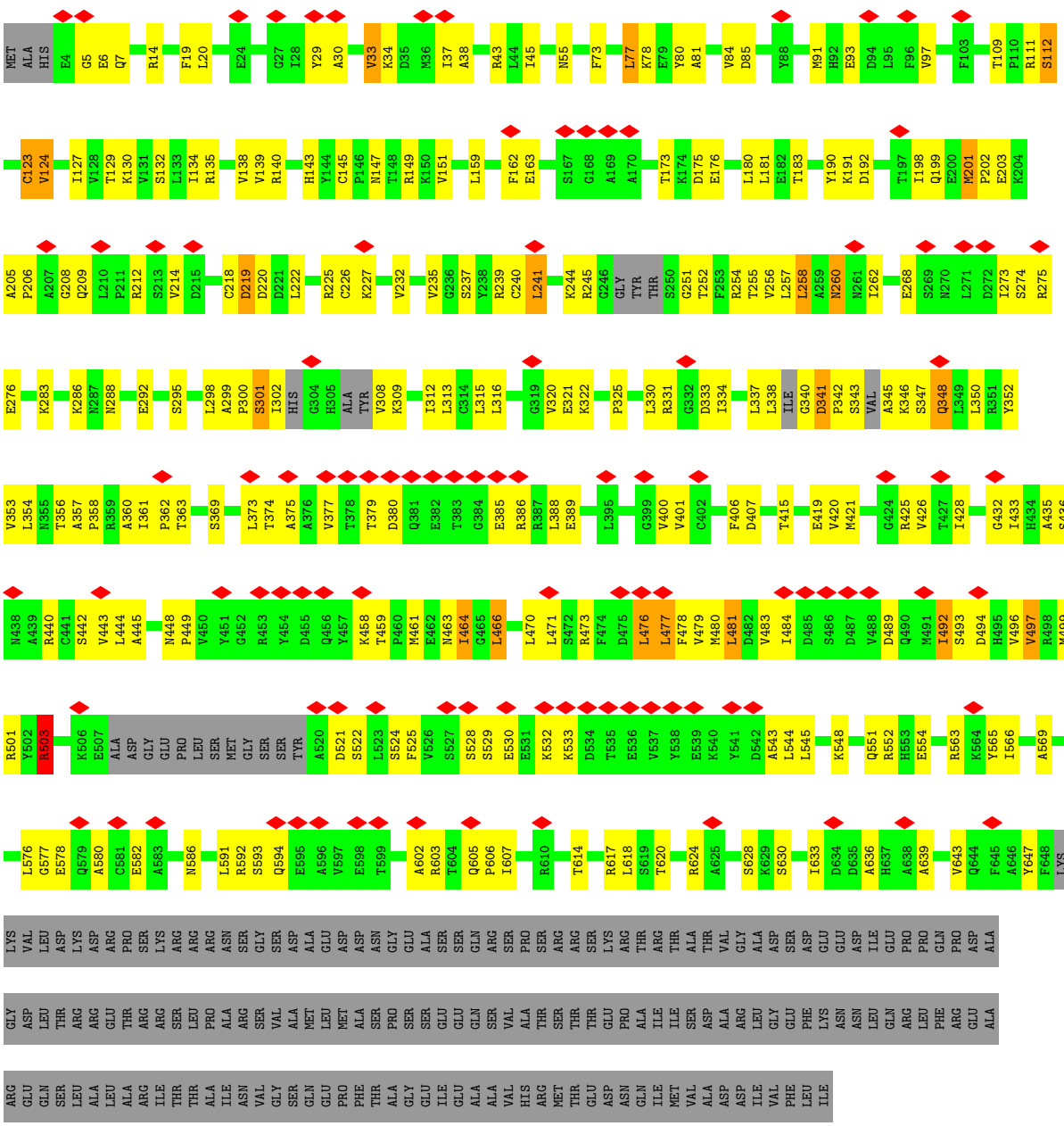
Chain 2:





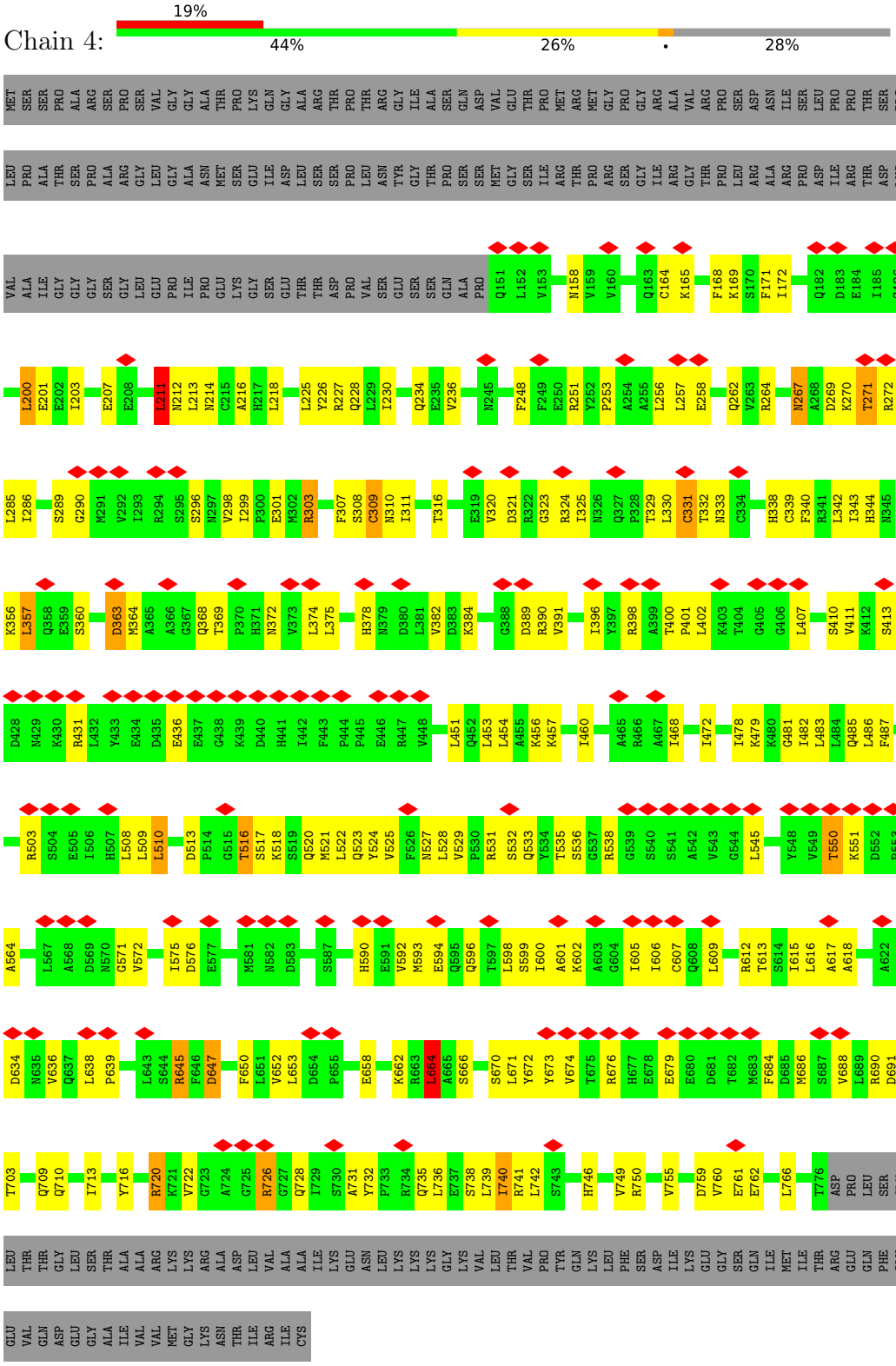
• Molecule 2: DNA replication licensing factor Mcm3

Chain 3:



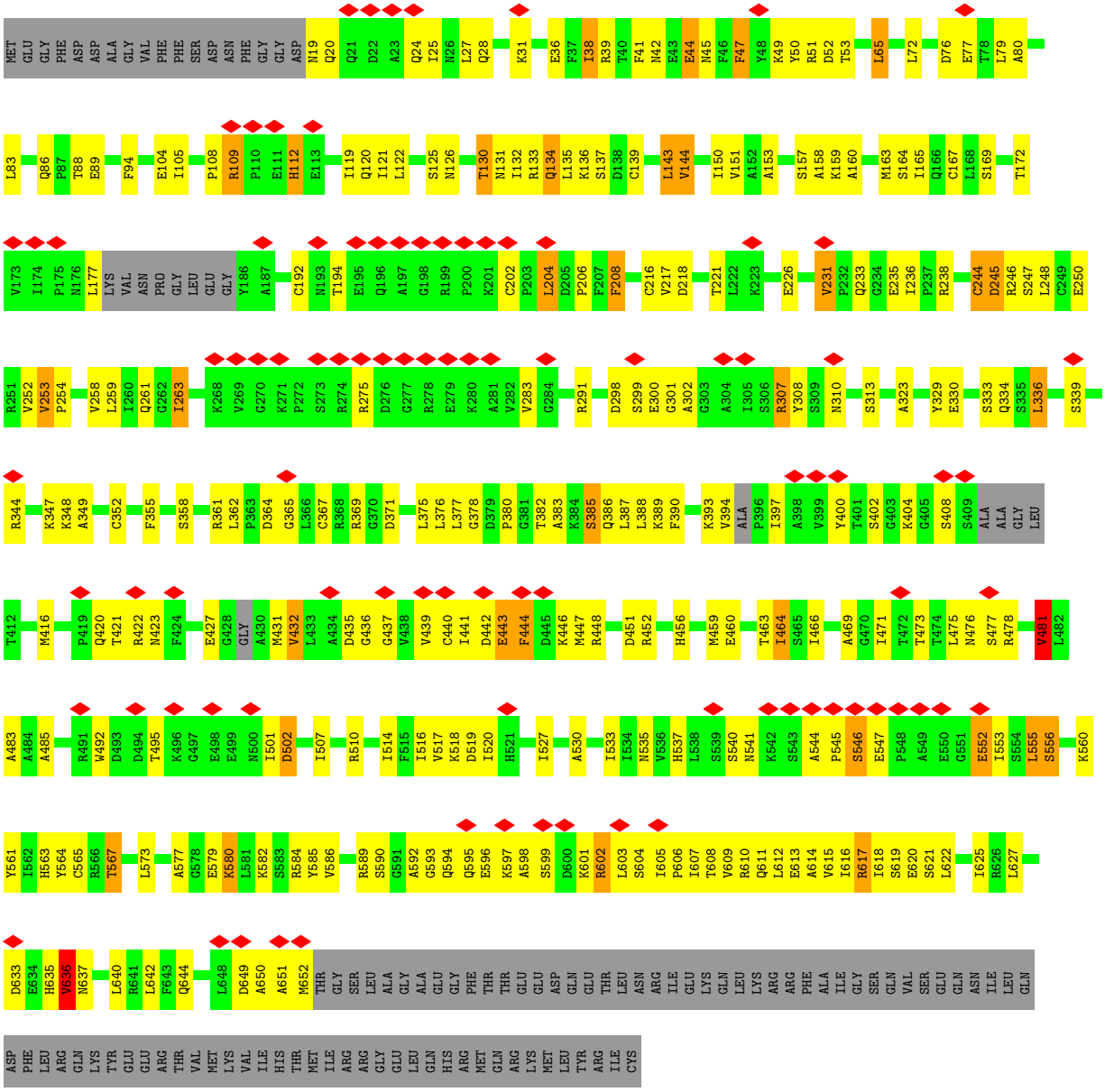
• Molecule 3: DNA replication licensing factor MCM4

Chain 4:



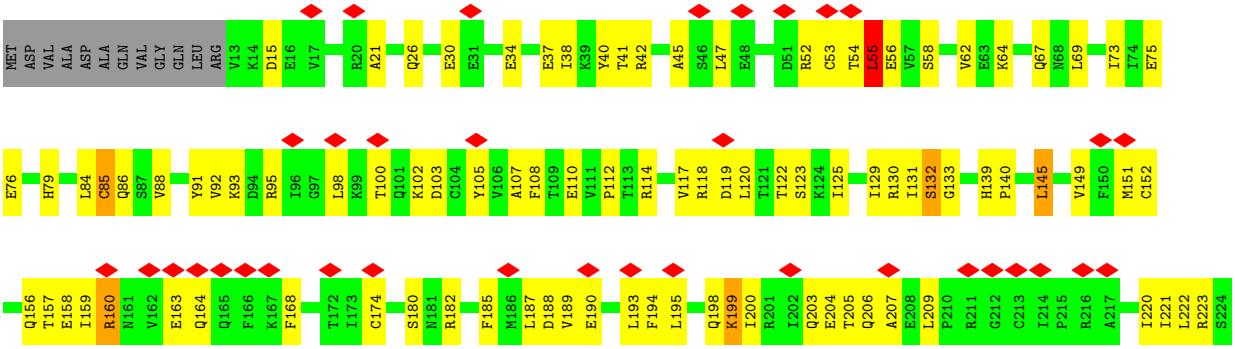
• Molecule 4: DNA replication licensing factor Mcm5

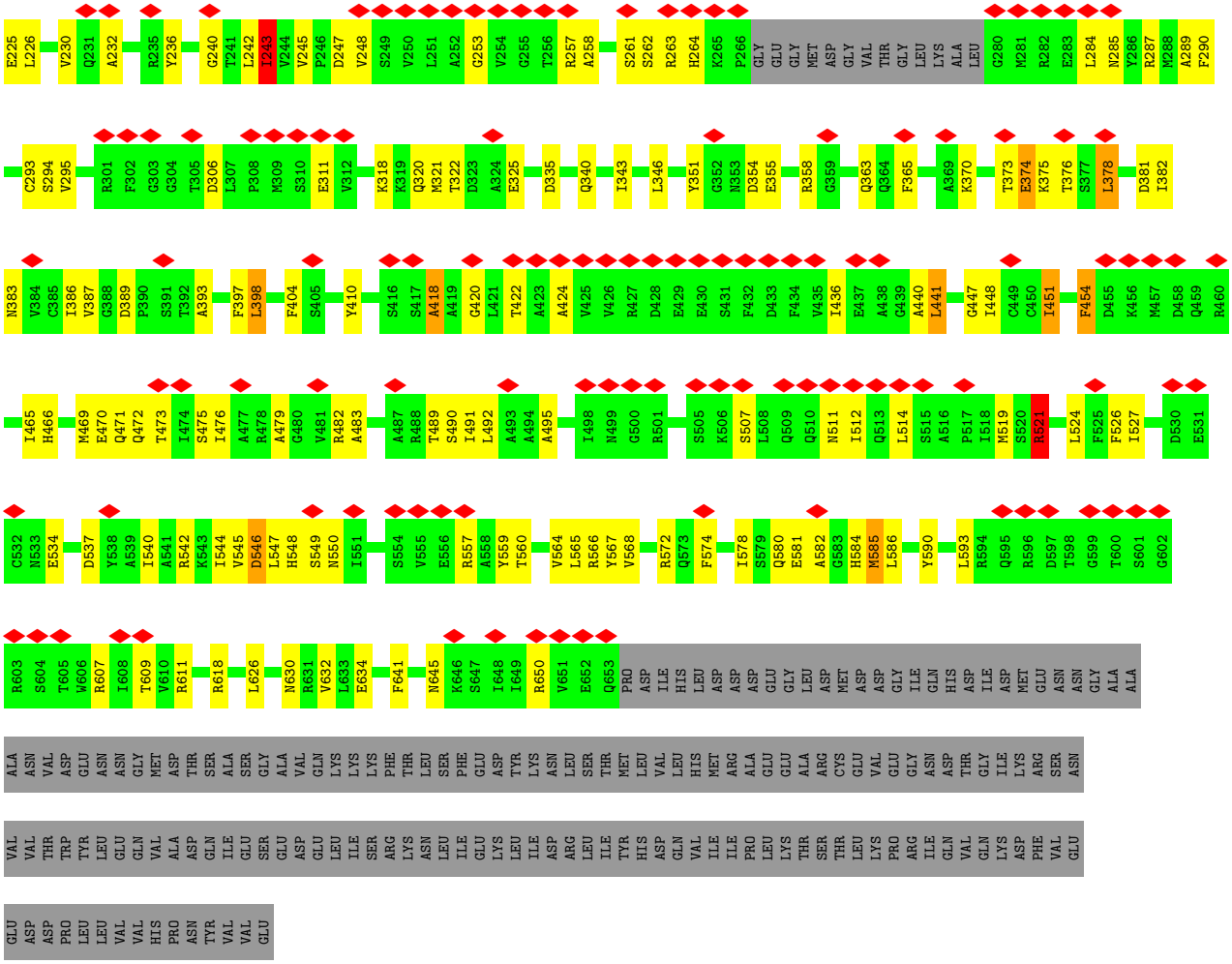
Chain 5:



• Molecule 5: DNA replication licensing factor Mcm6

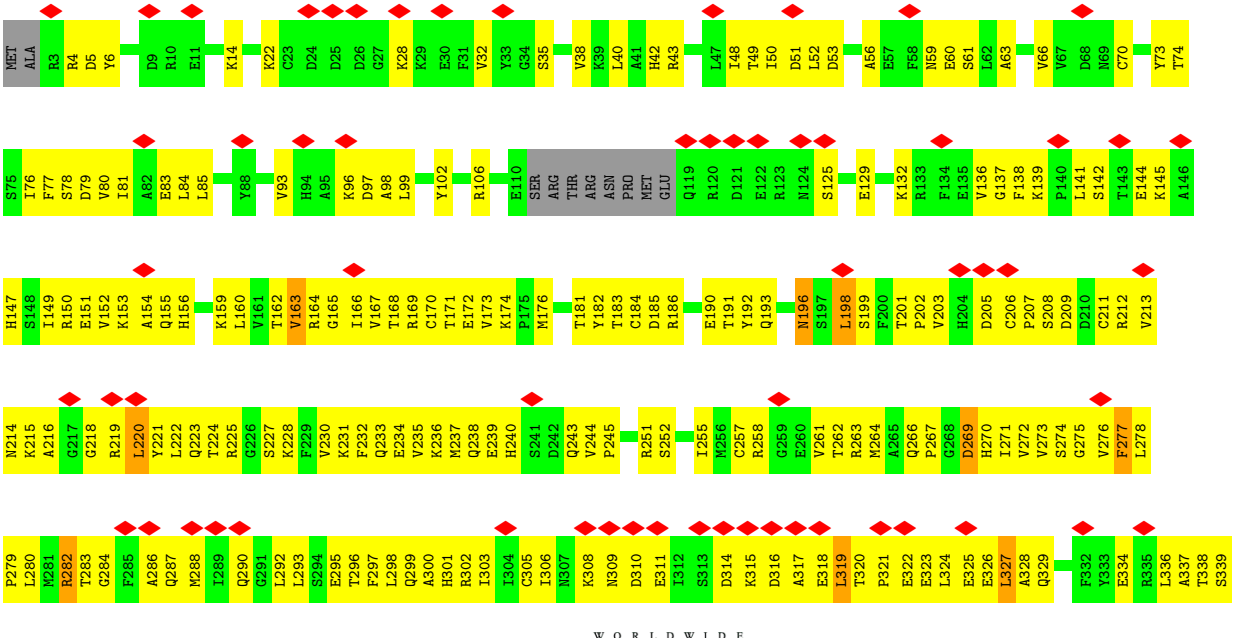
Chain 6:

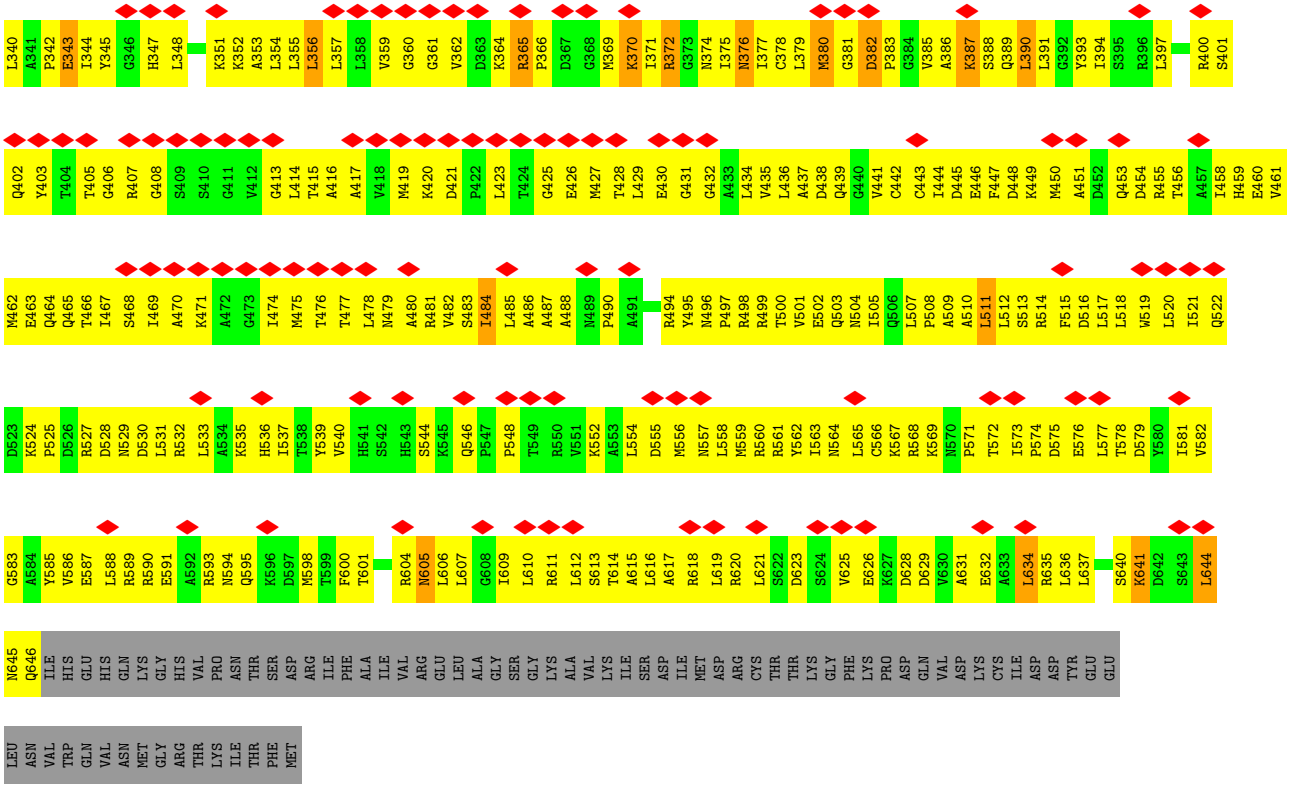




• Molecule 6: DNA replication licensing factor Mcm7

Chain 7:

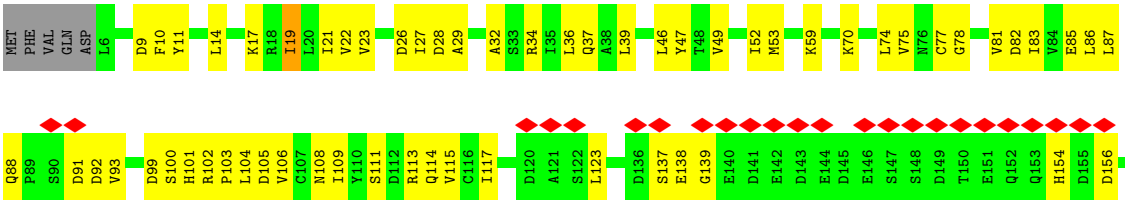


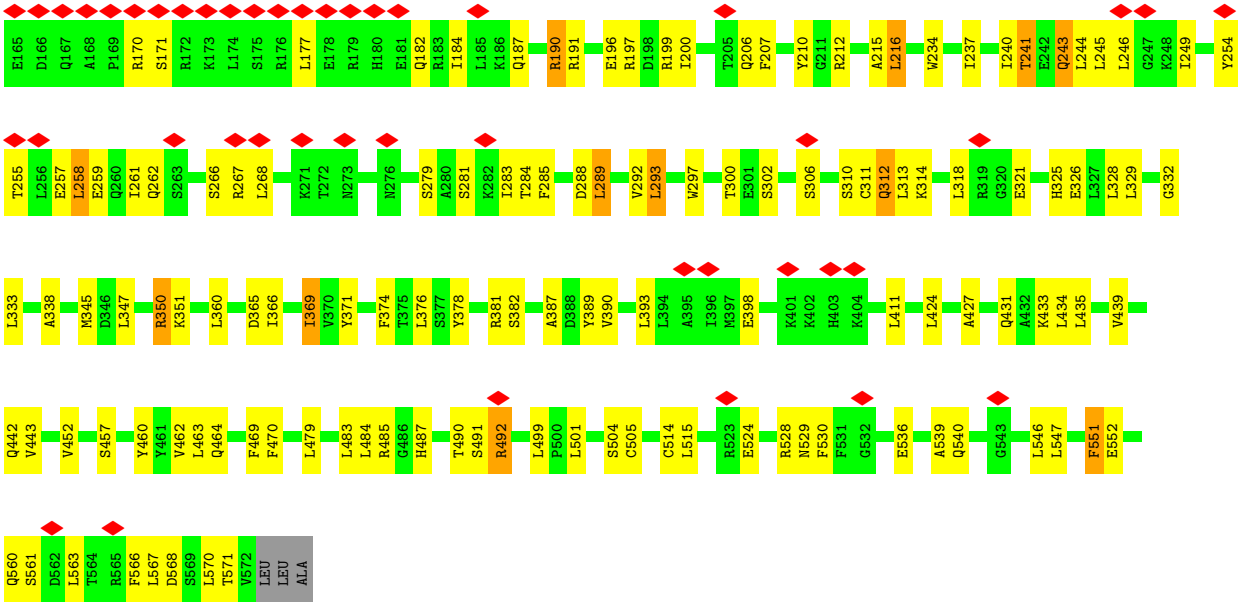


• Molecule 7: DNA

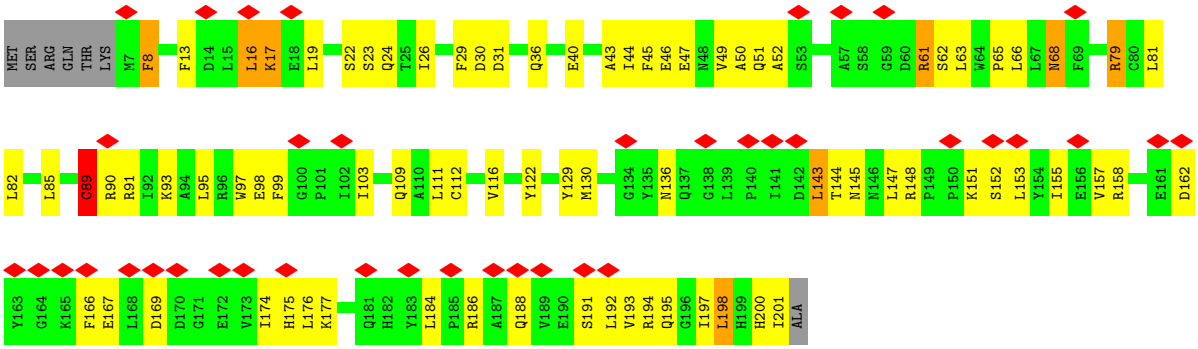
• Molecule 8: DNA

• Molecule 9: CDC45L

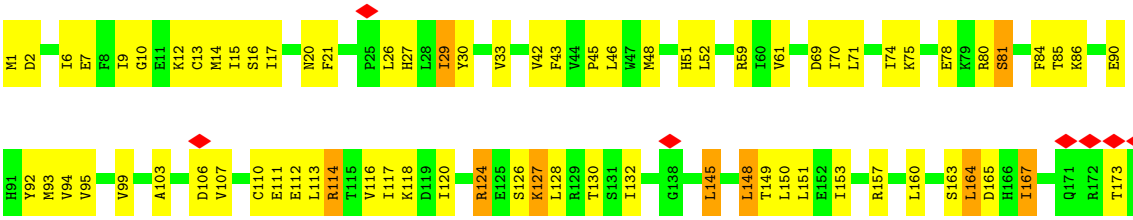




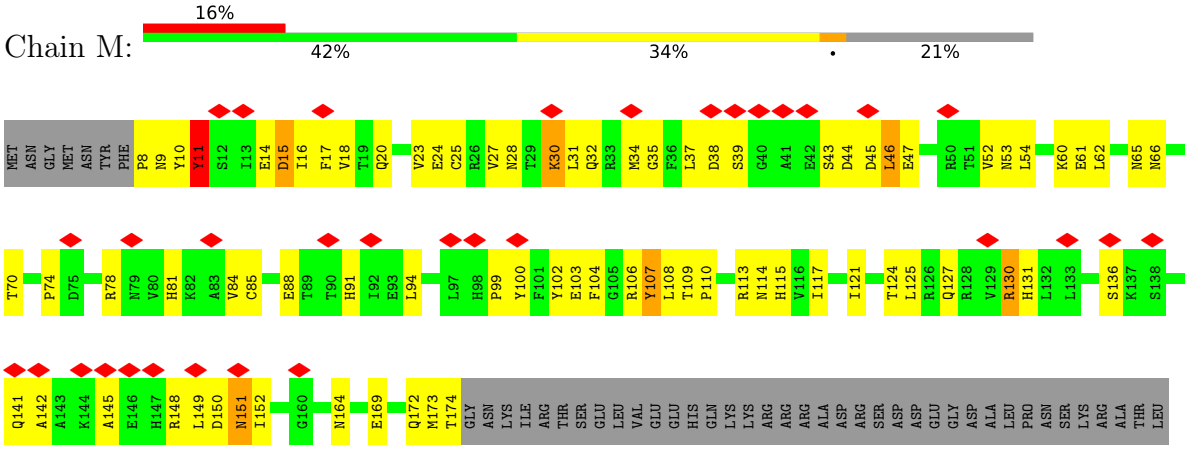
• Molecule 10: IP07275p



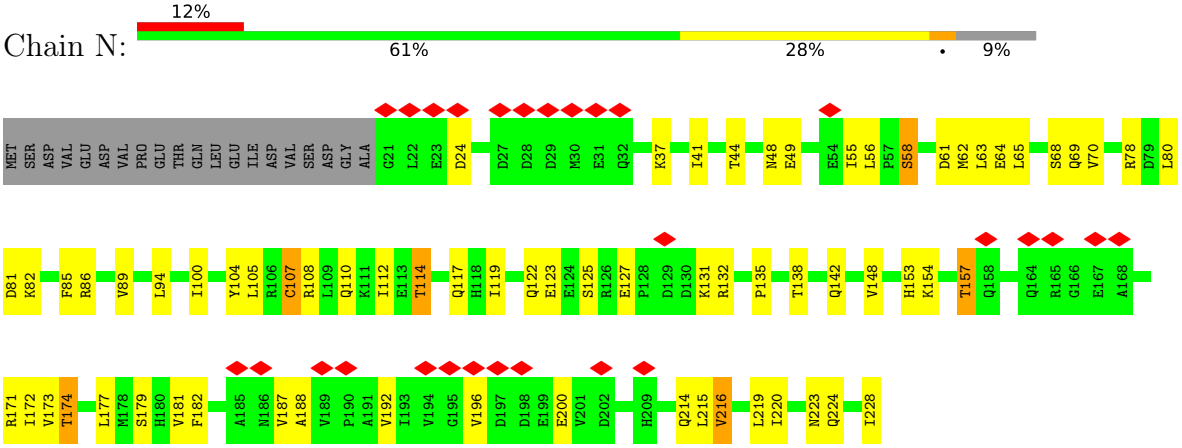
• Molecule 11: Probable DNA replication complex GINS protein PSF2



• Molecule 12: AT18545p



• Molecule 13: DNA replication complex GINS protein SLD5



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92754	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	0.066	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, 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	2	0.53	0/4874	1.00	32/6587 (0.5%)
2	3	0.51	1/4946 (0.0%)	0.85	13/6664 (0.2%)
3	4	0.44	0/5106	0.75	2/6912 (0.0%)
4	5	0.58	0/4939	0.85	11/6646 (0.2%)
5	6	0.49	1/5064 (0.0%)	0.82	9/6834 (0.1%)
6	7	0.36	0/5029	0.66	0/6775
7	X	0.81	0/469	1.47	5/722 (0.7%)
8	Y	0.60	0/183	1.04	0/280
9	A	0.58	1/4669 (0.0%)	0.82	5/6312 (0.1%)
10	H	0.61	1/1618 (0.1%)	0.85	2/2184 (0.1%)
11	L	0.65	0/1534	0.84	2/2076 (0.1%)
12	M	0.71	1/1413 (0.1%)	0.87	3/1914 (0.2%)
13	N	0.55	0/1703	0.78	0/2304
All	All	0.53	5/41547 (0.0%)	0.84	84/56210 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2	1	4
2	3	0	4
3	4	0	9
4	5	0	11
5	6	0	5
6	7	0	1
9	A	0	3
10	H	0	2
11	L	0	2
12	M	0	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	N	0	2
All	All	1	51

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	11	TYR	CD1-CE1	-7.23	1.28	1.39
10	H	89	CYS	CB-SG	-5.25	1.73	1.81
5	6	454	PHE	CD1-CE1	-5.11	1.29	1.39
9	A	297	TRP	CB-CG	-5.10	1.41	1.50
2	3	503	ARG	C-N	5.03	1.45	1.34

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	6	521	ARG	NE-CZ-NH2	-16.89	111.86	120.30
1	2	499	ARG	C-N-CA	11.83	147.14	122.30
1	2	466	MET	C-N-CA	11.03	149.28	121.70
1	2	518	LEU	CB-CG-CD1	10.78	129.33	111.00
7	X	0	DG	O4'-C1'-C2'	-10.69	97.35	105.90
9	A	551	PHE	CB-CG-CD1	-9.63	114.06	120.80
7	X	10	DT	O5'-P-OP1	-9.40	97.24	105.70
4	5	432	VAL	CG1-CB-CG2	9.38	125.92	110.90
9	A	551	PHE	CB-CG-CD2	9.28	127.29	120.80
1	2	749	ARG	NE-CZ-NH2	-9.08	115.76	120.30
4	5	636	VAL	CG1-CB-CG2	8.57	124.61	110.90
1	2	504	LEU	CB-CG-CD2	8.54	125.52	111.00
1	2	480	LEU	CB-CG-CD2	8.47	125.40	111.00
5	6	521	ARG	CD-NE-CZ	8.17	135.03	123.60
4	5	481	VAL	CG1-CB-CG2	8.09	123.85	110.90
1	2	639	LEU	CB-CG-CD2	8.06	124.70	111.00
1	2	783	GLN	C-N-CA	7.90	141.46	121.70
1	2	462	VAL	CG1-CB-CG2	7.78	123.35	110.90
9	A	289	LEU	CB-CG-CD2	-7.63	98.02	111.00
1	2	463	VAL	CG1-CB-CG2	7.53	122.94	110.90
1	2	530	PHE	C-N-CA	7.46	140.35	121.70
1	2	747	VAL	CG1-CB-CG2	7.38	122.70	110.90
2	3	481	LEU	CB-CG-CD2	7.38	123.54	111.00
2	3	483	VAL	CG1-CB-CG2	7.34	122.65	110.90
2	3	19	PHE	CB-CG-CD2	-7.28	115.70	120.80
5	6	365	PHE	CB-CG-CD2	-7.25	115.72	120.80
2	3	492	ILE	CG1-CB-CG2	7.20	127.23	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	611	VAL	CG1-CB-CG2	-7.11	99.53	110.90
2	3	19	PHE	CB-CG-CD1	6.93	125.65	120.80
1	2	585	ILE	CG1-CB-CG2	6.83	126.43	111.40
1	2	574	PHE	C-N-CA	6.82	138.76	121.70
5	6	287	ARG	NE-CZ-NH1	-6.70	116.95	120.30
2	3	497	VAL	CG1-CB-CG2	6.70	121.61	110.90
1	2	561	LEU	CB-CG-CD2	6.67	122.34	111.00
1	2	561	LEU	CA-CB-CG	6.66	130.61	115.30
12	M	130	ARG	NE-CZ-NH1	6.65	123.62	120.30
5	6	521	ARG	NH1-CZ-NH2	-6.56	112.18	119.40
1	2	562	VAL	CG1-CB-CG2	6.53	121.34	110.90
5	6	365	PHE	CB-CG-CD1	6.52	125.37	120.80
1	2	779	PHE	CB-CG-CD1	-6.51	116.24	120.80
12	M	46	LEU	CA-CB-CG	6.33	129.85	115.30
4	5	208	PHE	CB-CG-CD1	-6.31	116.39	120.80
4	5	275	ARG	NE-CZ-NH2	6.20	123.40	120.30
5	6	287	ARG	NE-CZ-NH2	6.15	123.37	120.30
1	2	556	LEU	CA-CB-CG	6.10	129.33	115.30
1	2	639	LEU	CA-CB-CG	6.06	129.24	115.30
1	2	576	LYS	C-N-CA	6.01	136.73	121.70
1	2	618	ILE	CG1-CB-CG2	5.99	124.58	111.40
11	L	124	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	2	647	VAL	CA-CB-CG2	5.94	119.81	110.90
5	6	145	LEU	CB-CG-CD1	5.93	121.08	111.00
1	2	605	LEU	CB-CG-CD1	5.92	121.07	111.00
3	4	664	LEU	CA-CB-CG	5.86	128.78	115.30
2	3	241	LEU	CB-CG-CD1	5.82	120.89	111.00
1	2	594	ILE	CG1-CB-CG2	5.78	124.11	111.40
1	2	499	ARG	NE-CZ-NH1	5.70	123.15	120.30
5	6	55	LEU	CB-CG-CD2	-5.66	101.37	111.00
4	5	109	ARG	N-CA-C	-5.66	95.72	111.00
4	5	192	CYS	CA-CB-SG	-5.66	103.81	114.00
2	3	477	LEU	CA-CB-CG	5.64	128.28	115.30
4	5	208	PHE	CB-CG-CD2	5.60	124.72	120.80
4	5	650	ALA	C-N-CA	5.59	135.66	121.70
9	A	34	ARG	NE-CZ-NH2	5.57	123.09	120.30
2	3	552	ARG	NE-CZ-NH1	5.53	123.06	120.30
3	4	211	LEU	CA-CB-CG	5.47	127.89	115.30
1	2	647	VAL	CG1-CB-CG2	5.45	119.61	110.90
2	3	239	ARG	NE-CZ-NH2	5.44	123.02	120.30
4	5	263	ILE	CG1-CB-CG2	-5.41	99.50	111.40
2	3	497	VAL	CA-CB-CG1	5.37	118.96	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	779	PHE	CB-CG-CD2	5.35	124.54	120.80
2	3	225	ARG	NE-CZ-NH1	-5.32	117.64	120.30
10	H	130	MET	CG-SD-CE	5.27	108.64	100.20
10	H	8	PHE	CB-CG-CD1	5.26	124.48	120.80
7	X	6	DT	O4'-C1'-N1	5.25	111.68	108.00
2	3	614	THR	OG1-CB-CG2	5.23	122.03	110.00
7	X	0	DG	C1'-O4'-C4'	-5.19	104.91	110.10
1	2	290	LEU	CA-CB-CG	5.19	127.24	115.30
1	2	562	VAL	CA-CB-CG1	5.16	118.64	110.90
12	M	11	TYR	CB-CG-CD1	-5.12	117.93	121.00
11	L	124	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	2	747	VAL	CA-CB-CG1	5.05	118.48	110.90
4	5	204	LEU	CB-CG-CD2	5.05	119.58	111.00
9	A	258	LEU	CA-CB-CG	5.04	126.89	115.30
7	X	0	DG	C4'-C3'-C2'	-5.03	98.58	103.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	2	585	ILE	CB

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	437	VAL	Peptide
1	2	497	LYS	Peptide
1	2	527	ARG	Peptide
1	2	569	CYS	Peptide
2	3	201	MET	Peptide
2	3	219	ASP	Peptide
2	3	251	GLY	Peptide
2	3	252	THR	Peptide
3	4	267	ASN	Peptide
3	4	271	THR	Peptide
3	4	321	ASP	Peptide
3	4	360	SER	Peptide
3	4	364	MET	Peptide
3	4	561	GLN	Peptide
3	4	615	ILE	Peptide
3	4	636	VAL	Peptide
3	4	720	ARG	Peptide
4	5	112	HIS	Peptide

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Mol	Chain	Res	Type	Group
4	5	143	LEU	Peptide
4	5	231	VAL	Peptide
4	5	248	LEU	Peptide
4	5	400	TYR	Peptide
4	5	42	ASN	Peptide
4	5	44	GLU	Peptide
4	5	47	PHE	Peptide
4	5	507	ILE	Peptide
4	5	540	SER	Peptide
4	5	552	GLU	Peptide
5	6	243	ILE	Peptide
5	6	418	ALA	Peptide
5	6	521	ARG	Sidechain
5	6	585	MET	Peptide
5	6	630	ASN	Peptide
6	7	382	ASP	Peptide
9	A	243	GLN	Peptide
9	A	360	LEU	Peptide
9	A	490	THR	Peptide
10	H	194	ARG	Peptide
10	H	198	LEU	Peptide
11	L	145	LEU	Peptide
11	L	21	PHE	Peptide
12	M	10	TYR	Peptide
12	M	106	ARG	Peptide
12	M	107	TYR	Peptide
12	M	114	ASN	Peptide
12	M	145	ALA	Peptide
12	M	149	LEU	Peptide
12	M	17	PHE	Peptide
12	M	62	LEU	Peptide
13	N	157	THR	Peptide
13	N	216	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	4788	0	4825	187	0
2	3	4879	0	4914	196	0
3	4	5013	0	4999	174	0
4	5	4864	0	4911	216	0
5	6	4986	0	4983	156	0
6	7	4964	0	4992	642	0
7	X	424	0	247	43	0
8	Y	164	0	91	6	0
9	A	4575	0	4493	136	0
10	H	1583	0	1567	61	0
11	L	1498	0	1519	61	0
12	M	1381	0	1352	55	0
13	N	1677	0	1623	58	0
14	2	31	0	12	2	0
14	3	31	0	11	10	0
14	5	31	0	12	5	0
15	4	27	0	12	2	0
15	6	27	0	12	3	0
15	7	27	0	12	8	0
All	All	40970	0	40587	1883	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 23.

All (1883) 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)
6:7:237:MET:HB2	6:7:255:ILE:HD11	1.27	1.10
6:7:441:VAL:HG22	6:7:483:SER:HB2	1.37	1.06
4:5:589:ARG:HB2	4:5:607:ILE:HG21	1.39	1.00
6:7:336:LEU:HD11	6:7:559:MET:HG2	1.42	1.00
6:7:206:CYS:HB2	6:7:211:CYS:HB3	1.40	0.99
4:5:584:ARG:HG2	4:5:640:LEU:HD11	1.43	0.97
6:7:508:PRO:HG2	6:7:511:LEU:HB2	1.44	0.96
4:5:596:GLU:HG2	4:5:602:ARG:HA	1.47	0.95
6:7:156:HIS:HA	6:7:159:LYS:HE2	1.47	0.94
6:7:571:PRO:HG3	6:7:617:ALA:HB3	1.49	0.94
6:7:445:ASP:HA	6:7:487:ALA:HB3	1.52	0.92
6:7:566:CYS:HB3	6:7:619:LEU:HA	1.49	0.91
6:7:587:GLU:HA	6:7:590:ARG:HG2	1.53	0.91
6:7:509:ALA:HA	6:7:512:LEU:HD13	1.51	0.91
6:7:448:ASP:HB3	6:7:507:LEU:HD11	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:331:ARG:O	2:3:617:ARG:NH2	2.06	0.89
6:7:262:THR:HG22	6:7:263:ARG:HG3	1.52	0.88
6:7:406:GLY:HA2	6:7:450:MET:HA	1.53	0.88
6:7:310:ASP:HA	6:7:316:ASP:HB2	1.55	0.87
5:6:512:ILE:HG22	5:6:514:LEU:HD13	1.57	0.87
6:7:439:GLN:HG2	6:7:481:ARG:HD2	1.57	0.86
3:4:407:LEU:HD21	7:X:3:DT:H5'	1.57	0.86
3:4:522:LEU:HD13	3:4:616:LEU:HD21	1.55	0.86
13:N:153:HIS:HA	13:N:157:THR:HG21	1.58	0.86
6:7:496:ASN:HB3	6:7:499:ARG:HB2	1.56	0.86
5:6:129:ILE:HG23	5:6:131:ILE:HD11	1.56	0.86
6:7:208:SER:HB3	6:7:211:CYS:HB2	1.55	0.86
6:7:462:MET:HB2	6:7:514:ARG:HH21	1.39	0.86
6:7:522:GLN:HB3	6:7:524:LYS:HE3	1.56	0.86
1:2:667:SER:O	1:2:670:LYS:NZ	2.10	0.85
6:7:558:LEU:HD13	6:7:561:ARG:HD2	1.59	0.85
6:7:458:ILE:HG23	6:7:511:LEU:HD21	1.56	0.84
6:7:431:GLY:HA3	6:7:435:VAL:HG11	1.59	0.84
1:2:571:ILE:HG22	1:2:612:ILE:HB	1.59	0.84
4:5:585:TYR:HB2	4:5:612:LEU:HD21	1.58	0.84
6:7:414:LEU:HD22	6:7:434:LEU:HD23	1.60	0.84
5:6:466:HIS:O	5:6:521:ARG:NH1	2.11	0.84
6:7:416:ALA:HA	6:7:431:GLY:HA2	1.60	0.83
6:7:374:ASN:HB3	6:7:483:SER:HA	1.60	0.83
10:H:23:SER:O	10:H:91:ARG:NH2	2.11	0.83
4:5:592:ALA:HB3	4:5:607:ILE:HD11	1.59	0.83
6:7:380:MET:HE2	6:7:520:LEU:HD13	1.62	0.82
4:5:589:ARG:HA	4:5:607:ILE:HG12	1.62	0.82
9:A:311:CYS:SG	9:A:312:GLN:NE2	2.53	0.82
2:3:377:VAL:HG22	7:X:8:DT:H4'	1.59	0.82
7:X:9:DT:H2"	7:X:10:DT:H71	1.62	0.81
6:7:438:ASP:HA	6:7:482:VAL:HB	1.60	0.81
6:7:441:VAL:HG11	6:7:485:LEU:HD23	1.61	0.81
7:X:0:DG:H1'	7:X:1:DT:H5'	1.62	0.81
5:6:243:ILE:HD12	5:6:245:VAL:HG22	1.62	0.80
9:A:237:ILE:O	9:A:241:THR:OG1	1.97	0.80
1:2:545:VAL:HG11	1:2:547:ARG:HH21	1.45	0.80
3:4:486:LEU:O	3:4:697:ARG:NH1	2.14	0.80
3:4:309:CYS:SG	3:4:310:ASN:N	2.55	0.80
6:7:386:ALA:HB1	6:7:389:GLN:HB2	1.62	0.80
7:X:8:DT:H2"	7:X:9:DT:H71	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:32:ALA:HB2	9:A:215:ALA:HB2	1.65	0.79
11:L:90:GLU:O	11:L:149:THR:OG1	2.00	0.79
1:2:349:ASN:ND2	1:2:351:GLU:O	2.16	0.79
3:4:203:ILE:O	3:4:207:GLU:N	2.15	0.79
5:6:355:GLU:OE1	5:6:650:ARG:NH2	2.15	0.79
1:2:278:GLU:O	1:2:281:THR:OG1	2.00	0.79
1:2:547:ARG:NH2	1:2:553:GLU:O	2.16	0.79
9:A:321:GLU:O	9:A:325:HIS:ND1	2.13	0.79
1:2:262:VAL:HG12	1:2:263:THR:HG23	1.63	0.78
5:6:420:GLY:O	5:6:440:ALA:N	2.16	0.78
6:7:464:GLN:HE21	6:7:481:ARG:HA	1.48	0.78
3:4:468:ILE:HD11	3:4:486:LEU:HD11	1.65	0.78
1:2:742:ARG:NH2	14:5:801:ATP:O3A	2.17	0.78
4:5:244:CYS:SG	4:5:245:ASP:N	2.58	0.77
6:7:626:GLU:HG2	6:7:629:ASP:H	1.48	0.77
3:4:296:SER:OG	3:4:353:GLN:NE2	2.18	0.77
5:6:469:MET:O	5:6:472:GLN:NE2	2.17	0.77
2:3:5:GLY:O	2:3:7:GLN:NE2	2.17	0.77
5:6:387:VAL:HB	5:6:527:ILE:HD12	1.65	0.77
5:6:418:ALA:O	5:6:422:THR:OG1	2.03	0.77
5:6:582:ALA:O	5:6:586:LEU:N	2.18	0.77
1:2:206:ARG:O	1:2:210:GLN:NE2	2.17	0.77
1:2:597:SER:OG	4:5:408:SER:O	2.02	0.77
4:5:594:GLN:O	4:5:598:ALA:N	2.16	0.76
5:6:351:TYR:O	15:6:901:ADP:N6	2.19	0.76
4:5:369:ARG:NH1	4:5:460:GLU:OE2	2.19	0.76
4:5:375:LEU:HD23	4:5:514:ILE:HG23	1.67	0.76
4:5:580:LYS:NZ	4:5:637:ASN:OD1	2.18	0.76
3:4:316:THR:CG2	3:4:331:CYS:HB2	2.16	0.76
6:7:129:GLU:O	6:7:228:LYS:NZ	2.17	0.76
6:7:421:ASP:HB2	6:7:425:GLY:H	1.48	0.76
6:7:459:HIS:O	6:7:514:ARG:NH2	2.18	0.76
9:A:85:GLU:O	9:A:88:GLN:NE2	2.19	0.76
5:6:567:TYR:OH	5:6:626:LEU:O	2.04	0.75
10:H:61:ARG:NH1	10:H:62:SER:OG	2.19	0.75
12:M:16:ILE:O	12:M:20:GLN:NE2	2.19	0.75
2:3:572:MET:O	2:3:624:ARG:NH2	2.19	0.75
11:L:78:GLU:OE1	11:L:81:SER:OG	2.03	0.75
1:2:467:ALA:O	1:2:477:LYS:NZ	2.19	0.75
6:7:320:THR:O	6:7:324:LEU:N	2.18	0.75
4:5:422:ARG:NH1	7:X:6:DT:O2	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:315:LYS:NZ	6:7:319:LEU:HG	2.01	0.75
6:7:372:ARG:NH2	6:7:374:ASN:O	2.20	0.75
1:2:565:ASP:OD2	1:2:608:ARG:NH1	2.19	0.75
2:3:203:GLU:OE2	4:5:476:ASN:ND2	2.19	0.75
3:4:353:GLN:NE2	3:4:354:LEU:O	2.20	0.74
5:6:581:GLU:O	5:6:585:MET:N	2.19	0.74
11:L:164:LEU:HD12	11:L:167:ILE:HD12	1.69	0.74
1:2:790:LYS:O	1:2:794:THR:OG1	2.02	0.74
5:6:151:MET:SD	5:6:152:CYS:N	2.61	0.74
6:7:170:CYS:HA	6:7:235:VAL:HG13	1.68	0.74
11:L:93:MET:HB2	11:L:151:LEU:HD22	1.69	0.74
2:3:499:MET:O	2:3:503:ARG:NE	2.21	0.74
9:A:22:VAL:HG12	9:A:29:ALA:HB1	1.70	0.74
9:A:210:TYR:OH	9:A:552:GLU:OE1	2.05	0.74
1:2:611:VAL:HG12	1:2:612:ILE:O	1.86	0.73
4:5:421:THR:OG1	4:5:423:ASN:ND2	2.20	0.73
6:7:447:PHE:N	6:7:487:ALA:O	2.20	0.73
5:6:158:GLU:OE2	5:6:160:ARG:NH2	2.21	0.73
6:7:357:LEU:HG	6:7:375:ILE:HG21	1.70	0.73
3:4:410:SER:OG	6:7:199:SER:OG	2.04	0.73
6:7:535:LYS:O	6:7:546:GLN:NE2	2.21	0.73
9:A:524:GLU:O	9:A:528:ARG:NH1	2.22	0.73
1:2:397:LEU:O	1:2:432:LYS:NZ	2.21	0.73
3:4:575:ILE:O	3:4:618:ALA:N	2.22	0.73
12:M:46:LEU:HD23	12:M:47:GLU:H	1.54	0.73
5:6:102:LYS:NZ	5:6:103:ASP:O	2.22	0.73
5:6:557:ARG:NH2	5:6:559:TYR:O	2.21	0.73
6:7:171:THR:HB	6:7:423:LEU:HD22	1.69	0.73
10:H:111:LEU:HD21	10:H:116:VAL:N	2.04	0.73
13:N:58:SER:N	13:N:131:LYS:O	2.21	0.72
2:3:532:LYS:NZ	12:M:20:GLN:O	2.22	0.72
4:5:77:GLU:OE1	9:A:351:LYS:NZ	2.21	0.72
6:7:372:ARG:O	6:7:611:ARG:NH2	2.22	0.72
6:7:317:ALA:HB3	6:7:564:ASN:HB2	1.70	0.72
12:M:121:ILE:O	12:M:124:THR:OG1	2.06	0.72
3:4:431:ARG:NH2	3:4:527:ASN:O	2.22	0.72
12:M:43:SER:OG	12:M:45:ASP:O	2.08	0.72
2:3:299:ALA:HB1	2:3:302:ILE:HD11	1.70	0.72
3:4:673:TYR:OH	6:7:573:ILE:O	2.07	0.72
1:2:528:ALA:HA	1:2:568:VAL:O	1.90	0.72
6:7:614:THR:OG1	6:7:618:ARG:NH2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:77:CYS:SG	9:A:78:GLY:N	2.63	0.72
4:5:404:LYS:NZ	4:5:446:LYS:O	2.18	0.71
6:7:407:ARG:NH2	6:7:449:LYS:O	2.23	0.71
13:N:81:ASP:OD1	13:N:82:LYS:NZ	2.17	0.71
3:4:726:ARG:O	3:4:728:GLN:NE2	2.23	0.71
10:H:145:ASN:ND2	10:H:191:SER:O	2.23	0.71
6:7:455:ARG:HG2	6:7:508:PRO:CD	2.20	0.71
3:4:529:VAL:O	3:4:532:SER:OG	2.07	0.71
4:5:120:GLN:NE2	4:5:247:SER:OG	2.22	0.71
12:M:61:GLU:OE1	12:M:61:GLU:N	2.23	0.71
12:M:32:GLN:NE2	12:M:44:ASP:O	2.24	0.71
12:M:104:PHE:CE2	12:M:108:LEU:HD13	2.26	0.71
1:2:504:LEU:HB2	1:2:644:VAL:HB	1.72	0.71
1:2:544:TYR:OH	4:5:404:LYS:O	2.07	0.71
2:3:522:SER:OG	10:H:36:GLN:NE2	2.23	0.71
6:7:631:ALA:HA	6:7:634:LEU:HD21	1.72	0.71
9:A:23:VAL:HG22	9:A:75:VAL:O	1.90	0.71
2:3:565:TYR:OH	2:3:624:ARG:O	2.07	0.71
4:5:593:GLY:O	4:5:597:LYS:HG2	1.91	0.71
5:6:151:MET:O	5:6:185:PHE:N	2.23	0.71
3:4:555:THR:O	3:4:557:GLN:NE2	2.24	0.71
4:5:72:LEU:HD13	4:5:79:LEU:HB2	1.73	0.71
6:7:628:ASP:HA	6:7:631:ALA:HB3	1.71	0.71
2:3:459:THR:O	2:3:463:ASN:ND2	2.24	0.71
3:4:735:GLN:O	3:4:738:SER:OG	2.08	0.71
6:7:479:ASN:HB2	6:7:481:ARG:HH21	1.56	0.70
9:A:328:LEU:O	9:A:332:GLY:N	2.23	0.70
13:N:220:ILE:O	13:N:223:ASN:ND2	2.24	0.70
6:7:438:ASP:HB2	6:7:481:ARG:H	1.54	0.70
6:7:382:ASP:O	6:7:385:VAL:HG13	1.91	0.70
3:4:531:ARG:O	3:4:533:GLN:NE2	2.24	0.70
7:X:11:DT:H2”	7:X:12:DT:H71	1.74	0.70
4:5:592:ALA:HB1	4:5:604:SER:HB3	1.72	0.70
9:A:398:GLU:OE1	9:A:431:GLN:NE2	2.23	0.70
4:5:133:ARG:NH2	4:5:231:VAL:O	2.24	0.70
5:6:546:ASP:OD1	5:6:546:ASP:N	2.21	0.70
6:7:587:GLU:HG3	6:7:590:ARG:HE	1.56	0.70
5:6:118:ARG:NH1	5:6:204:GLU:OE2	2.25	0.70
10:H:103:ILE:HG23	10:H:166:PHE:HB2	1.73	0.70
6:7:334:GLU:OE2	6:7:338:THR:OG1	2.10	0.70
10:H:169:ASP:O	10:H:188:GLN:NE2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:613:GLU:O	4:5:617:ARG:NE	2.25	0.70
4:5:564:TYR:O	4:5:567:THR:OG1	2.07	0.69
1:2:660:LEU:O	1:2:664:VAL:HG23	1.92	0.69
3:4:716:TYR:OH	3:4:720:ARG:NH1	2.26	0.69
6:7:585:TYR:CE1	6:7:605:ASN:HB2	2.27	0.69
1:2:306:GLN:OE1	1:2:356:ARG:NH2	2.24	0.69
6:7:266:GLN:HG3	6:7:269:ASP:OD1	1.93	0.69
6:7:589:ARG:NH2	6:7:601:THR:O	2.25	0.69
13:N:65:LEU:O	13:N:69:GLN:NE2	2.25	0.69
3:4:497:LEU:HD21	3:4:499:ARG:HE	1.56	0.69
6:7:209:ASP:HA	6:7:212:ARG:HB2	1.73	0.69
2:3:628:SER:OG	2:3:630:SER:OG	2.08	0.69
9:A:452:VAL:HG21	9:A:487:HIS:CD2	2.28	0.69
10:H:68:ASN:ND2	12:M:61:GLU:OE2	2.26	0.69
11:L:164:LEU:HA	11:L:167:ILE:HD12	1.74	0.69
1:2:233:LEU:HD12	1:2:290:LEU:HD21	1.74	0.69
5:6:152:CYS:SG	5:6:180:SER:OG	2.47	0.69
1:2:749:ARG:NH1	1:2:752:GLU:OE2	2.26	0.68
9:A:302:SER:OG	9:A:433:LYS:NZ	2.25	0.68
2:3:159:LEU:CD2	2:3:241:LEU:HD13	2.23	0.68
9:A:312:GLN:O	9:A:313:LEU:HD23	1.93	0.68
12:M:8:PRO:N	12:M:11:TYR:HH	1.90	0.68
2:3:448:ASN:ND2	2:3:449:PRO:O	2.26	0.68
2:3:524:SER:OG	2:3:525:PHE:N	2.25	0.68
1:2:258:THR:O	1:2:261:ARG:NH1	2.26	0.68
4:5:618:ILE:O	4:5:622:LEU:HG	1.94	0.68
6:7:463:GLU:OE1	6:7:466:THR:OG1	2.06	0.68
1:2:533:GLY:N	1:2:572:ASP:O	2.27	0.68
3:4:316:THR:HG21	3:4:332:THR:HG23	1.74	0.68
4:5:144:VAL:O	4:5:261:GLN:NE2	2.26	0.68
6:7:421:ASP:OD2	6:7:427:MET:N	2.25	0.68
6:7:319:LEU:HB2	6:7:322:GLU:HB3	1.75	0.68
6:7:372:ARG:HH11	6:7:464:GLN:HG3	1.58	0.68
4:5:385:SER:O	4:5:389:LYS:HG2	1.94	0.68
6:7:171:THR:CB	6:7:423:LEU:HD22	2.24	0.68
6:7:270:HIS:O	6:7:306:ILE:HG22	1.93	0.68
13:N:123:GLU:O	13:N:127:GLU:N	2.27	0.68
3:4:626:TRP:NE1	3:4:630:LYS:O	2.28	0.67
9:A:300:THR:OG1	9:A:338:ALA:O	2.05	0.67
11:L:7:GLU:N	11:L:7:GLU:OE2	2.27	0.67
1:2:270:ILE:O	1:2:428:HIS:ND1	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:480:MET:O	2:3:481:LEU:HD23	1.93	0.67
2:3:202:PRO:O	2:3:205:ALA:N	2.27	0.67
2:3:548:LYS:O	2:3:551:GLN:NE2	2.27	0.67
3:4:686:MET:O	3:4:690:ARG:NH2	2.27	0.67
5:6:383:ASN:ND2	5:6:521:ARG:O	2.27	0.67
5:6:641:PHE:O	5:6:645:ASN:ND2	2.28	0.67
6:7:325:GLU:O	6:7:329:GLN:HB2	1.94	0.67
5:6:108:PHE:O	5:6:294:SER:OG	2.03	0.67
3:4:158:ASN:O	3:4:228:GLN:NE2	2.28	0.67
6:7:585:TYR:HE1	6:7:605:ASN:HB2	1.59	0.67
7:X:-2:DT:H2'	7:X:-1:DC:H6	1.60	0.67
12:M:35:GLY:N	12:M:39:SER:OG	2.27	0.67
13:N:219:LEU:O	13:N:223:ASN:N	2.27	0.67
1:2:788:MET:O	1:2:792:ARG:NE	2.26	0.67
2:3:321:GLU:OE1	2:3:440:ARG:NH1	2.28	0.67
6:7:366:PRO:HG3	6:7:371:ILE:HG23	1.76	0.67
1:2:545:VAL:HG13	1:2:554:TRP:HD1	1.58	0.67
2:3:426:VAL:O	2:3:436:SER:OG	2.07	0.67
4:5:535:ASN:O	4:5:541:ASN:ND2	2.28	0.67
5:6:537:ASP:HA	5:6:540:ILE:HD12	1.76	0.67
6:7:168:THR:OG1	6:7:169:ARG:NH1	2.28	0.67
6:7:385:VAL:HG11	6:7:521:ILE:CG2	2.25	0.67
2:3:43:ARG:NH2	2:3:260:ASN:O	2.28	0.67
6:7:317:ALA:CB	6:7:561:ARG:HA	2.24	0.67
6:7:359:VAL:HG23	6:7:567:LYS:HB2	1.75	0.67
6:7:464:GLN:NE2	6:7:481:ARG:HA	2.09	0.67
2:3:190:TYR:OH	6:7:153:LYS:O	2.09	0.67
2:3:286:LYS:O	2:3:288:ASN:ND2	2.28	0.67
3:4:308:SER:OG	3:4:309:CYS:N	2.28	0.67
4:5:79:LEU:O	4:5:83:LEU:N	2.27	0.67
11:L:160:LEU:O	11:L:163:SER:OG	2.08	0.67
6:7:374:ASN:HB3	6:7:483:SER:CA	2.24	0.66
5:6:15:ASP:OD2	5:6:79:HIS:NE2	2.27	0.66
6:7:344:ILE:HD13	15:7:801:ADP:C2	2.29	0.66
13:N:37:LYS:O	13:N:41:ILE:HG23	1.95	0.66
1:2:503:ASN:O	1:2:643:ASP:HB2	1.95	0.66
2:3:190:TYR:CE2	6:7:154:ALA:HA	2.30	0.66
3:4:693:ILE:O	3:4:697:ARG:NH2	2.28	0.66
1:2:316:LYS:CG	1:2:343:THR:HG23	2.26	0.66
2:3:341:ASP:N	2:3:341:ASP:OD1	2.27	0.66
3:4:307:PHE:HD2	3:4:316:THR:HG23	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:439:GLN:HG2	6:7:481:ARG:CD	2.25	0.66
6:7:339:SER:HA	6:7:342:PRO:HG3	1.76	0.66
1:2:586:HIS:NE2	1:2:638:ILE:HA	2.11	0.66
6:7:184:CYS:SG	6:7:220:LEU:HD23	2.36	0.66
6:7:372:ARG:HE	6:7:464:GLN:HB2	1.61	0.66
2:3:127:ILE:HD11	2:3:201:MET:SD	2.35	0.66
6:7:176:MET:HB2	6:7:232:PHE:HB2	1.76	0.66
6:7:302:ARG:NH1	6:7:303:ILE:O	2.24	0.66
11:L:29:ILE:HG23	11:L:33:VAL:HG11	1.77	0.66
4:5:431:MET:CE	4:5:439:VAL:HG21	2.25	0.66
2:3:260:ASN:OD1	2:3:260:ASN:N	2.28	0.65
2:3:240:CYS:SG	2:3:255:THR:HG22	2.35	0.65
4:5:72:LEU:HD12	4:5:80:ALA:HB2	1.77	0.65
6:7:176:MET:N	6:7:230:VAL:O	2.25	0.65
6:7:275:GLY:HA3	6:7:300:ALA:HA	1.77	0.65
6:7:379:LEU:HB2	6:7:487:ALA:CB	2.26	0.65
4:5:612:LEU:HA	4:5:615:VAL:HG12	1.78	0.65
6:7:193:GLN:HE22	6:7:202:PRO:HA	1.62	0.65
6:7:207:PRO:HD2	6:7:220:LEU:HD21	1.78	0.65
10:H:97:TRP:O	10:H:144:THR:OG1	2.10	0.65
11:L:124:ARG:HH21	11:L:149:THR:HG22	1.60	0.65
11:L:145:LEU:HD12	11:L:148:LEU:HB3	1.76	0.65
1:2:475:TYR:OH	1:2:774:MET:O	2.13	0.65
2:3:299:ALA:HA	2:3:352:TYR:CE2	2.30	0.65
5:6:139:HIS:HB2	5:6:199:LYS:O	1.96	0.65
6:7:536:HIS:O	6:7:540:VAL:HG13	1.97	0.65
6:7:617:ALA:HB2	6:7:625:VAL:HG22	1.78	0.65
2:3:147:ASN:N	2:3:180:LEU:HD12	2.12	0.65
3:4:516:THR:HG21	3:4:652:VAL:HG11	1.78	0.65
2:3:199:GLN:NE2	2:3:212:ARG:O	2.30	0.65
3:4:673:TYR:HE1	6:7:573:ILE:HB	1.60	0.65
5:6:475:SER:OG	5:6:483:ALA:O	2.05	0.65
6:7:415:THR:HG22	6:7:416:ALA:H	1.60	0.65
6:7:527:ARG:HH12	6:7:528:ASP:HB2	1.61	0.65
1:2:694:GLN:O	1:2:698:ARG:NE	2.29	0.65
4:5:157:SER:OG	4:5:158:ALA:N	2.30	0.65
5:6:534:GLU:OE1	5:6:534:GLU:N	2.30	0.65
3:4:594:GLU:OE1	3:4:645:ARG:NE	2.30	0.65
6:7:527:ARG:NH1	6:7:528:ASP:HB2	2.12	0.65
6:7:528:ASP:O	6:7:532:ARG:HG3	1.96	0.65
7:X:4:DT:H2”	7:X:5:DT:H5”	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:169:GLU:OE1	12:M:169:GLU:N	2.29	0.65
4:5:233:GLN:N	4:5:235:GLU:OE2	2.29	0.64
4:5:614:ALA:HA	4:5:617:ARG:HE	1.62	0.64
3:4:510:LEU:HD11	3:4:522:LEU:HD11	1.79	0.64
6:7:344:ILE:HA	6:7:536:HIS:HB3	1.80	0.64
6:7:370:LYS:NZ	6:7:464:GLN:OE1	2.31	0.64
6:7:385:VAL:HG11	6:7:521:ILE:HG21	1.79	0.64
6:7:511:LEU:HD22	6:7:515:PHE:CE2	2.32	0.64
13:N:78:ARG:NH2	13:N:81:ASP:OD2	2.29	0.64
1:2:244:PHE:CD2	1:2:268:VAL:HG21	2.32	0.64
2:3:379:THR:HG23	7:X:5:DT:O2	1.97	0.64
5:6:544:ILE:HG13	5:6:547:LEU:HD12	1.79	0.64
10:H:36:GLN:NE2	10:H:36:GLN:O	2.28	0.64
3:4:454:LEU:HD11	3:4:688:VAL:HG12	1.77	0.64
3:4:533:GLN:NE2	3:4:572:VAL:O	2.30	0.64
6:7:59:ASN:ND2	6:7:61:SER:O	2.30	0.64
6:7:415:THR:HG21	6:7:469:ILE:HG13	1.79	0.64
9:A:283:ILE:HA	9:A:376:LEU:HD13	1.78	0.64
12:M:15:ASP:O	12:M:16:ILE:HD13	1.97	0.64
12:M:102:TYR:CD1	12:M:125:LEU:HD11	2.33	0.64
1:2:744:ILE:O	1:2:747:VAL:HB	1.98	0.64
6:7:499:ARG:HB3	6:7:504:ASN:HD22	1.62	0.64
6:7:626:GLU:HG2	6:7:629:ASP:N	2.12	0.64
1:2:495:LYS:NZ	4:5:339:SER:OG	2.30	0.64
3:4:517:SER:HA	15:4:901:ADP:H5'1	1.79	0.64
12:M:84:VAL:O	12:M:88:GLU:N	2.28	0.64
5:6:52:ARG:NH1	5:6:225:GLU:OE1	2.31	0.64
6:7:571:PRO:CB	6:7:623:ASP:HA	2.28	0.64
12:M:109:THR:HG23	12:M:117:ILE:HB	1.80	0.64
6:7:156:HIS:HA	6:7:159:LYS:CE	2.25	0.64
6:7:264:MET:HB3	6:7:303:ILE:HD12	1.80	0.64
6:7:380:MET:CE	6:7:520:LEU:HD13	2.28	0.64
10:H:89:CYS:SG	10:H:90:ARG:NH1	2.71	0.64
13:N:110:GLN:O	13:N:114:THR:OG1	2.15	0.64
1:2:546:ARG:NH2	7:X:11:DT:O4'	2.31	0.63
3:4:521:MET:O	3:4:525:VAL:HG23	1.98	0.63
6:7:287:GLN:HG2	6:7:288:MET:H	1.63	0.63
13:N:200:GLU:N	13:N:200:GLU:OE1	2.32	0.63
2:3:377:VAL:HG21	7:X:9:DT:H5'	1.80	0.63
4:5:36:GLU:OE2	4:5:39:ARG:NH2	2.30	0.63
4:5:165:ILE:HG22	4:5:167:CYS:H	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:537:ILE:O	6:7:540:VAL:HG22	1.98	0.63
10:H:152:SER:O	10:H:186:ARG:NH2	2.31	0.63
2:3:292:GLU:O	2:3:295:SER:OG	2.09	0.63
4:5:595:GLN:CD	4:5:603:LEU:HB3	2.18	0.63
6:7:102:TYR:OH	6:7:225:ARG:NH2	2.31	0.63
6:7:575:ASP:HA	6:7:578:THR:HG23	1.81	0.63
11:L:111:GLU:OE1	11:L:111:GLU:N	2.32	0.63
6:7:164:ARG:HG2	6:7:271:ILE:O	1.99	0.63
6:7:540:VAL:HG12	6:7:546:GLN:HB2	1.80	0.63
6:7:565:LEU:HG	6:7:621:LEU:HD21	1.80	0.63
2:3:602:ALA:O	2:3:605:GLN:NE2	2.31	0.63
6:7:326:GLU:HA	6:7:329:GLN:HB3	1.81	0.63
1:2:174:LEU:HD22	1:2:177:ARG:HG3	1.81	0.63
2:3:315:LEU:HD22	2:3:444:LEU:HD21	1.80	0.63
3:4:351:ASP:OD2	5:6:122:THR:HG23	1.99	0.63
3:4:375:LEU:HD11	3:4:419:VAL:HB	1.81	0.63
6:7:174:LYS:HD3	6:7:423:LEU:HD21	1.81	0.63
13:N:138:THR:O	13:N:142:GLN:NE2	2.32	0.63
2:3:159:LEU:HD23	2:3:241:LEU:HD13	1.80	0.63
3:4:605:ILE:HG13	5:6:232:ALA:HB1	1.80	0.63
4:5:250:GLU:O	4:5:308:TYR:OH	2.16	0.63
8:Y:8:DG:H2'	8:Y:9:DA:C8	2.34	0.63
1:2:706:GLU:O	1:2:709:ARG:NH2	2.31	0.63
6:7:458:ILE:HG21	6:7:511:LEU:HD11	1.81	0.63
6:7:379:LEU:HD13	6:7:387:LYS:HB2	1.80	0.63
7:X:10:DT:H2"	7:X:11:DT:C5	2.34	0.63
9:A:491:SER:O	9:A:492:ARG:NE	2.28	0.63
4:5:375:LEU:HD23	4:5:514:ILE:CG2	2.29	0.62
6:7:261:VAL:HA	6:7:264:MET:CE	2.29	0.62
2:3:237:SER:O	2:3:257:LEU:HD12	1.99	0.62
4:5:444:PHE:O	4:5:452:ARG:NH2	2.32	0.62
6:7:233:GLN:OE1	6:7:234:GLU:N	2.32	0.62
1:2:528:ALA:O	5:6:482:ARG:NH1	2.31	0.62
3:4:303:ARG:O	3:4:320:VAL:N	2.32	0.62
5:6:85:CYS:SG	5:6:86:GLN:N	2.72	0.62
6:7:376:ASN:HA	6:7:484:ILE:O	1.99	0.62
5:6:507:SER:O	5:6:511:ASN:N	2.32	0.62
2:3:494:ASP:HA	2:3:497:VAL:HG12	1.81	0.62
4:5:404:LYS:N	4:5:447:MET:SD	2.72	0.62
6:7:50:ILE:O	6:7:139:LYS:N	2.32	0.62
6:7:326:GLU:HB3	6:7:562:TYR:OH	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:336:LEU:CD1	6:7:559:MET:HG2	2.26	0.62
9:A:281:SER:O	9:A:376:LEU:HD21	1.99	0.62
9:A:435:LEU:HD12	9:A:469:PHE:CD1	2.34	0.62
1:2:279:LEU:O	1:2:281:THR:HG23	1.99	0.62
1:2:660:LEU:HD23	1:2:661:ALA:N	2.15	0.62
3:4:201:GLU:HA	3:4:251:ARG:HE	1.63	0.62
4:5:589:ARG:NH1	4:5:590:SER:HA	2.13	0.62
6:7:152:VAL:HA	6:7:156:HIS:CE1	2.34	0.62
6:7:169:ARG:HD3	6:7:419:MET:HE1	1.82	0.62
2:3:208:GLY:N	4:5:435:ASP:OD2	2.33	0.62
3:4:503:ARG:O	3:4:741:ARG:NH2	2.33	0.62
6:7:391:LEU:HD21	6:7:443:CYS:HB3	1.81	0.62
2:3:347:SER:N	14:3:901:ATP:O2B	2.28	0.62
5:6:257:ARG:NH1	5:6:285:ASN:OD1	2.33	0.62
5:6:311:GLU:O	5:6:566:ARG:NH2	2.32	0.62
2:3:123:CYS:SG	2:3:124:VAL:N	2.73	0.62
2:3:489:ASP:OD1	4:5:586:VAL:HG13	1.98	0.62
4:5:330:GLU:O	4:5:333:SER:OG	2.17	0.62
6:7:344:ILE:HG21	15:7:801:ADP:C2	2.34	0.62
6:7:379:LEU:H	6:7:487:ALA:HA	1.63	0.62
6:7:574:PRO:HG3	6:7:625:VAL:O	1.99	0.62
3:4:672:TYR:CD1	6:7:366:PRO:HB3	2.34	0.62
9:A:283:ILE:HG13	9:A:376:LEU:HD22	1.81	0.62
3:4:269:ASP:OD1	3:4:270:LYS:N	2.33	0.61
6:7:277:PHE:O	6:7:278:LEU:HD12	2.00	0.61
6:7:437:ALA:HB3	6:7:442:CYS:HB2	1.80	0.61
6:7:517:LEU:HD13	6:7:519:TRP:HZ2	1.64	0.61
12:M:25:CYS:N	12:M:52:VAL:O	2.33	0.61
1:2:303:VAL:O	1:2:304:LEU:HD23	2.01	0.61
2:3:369:SER:HA	2:3:373:LEU:HD13	1.80	0.61
6:7:340:LEU:HB2	6:7:351:LYS:CE	2.30	0.61
1:2:518:LEU:O	1:2:521:THR:OG1	2.08	0.61
1:2:570:LEU:HA	1:2:612:ILE:HG13	1.82	0.61
7:X:-7:DA:H2'	7:X:-6:DT:H72	1.82	0.61
6:7:571:PRO:HB3	6:7:623:ASP:HA	1.80	0.61
1:2:570:LEU:HD13	1:2:612:ILE:HG13	1.83	0.61
2:3:582:GLU:O	2:3:586:ASN:ND2	2.33	0.61
6:7:147:HIS:HB2	6:7:162:THR:O	2.01	0.61
1:2:465:SER:OG	1:2:694:GLN:NE2	2.34	0.61
2:3:386:ARG:NH1	7:X:5:DT:H4'	2.16	0.61
1:2:297:VAL:CG2	1:2:397:LEU:HD11	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:80:TYR:O	2:3:84:VAL:HG23	2.01	0.61
3:4:520:GLN:NE2	3:4:520:GLN:O	2.34	0.61
6:7:386:ALA:O	6:7:390:LEU:HD12	2.00	0.61
9:A:22:VAL:CG1	9:A:29:ALA:HB1	2.30	0.61
10:H:162:ASP:OD1	10:H:197:ILE:HD11	2.00	0.61
13:N:85:PHE:O	13:N:89:VAL:HG23	2.00	0.61
1:2:316:LYS:HG2	1:2:343:THR:HG23	1.81	0.61
3:4:560:LEU:O	5:6:203:GLN:NE2	2.34	0.61
6:7:40:LEU:HD11	6:7:48:ILE:HD11	1.82	0.61
6:7:377:ILE:O	6:7:486:ALA:N	2.25	0.61
6:7:505:ILE:HG22	6:7:507:LEU:HD13	1.81	0.61
5:6:26:GLN:O	5:6:30:GLU:N	2.30	0.61
6:7:170:CYS:CA	6:7:235:VAL:HG13	2.30	0.61
6:7:345:TYR:CE1	6:7:348:LEU:HD11	2.35	0.61
3:4:662:LYS:NZ	6:7:579:ASP:O	2.32	0.61
6:7:151:GLU:HA	6:7:153:LYS:NZ	2.16	0.61
9:A:378:TYR:HH	9:A:389:TYR:HH	1.45	0.61
10:H:68:ASN:N	10:H:68:ASN:OD1	2.32	0.61
1:2:545:VAL:HG13	1:2:554:TRP:CD1	2.35	0.60
4:5:459:MET:CE	4:5:481:VAL:HB	2.31	0.60
6:7:286:ALA:HA	6:7:290:GLN:HB2	1.82	0.60
6:7:390:LEU:O	6:7:394:ILE:HG12	2.01	0.60
2:3:237:SER:N	2:3:258:LEU:O	2.33	0.60
3:4:732:TYR:O	3:4:735:GLN:NE2	2.34	0.60
5:6:205:THR:HG22	5:6:207:ALA:H	1.65	0.60
6:7:212:ARG:HG3	6:7:213:VAL:H	1.66	0.60
11:L:153:ILE:HD11	13:N:182:PHE:CE2	2.36	0.60
1:2:534:GLN:NE2	1:2:576:LYS:O	2.34	0.60
2:3:190:TYR:OH	6:7:156:HIS:N	2.28	0.60
3:4:407:LEU:HD11	7:X:3:DT:H4'	1.82	0.60
4:5:592:ALA:CB	4:5:607:ILE:HD11	2.29	0.60
6:7:587:GLU:HA	6:7:590:ARG:CG	2.29	0.60
9:A:32:ALA:CB	9:A:215:ALA:HB2	2.31	0.60
13:N:179:SER:O	13:N:181:VAL:HG13	2.01	0.60
3:4:298:VAL:O	3:4:299:ILE:HD13	2.02	0.60
4:5:593:GLY:O	4:5:596:GLU:HB2	2.01	0.60
6:7:609:ILE:HA	6:7:612:LEU:CD2	2.31	0.60
3:4:478:ILE:O	3:4:481:GLY:N	2.33	0.60
3:4:598:LEU:HD23	3:4:609:LEU:HD21	1.83	0.60
6:7:380:MET:HE2	6:7:380:MET:O	2.01	0.60
6:7:609:ILE:HA	6:7:612:LEU:HG	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:135:PRO:O	13:N:138:THR:OG1	2.13	0.60
1:2:343:THR:HG22	1:2:345:PRO:O	2.01	0.60
1:2:479:ALA:HB1	1:2:644:VAL:HG11	1.83	0.60
4:5:72:LEU:O	4:5:76:ASP:N	2.33	0.60
5:6:590:TYR:CD1	5:6:593:LEU:HD13	2.36	0.60
6:7:379:LEU:HB2	6:7:487:ALA:HA	1.83	0.60
6:7:439:GLN:HE21	6:7:481:ARG:HD3	1.67	0.60
9:A:536:GLU:O	9:A:540:GLN:NE2	2.35	0.60
4:5:88:THR:OG1	4:5:89:GLU:OE2	2.16	0.60
4:5:443:GLU:OE2	4:5:446:LYS:NZ	2.30	0.60
4:5:595:GLN:NE2	4:5:651:ALA:O	2.35	0.60
6:7:556:MET:O	6:7:560:ARG:HG2	2.02	0.60
9:A:23:VAL:HG21	9:A:77:CYS:HB2	1.83	0.60
4:5:377:LEU:HB3	4:5:485:ALA:HB3	1.83	0.59
6:7:482:VAL:HG22	6:7:483:SER:O	2.02	0.59
6:7:524:LYS:HB3	6:7:525:PRO:HD2	1.84	0.59
9:A:484:LEU:HD13	9:A:501:LEU:HD22	1.83	0.59
2:3:375:ALA:HB1	7:X:9:DT:H5”	1.83	0.59
4:5:376:LEU:HD23	4:5:483:ALA:O	2.02	0.59
6:7:389:GLN:OE1	15:7:801:ADP:H3’	2.02	0.59
6:7:494:ARG:NH1	6:7:524:LYS:HE2	2.18	0.59
4:5:593:GLY:HA2	4:5:596:GLU:OE1	2.03	0.59
10:H:129:TYR:CE1	13:N:105:LEU:HD12	2.37	0.59
11:L:132:ILE:O	12:M:130:ARG:NH1	2.35	0.59
2:3:226:CYS:SG	2:3:227:LYS:N	2.75	0.59
3:4:351:ASP:OD2	5:6:122:THR:N	2.34	0.59
3:4:451:LEU:HA	3:4:454:LEU:HD12	1.83	0.59
9:A:560:GLN:NE2	9:A:561:SER:OG	2.35	0.59
10:H:111:LEU:HD21	10:H:116:VAL:H	1.66	0.59
11:L:124:ARG:NH2	11:L:149:THR:HG22	2.18	0.59
2:3:471:LEU:HD23	2:3:477:LEU:HD21	1.84	0.59
3:4:672:TYR:CE2	6:7:610:LEU:HD11	2.37	0.59
7:X:-2:DT:H2’	7:X:-1:DC:C6	2.38	0.59
1:2:783:GLN:HG2	1:2:784:LYS:H	1.67	0.59
6:7:52:LEU:O	6:7:56:ALA:N	2.34	0.59
6:7:376:ASN:HB3	6:7:484:ILE:HB	1.84	0.59
9:A:26:ASP:OD1	9:A:27:ILE:N	2.35	0.59
2:3:73:PHE:CD2	2:3:97:VAL:HG21	2.38	0.59
2:3:618:LEU:HD12	2:3:639:ALA:HB1	1.83	0.59
5:6:41:THR:O	5:6:45:ALA:N	2.36	0.59
5:6:56:GLU:HG2	5:6:107:ALA:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:357:LEU:HG	6:7:375:ILE:CG2	2.32	0.59
6:7:566:CYS:SG	6:7:621:LEU:HD11	2.41	0.59
1:2:186:SER:O	1:2:190:THR:OG1	2.12	0.59
1:2:547:ARG:NH1	1:2:556:LEU:HD22	2.17	0.59
6:7:494:ARG:HH12	6:7:524:LYS:HE2	1.67	0.59
6:7:556:MET:HA	6:7:559:MET:SD	2.43	0.59
12:M:103:GLU:OE2	12:M:152:ILE:HG21	2.03	0.59
2:3:43:ARG:CD	2:3:222:LEU:HD21	2.33	0.59
2:3:192:ASP:OD1	6:7:154:ALA:HB2	2.03	0.59
2:3:299:ALA:HB1	2:3:302:ILE:CG1	2.33	0.59
5:6:470:GLU:OE2	5:6:611:ARG:NE	2.35	0.59
6:7:32:VAL:O	6:7:35:SER:OG	2.14	0.59
6:7:446:GLU:N	6:7:487:ALA:O	2.35	0.59
6:7:518:LEU:HD21	6:7:641:LYS:HD3	1.83	0.59
6:7:585:TYR:CZ	6:7:606:LEU:HG	2.37	0.59
9:A:137:SER:OG	9:A:160:GLY:O	2.16	0.59
10:H:97:TRP:HZ3	10:H:143:LEU:HD22	1.67	0.59
2:3:219:ASP:OD1	2:3:220:ASP:N	2.35	0.58
4:5:132:ILE:HD12	4:5:226:GLU:HB3	1.85	0.58
6:7:185:ASP:HB2	6:7:186:ARG:NH2	2.18	0.58
6:7:462:MET:HB2	6:7:514:ARG:NH2	2.15	0.58
6:7:508:PRO:HG2	6:7:511:LEU:CB	2.27	0.58
4:5:259:LEU:HD13	4:5:298:ASP:HA	1.84	0.58
6:7:165:GLY:O	6:7:166:ILE:HD13	2.03	0.58
6:7:182:TYR:HB3	6:7:220:LEU:HB2	1.85	0.58
6:7:203:VAL:CG1	6:7:207:PRO:HG3	2.33	0.58
6:7:209:ASP:HA	6:7:212:ARG:HE	1.68	0.58
6:7:415:THR:HA	6:7:435:VAL:CG2	2.33	0.58
6:7:458:ILE:CG2	6:7:511:LEU:HD11	2.33	0.58
2:3:309:LYS:HA	2:3:312:ILE:HD12	1.86	0.58
3:4:234:GLN:NE2	3:4:396:ILE:HG21	2.19	0.58
6:7:174:LYS:HD3	6:7:423:LEU:CD2	2.34	0.58
6:7:385:VAL:CG2	6:7:387:LYS:HB3	2.33	0.58
11:L:94:VAL:HB	11:L:151:LEU:HD21	1.86	0.58
6:7:280:LEU:HB2	6:7:297:PHE:CD1	2.38	0.58
2:3:401:VAL:HB	2:3:443:VAL:HG23	1.85	0.58
6:7:168:THR:OG1	6:7:169:ARG:HG2	2.03	0.58
9:A:366:ILE:HB	9:A:369:ILE:HD11	1.84	0.58
2:3:386:ARG:HH12	7:X:5:DT:H4'	1.68	0.58
4:5:329:TYR:OH	4:5:348:LYS:O	2.15	0.58
5:6:243:ILE:HD11	5:6:289:ALA:C	2.24	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:524:LEU:HD11	5:6:526:PHE:CZ	2.38	0.58
6:7:566:CYS:CB	6:7:619:LEU:HA	2.27	0.58
1:2:272:GLU:O	1:2:273:LEU:HD22	2.04	0.58
1:2:292:ARG:O	1:2:293:THR:OG1	2.20	0.58
3:4:169:LYS:HD3	3:4:172:ILE:HD11	1.85	0.58
6:7:190:GLU:HG2	6:7:192:TYR:CZ	2.39	0.58
6:7:583:GLY:O	6:7:586:VAL:HB	2.04	0.58
4:5:380:PRO:HB3	14:5:801:ATP:O3G	2.04	0.58
6:7:386:ALA:HA	6:7:389:GLN:HG3	1.86	0.58
6:7:631:ALA:HA	6:7:634:LEU:CD2	2.34	0.58
1:2:297:VAL:HG13	1:2:361:ILE:HD11	1.86	0.58
3:4:523:GLN:O	3:4:523:GLN:NE2	2.36	0.58
6:7:284:GLY:O	6:7:290:GLN:NE2	2.37	0.58
1:2:297:VAL:HG22	1:2:361:ILE:HD11	1.86	0.58
4:5:589:ARG:CA	4:5:607:ILE:HG12	2.32	0.58
5:6:54:THR:HG21	5:6:225:GLU:HB2	1.85	0.58
6:7:149:ILE:HG22	6:7:239:GLU:HG3	1.86	0.58
2:3:299:ALA:HB1	2:3:302:ILE:CD1	2.33	0.57
9:A:59:LYS:NZ	9:A:86:LEU:O	2.35	0.57
9:A:268:LEU:HD12	9:A:268:LEU:O	2.04	0.57
11:L:110:CYS:N	11:L:111:GLU:OE1	2.36	0.57
13:N:48:ASN:OD1	13:N:49:GLU:N	2.36	0.57
3:4:330:LEU:HD13	3:4:338:HIS:CE1	2.39	0.57
4:5:333:SER:OG	4:5:334:GLN:NE2	2.37	0.57
4:5:369:ARG:O	4:5:617:ARG:NH1	2.37	0.57
6:7:571:PRO:HD2	6:7:618:ARG:CZ	2.35	0.57
2:3:147:ASN:H	2:3:180:LEU:HD12	1.67	0.57
4:5:369:ARG:HH12	4:5:610:ARG:HG2	1.69	0.57
9:A:105:ASP:OD1	9:A:106:VAL:N	2.37	0.57
3:4:524:TYR:CE2	3:4:528:LEU:HD11	2.40	0.57
4:5:89:GLU:OE2	4:5:89:GLU:N	2.37	0.57
6:7:465:GLN:NE2	6:7:481:ARG:HB3	2.20	0.57
9:A:258:LEU:O	9:A:262:GLN:NE2	2.38	0.57
1:2:296:VAL:N	1:2:364:GLN:O	2.33	0.57
1:2:453:SER:OG	1:2:454:LYS:NZ	2.21	0.57
3:4:283:ASP:OD1	6:7:102:TYR:OH	2.22	0.57
6:7:414:LEU:O	6:7:435:VAL:HG23	2.04	0.57
9:A:288:ASP:O	9:A:371:TYR:N	2.36	0.57
10:H:145:ASN:ND2	10:H:193:VAL:HG22	2.19	0.57
1:2:480:LEU:HD13	1:2:517:PHE:HE1	1.67	0.57
6:7:403:TYR:HA	6:7:443:CYS:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:604:ARG:NE	6:7:604:ARG:HA	2.20	0.57
1:2:502:ILE:H	1:2:610:THR:HG23	1.70	0.57
1:2:541:LEU:HD22	5:6:479:ALA:HA	1.85	0.57
6:7:174:LYS:HA	6:7:174:LYS:HE3	1.86	0.57
6:7:261:VAL:HG21	6:7:301:HIS:O	2.05	0.57
6:7:375:ILE:HG12	6:7:516:ASP:OD2	2.05	0.57
6:7:554:LEU:HD21	6:7:562:TYR:CD1	2.39	0.57
10:H:30:ASP:OD1	10:H:109:GLN:NE2	2.37	0.57
10:H:63:LEU:O	10:H:66:LEU:N	2.37	0.57
11:L:92:TYR:HA	11:L:95:VAL:HG12	1.85	0.57
5:6:393:ALA:HB2	15:6:901:ADP:H2'	1.87	0.57
6:7:326:GLU:HA	6:7:329:GLN:CB	2.35	0.57
6:7:397:LEU:HB3	6:7:560:ARG:CZ	2.35	0.57
6:7:431:GLY:HA3	6:7:435:VAL:CG1	2.32	0.57
1:2:480:LEU:HD13	1:2:517:PHE:CE1	2.38	0.57
2:3:334:ILE:HD11	2:3:617:ARG:HB3	1.86	0.57
6:7:324:LEU:HA	6:7:327:LEU:HB3	1.86	0.57
6:7:465:GLN:HE22	6:7:481:ARG:HB3	1.70	0.57
6:7:315:LYS:NZ	6:7:318:GLU:H	2.03	0.57
6:7:450:MET:HG3	6:7:454:ASP:OD2	2.04	0.57
12:M:150:ASP:OD1	12:M:152:ILE:N	2.36	0.57
3:4:538:ARG:HG3	6:7:456:THR:HG21	1.86	0.56
6:7:589:ARG:O	6:7:593:ARG:NH2	2.38	0.56
1:2:541:LEU:HD13	5:6:479:ALA:HA	1.86	0.56
1:2:575:ASP:HB2	1:2:615:ALA:HB1	1.86	0.56
2:3:274:SER:OG	2:3:276:GLU:OE1	2.11	0.56
3:4:389:ASP:OD1	3:4:390:ARG:N	2.38	0.56
3:4:509:LEU:HD12	3:4:617:ALA:HB3	1.88	0.56
3:4:571:GLY:O	3:4:613:THR:OG1	2.23	0.56
4:5:109:ARG:NH1	11:L:78:GLU:O	2.38	0.56
5:6:200:ILE:CD1	5:6:230:VAL:HG21	2.36	0.56
5:6:580:GLN:NE2	5:6:634:GLU:OE1	2.37	0.56
6:7:196:ASN:N	6:7:196:ASN:OD1	2.37	0.56
6:7:340:LEU:HD13	6:7:393:TYR:HE2	1.70	0.56
1:2:534:GLN:N	1:2:577:MET:SD	2.77	0.56
11:L:84:PHE:HZ	11:L:148:LEU:HD12	1.70	0.56
12:M:9:ASN:HD21	12:M:18:VAL:HG11	1.69	0.56
13:N:177:LEU:HD12	13:N:214:GLN:NE2	2.21	0.56
2:3:345:ALA:O	2:3:348:GLN:NE2	2.37	0.56
4:5:390:PHE:O	4:5:394:VAL:HG23	2.04	0.56
4:5:431:MET:HE3	4:5:439:VAL:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:66:VAL:HG22	6:7:73:TYR:CG	2.41	0.56
3:4:679:GLU:OE1	3:4:684:PHE:N	2.38	0.56
4:5:579:GLU:N	4:5:579:GLU:OE2	2.37	0.56
6:7:554:LEU:HD23	6:7:559:MET:HA	1.88	0.56
6:7:574:PRO:HB2	6:7:576:GLU:HG3	1.88	0.56
7:X:6:DT:H2"	7:X:8:DT:H72	1.87	0.56
11:L:9:ILE:O	11:L:12:LYS:NZ	2.24	0.56
1:2:737:LEU:O	1:2:739:ILE:HG23	2.05	0.56
3:4:561:GLN:HG3	3:4:562:THR:HG23	1.88	0.56
4:5:595:GLN:NE2	4:5:603:LEU:HB3	2.20	0.56
4:5:616:ILE:O	4:5:620:GLU:HG3	2.05	0.56
6:7:190:GLU:HG2	6:7:192:TYR:OH	2.05	0.56
11:L:1:MET:SD	11:L:1:MET:N	2.73	0.56
6:7:378:CYS:HA	6:7:486:ALA:O	2.05	0.56
12:M:25:CYS:O	12:M:52:VAL:N	2.39	0.56
1:2:692:ILE:HG22	1:2:693:PRO:O	2.05	0.56
2:3:331:ARG:NE	2:3:421:MET:O	2.39	0.56
5:6:163:GLU:OE1	5:6:163:GLU:N	2.36	0.56
6:7:377:ILE:HG21	6:7:519:TRP:HE1	1.71	0.56
6:7:539:TYR:HB3	6:7:546:GLN:HE21	1.69	0.56
2:3:343:SER:HA	14:3:901:ATP:C5'	2.35	0.56
2:3:443:VAL:HG22	2:3:444:LEU:O	2.06	0.56
4:5:582:LYS:O	4:5:586:VAL:HG23	2.05	0.56
6:7:438:ASP:HA	6:7:482:VAL:CB	2.35	0.56
11:L:93:MET:CB	11:L:151:LEU:HD22	2.35	0.56
1:2:192:VAL:HG22	1:2:198:TYR:HB2	1.88	0.55
2:3:298:LEU:HB3	2:3:309:LYS:NZ	2.21	0.55
2:3:299:ALA:HA	2:3:352:TYR:HE2	1.69	0.55
3:4:761:GLU:N	3:4:761:GLU:OE2	2.39	0.55
6:7:174:LYS:HG2	6:7:423:LEU:HD11	1.87	0.55
6:7:298:LEU:HD23	6:7:299:GLN:N	2.21	0.55
6:7:314:ASP:OD2	6:7:561:ARG:NH2	2.39	0.55
12:M:34:MET:HB3	12:M:37:LEU:HD13	1.87	0.55
1:2:204:ILE:HD11	1:2:215:PHE:CZ	2.41	0.55
5:6:129:ILE:HG22	5:6:240:GLY:HA3	1.88	0.55
6:7:147:HIS:HA	6:7:151:GLU:OE2	2.06	0.55
6:7:208:SER:O	6:7:212:ARG:NE	2.39	0.55
6:7:372:ARG:NH1	6:7:374:ASN:HB2	2.21	0.55
10:H:40:GLU:O	10:H:43:ALA:N	2.38	0.55
6:7:571:PRO:HG3	6:7:617:ALA:CB	2.31	0.55
2:3:127:ILE:N	2:3:199:GLN:O	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:607:ILE:HA	4:5:611:GLN:NE2	2.21	0.55
6:7:455:ARG:O	6:7:458:ILE:HG22	2.06	0.55
7:X:4:DT:H2"	7:X:5:DT:C5'	2.36	0.55
2:3:345:ALA:HB1	2:3:348:GLN:NE2	2.22	0.55
6:7:337:ALA:O	6:7:340:LEU:HD23	2.06	0.55
10:H:136:ASN:HA	13:N:63:LEU:HD21	1.88	0.55
13:N:187:VAL:HG11	13:N:224:GLN:HG3	1.89	0.55
1:2:545:VAL:HG21	1:2:555:THR:O	2.06	0.55
6:7:132:LYS:NZ	6:7:258:ARG:HH12	2.05	0.55
6:7:155:GLN:O	6:7:159:LYS:HD3	2.06	0.55
6:7:340:LEU:HA	6:7:393:TYR:CE2	2.42	0.55
6:7:381:GLY:HA2	6:7:490:PRO:HD3	1.89	0.55
3:4:164:CYS:SG	3:4:165:LYS:N	2.80	0.55
3:4:214:ASN:ND2	3:4:216:ALA:HB3	2.22	0.55
3:4:516:THR:HG23	3:4:518:LYS:HG3	1.88	0.55
6:7:168:THR:HG23	6:7:236:LYS:HB3	1.88	0.55
6:7:274:SER:OG	6:7:302:ARG:HB3	2.07	0.55
6:7:528:ASP:HB3	6:7:532:ARG:HH22	1.71	0.55
6:7:605:ASN:O	6:7:609:ILE:HG12	2.07	0.55
11:L:85:THR:OG1	11:L:86:LYS:N	2.40	0.55
1:2:199:THR:O	1:2:202:ASP:N	2.35	0.55
6:7:610:LEU:O	6:7:614:THR:HG22	2.07	0.55
10:H:22:SER:OG	10:H:26:ILE:HG23	2.06	0.55
2:3:299:ALA:HB2	2:3:309:LYS:NZ	2.22	0.55
2:3:428:ILE:O	2:3:435:ALA:HB3	2.07	0.55
3:4:522:LEU:HD13	3:4:616:LEU:CD2	2.33	0.55
2:3:139:VAL:HG22	2:3:191:LYS:NZ	2.22	0.55
2:3:299:ALA:HB2	2:3:309:LYS:HZ2	1.71	0.55
14:3:901:ATP:H8	4:5:609:VAL:HG21	1.72	0.55
4:5:355:PHE:CD2	4:5:625:ILE:HG12	2.42	0.55
6:7:77:PHE:CE2	6:7:81:ILE:HD11	2.42	0.55
6:7:78:SER:OG	6:7:79:ASP:N	2.39	0.55
6:7:230:VAL:HG12	6:7:231:LYS:O	2.07	0.55
6:7:391:LEU:HD21	6:7:443:CYS:CB	2.37	0.55
6:7:616:LEU:HB3	6:7:629:ASP:OD2	2.07	0.55
10:H:19:LEU:HD12	10:H:22:SER:HB2	1.89	0.55
11:L:13:CYS:SG	11:L:14:MET:N	2.80	0.55
2:3:352:TYR:O	2:3:356:THR:OG1	2.14	0.54
3:4:749:VAL:HG22	3:4:750:ARG:HD2	1.89	0.54
6:7:182:TYR:N	6:7:191:THR:OG1	2.33	0.54
10:H:31:ASP:OD1	10:H:112:CYS:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:112:GLU:O	11:L:116:VAL:HG13	2.06	0.54
2:3:347:SER:OG	14:3:901:ATP:O2G	2.25	0.54
3:4:262:GLN:OE1	3:4:264:ARG:NH2	2.40	0.54
4:5:108:PRO:HG3	11:L:130:THR:HG21	1.87	0.54
6:7:497:PRO:HB2	6:7:498:ARG:NH2	2.21	0.54
11:L:103:ALA:O	11:L:107:VAL:HG23	2.07	0.54
1:2:195:ARG:NH2	1:2:444:GLU:OE2	2.40	0.54
2:3:145:CYS:O	2:3:149:ARG:N	2.38	0.54
4:5:27:LEU:HD13	4:5:31:LYS:HE3	1.90	0.54
4:5:605:ILE:HG12	4:5:606:PRO:HD2	1.88	0.54
2:3:173:THR:HA	2:3:181:LEU:HD12	1.90	0.54
4:5:599:SER:HB3	4:5:603:LEU:HD12	1.89	0.54
4:5:606:PRO:O	4:5:611:GLN:NE2	2.40	0.54
5:6:54:THR:HG22	5:6:105:TYR:HB2	1.88	0.54
6:7:160:LEU:HA	6:7:276:VAL:HG22	1.89	0.54
6:7:320:THR:HB	6:7:321:PRO:HD3	1.89	0.54
6:7:459:HIS:ND1	6:7:514:ARG:HG3	2.22	0.54
6:7:511:LEU:HD13	6:7:515:PHE:HZ	1.73	0.54
2:3:442:SER:OG	2:3:443:VAL:N	2.40	0.54
3:4:330:LEU:HD12	3:4:333:ASN:HA	1.90	0.54
6:7:183:THR:O	6:7:220:LEU:HA	2.08	0.54
6:7:223:GLN:CD	6:7:225:ARG:HG3	2.27	0.54
6:7:536:HIS:HA	6:7:546:GLN:NE2	2.21	0.54
6:7:539:TYR:HB3	6:7:546:GLN:HG2	1.89	0.54
9:A:563:LEU:HD23	9:A:563:LEU:H	1.72	0.54
13:N:55:ILE:HD12	13:N:112:ILE:HD11	1.90	0.54
1:2:586:HIS:CD2	1:2:638:ILE:HA	2.42	0.54
1:2:754:HIS:HA	1:2:757:MET:SD	2.48	0.54
4:5:516:ILE:HD12	4:5:649:ASP:OD2	2.06	0.54
6:7:240:HIS:HB3	6:7:243:GLN:HE22	1.71	0.54
13:N:153:HIS:O	13:N:157:THR:OG1	2.16	0.54
3:4:325:ILE:O	5:6:261:SER:OG	2.19	0.54
4:5:584:ARG:HH11	4:5:644:GLN:HE22	1.56	0.54
6:7:340:LEU:HB2	6:7:351:LYS:HE3	1.90	0.54
6:7:520:LEU:HD21	6:7:522:GLN:OE1	2.07	0.54
1:2:251:MET:O	1:2:255:ILE:HD12	2.07	0.54
1:2:545:VAL:HB	1:2:556:LEU:HD12	1.90	0.54
1:2:794:THR:O	1:2:798:TYR:N	2.34	0.54
2:3:340:GLY:O	2:3:346:LYS:HE2	2.07	0.54
3:4:413:SER:N	6:7:198:LEU:O	2.41	0.54
3:4:647:ASP:N	3:4:647:ASP:OD1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:736:LEU:O	3:4:740:ILE:HG23	2.07	0.54
5:6:363:GLN:OE1	5:6:492:LEU:HD21	2.08	0.54
6:7:141:LEU:HD23	6:7:142:SER:N	2.23	0.54
6:7:362:VAL:HA	6:7:618:ARG:NH1	2.23	0.54
6:7:585:TYR:CE2	6:7:589:ARG:HD2	2.43	0.54
9:A:11:TYR:HD1	9:A:14:LEU:HD22	1.72	0.54
9:A:37:GLN:O	9:A:47:TYR:OH	2.25	0.54
9:A:487:HIS:NE2	9:A:491:SER:OG	2.40	0.54
13:N:114:THR:C	13:N:173:VAL:HG11	2.28	0.54
2:3:298:LEU:HB3	2:3:309:LYS:HZ1	1.73	0.54
3:4:213:LEU:HD12	3:4:214:ASN:H	1.73	0.54
3:4:550:THR:OG1	3:4:551:LYS:N	2.40	0.54
4:5:459:MET:HE1	4:5:481:VAL:HB	1.88	0.54
5:6:397:PHE:HB3	5:6:398:LEU:HD23	1.89	0.54
5:6:441:LEU:CD1	5:6:465:ILE:HD11	2.37	0.54
6:7:448:ASP:HB3	6:7:507:LEU:CD1	2.34	0.54
6:7:528:ASP:HB3	6:7:532:ARG:NH2	2.23	0.54
11:L:78:GLU:O	11:L:81:SER:OG	2.25	0.54
13:N:171:ARG:C	13:N:172:ILE:HD12	2.28	0.54
3:4:339:CYS:SG	3:4:340:PHE:N	2.79	0.54
6:7:305:CYS:SG	6:7:309:ASN:HB2	2.48	0.54
13:N:188:ALA:HB3	13:N:192:VAL:HB	1.90	0.54
6:7:572:THR:HG23	6:7:623:ASP:OD1	2.08	0.53
9:A:111:SER:O	9:A:113:ARG:N	2.41	0.53
6:7:151:GLU:HA	6:7:153:LYS:HZ2	1.73	0.53
6:7:337:ALA:HA	6:7:355:LEU:HD12	1.89	0.53
6:7:379:LEU:O	6:7:488:ALA:N	2.27	0.53
6:7:517:LEU:HD13	6:7:519:TRP:CZ2	2.42	0.53
9:A:102:ARG:O	9:A:104:LEU:N	2.42	0.53
9:A:435:LEU:O	9:A:439:VAL:HG23	2.08	0.53
13:N:56:LEU:O	13:N:108:ARG:NH2	2.41	0.53
6:7:201:THR:HG23	6:7:202:PRO:HD2	1.89	0.53
6:7:475:MET:HG2	6:7:477:THR:H	1.72	0.53
6:7:612:LEU:HD12	6:7:613:SER:N	2.23	0.53
6:7:615:ALA:HA	6:7:618:ARG:HD3	1.91	0.53
1:2:610:THR:O	1:2:611:VAL:HG23	2.08	0.53
1:2:712:LEU:HD23	1:2:713:THR:N	2.23	0.53
4:5:177:LEU:O	4:5:291:ARG:NH2	2.42	0.53
6:7:437:ALA:CB	6:7:442:CYS:HB2	2.39	0.53
6:7:518:LEU:HD21	6:7:641:LYS:CD	2.37	0.53
3:4:216:ALA:HB2	3:4:267:ASN:ND2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:323:ALA:CB	4:5:627:LEU:HD12	2.38	0.53
6:7:203:VAL:HG11	6:7:207:PRO:HG3	1.91	0.53
11:L:15:ILE:HG12	11:L:46:LEU:HD11	1.90	0.53
5:6:548:HIS:O	5:6:550:ASN:ND2	2.41	0.53
6:7:413:GLY:O	6:7:432:GLY:HA3	2.09	0.53
1:2:398:GLU:OE1	1:2:432:LYS:NZ	2.41	0.53
1:2:545:VAL:HG11	1:2:547:ARG:NH2	2.20	0.53
1:2:700:TYR:OH	1:2:757:MET:O	2.27	0.53
2:3:6:GLU:OE1	2:3:6:GLU:N	2.40	0.53
2:3:159:LEU:HD12	2:3:162:PHE:O	2.09	0.53
2:3:379:THR:HG22	2:3:380:ASP:OD1	2.08	0.53
4:5:612:LEU:HA	4:5:615:VAL:CG1	2.39	0.53
5:6:38:ILE:HG22	5:6:40:TYR:H	1.72	0.53
6:7:609:ILE:HA	6:7:612:LEU:CG	2.39	0.53
8:Y:13:DA:H2"	8:Y:14:DT:C5	2.43	0.53
1:2:405:ASN:N	1:2:405:ASN:OD1	2.40	0.53
1:2:760:ARG:HE	1:2:763:VAL:HA	1.74	0.53
5:6:382:ILE:O	5:6:490:SER:OG	2.07	0.53
6:7:455:ARG:HB3	6:7:508:PRO:HG3	1.91	0.53
7:X:4:DT:C2'	7:X:5:DT:H5"	2.38	0.53
9:A:284:THR:OG1	9:A:285:PHE:N	2.42	0.53
12:M:136:SER:O	12:M:164:ASN:ND2	2.42	0.53
4:5:361:ARG:O	4:5:362:LEU:HD23	2.09	0.53
5:6:47:LEU:HD11	5:6:53:CYS:H	1.74	0.53
6:7:417:ALA:O	6:7:429:LEU:HA	2.09	0.53
9:A:240:ILE:O	9:A:244:LEU:N	2.41	0.53
10:H:147:LEU:O	10:H:147:LEU:HD23	2.09	0.53
3:4:479:LYS:HA	3:4:482:ILE:HD12	1.90	0.53
4:5:621:SER:O	4:5:625:ILE:HG13	2.08	0.53
5:6:75:GLU:N	5:6:75:GLU:OE1	2.42	0.53
6:7:4:ARG:NH1	6:7:61:SER:OG	2.41	0.53
6:7:344:ILE:HA	6:7:536:HIS:CB	2.39	0.53
6:7:366:PRO:HG3	6:7:371:ILE:CG2	2.39	0.53
6:7:478:LEU:CD2	6:7:480:ALA:HB2	2.39	0.53
2:3:109:THR:OG1	2:3:112:SER:OG	2.13	0.52
2:3:415:THR:HG21	6:7:407:ARG:HG2	1.91	0.52
6:7:391:LEU:HD22	6:7:403:TYR:CE2	2.44	0.52
9:A:9:ASP:OD1	9:A:10:PHE:N	2.41	0.52
1:2:480:LEU:HD11	1:2:521:THR:CG2	2.38	0.52
1:2:528:ALA:HB2	1:2:568:VAL:HG23	1.90	0.52
1:2:550:VAL:O	1:2:551:SER:OG	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:592:VAL:O	3:4:596:GLN:NE2	2.42	0.52
4:5:563:HIS:O	4:5:567:THR:OG1	2.27	0.52
6:7:166:ILE:HD13	6:7:270:HIS:HA	1.91	0.52
6:7:218:GLY:O	6:7:219:ARG:HG2	2.09	0.52
6:7:353:ALA:O	6:7:357:LEU:HD13	2.09	0.52
6:7:587:GLU:CA	6:7:590:ARG:HG2	2.34	0.52
6:7:632:GLU:O	6:7:636:LEU:HD23	2.09	0.52
1:2:480:LEU:HD11	1:2:521:THR:HG21	1.90	0.52
2:3:415:THR:CG2	6:7:407:ARG:HG2	2.39	0.52
3:4:605:ILE:CG1	5:6:232:ALA:HB1	2.39	0.52
3:4:664:LEU:HD23	3:4:664:LEU:H	1.73	0.52
11:L:160:LEU:O	11:L:164:LEU:N	2.43	0.52
13:N:173:VAL:HG12	13:N:174:THR:OG1	2.09	0.52
3:4:672:TYR:CE1	6:7:366:PRO:HB3	2.43	0.52
4:5:460:GLU:OE2	4:5:610:ARG:NE	2.27	0.52
5:6:69:LEU:O	5:6:73:ILE:N	2.43	0.52
5:6:117:VAL:HG23	5:6:118:ARG:HD3	1.90	0.52
5:6:149:VAL:HG12	5:6:157:THR:HG22	1.91	0.52
6:7:405:THR:HG22	6:7:408:GLY:HA3	1.91	0.52
6:7:500:THR:O	6:7:504:ASN:ND2	2.43	0.52
9:A:328:LEU:HD12	9:A:333:LEU:HB3	1.92	0.52
13:N:112:ILE:HD12	13:N:119:ILE:HD12	1.92	0.52
2:3:320:VAL:HB	2:3:620:THR:HG21	1.90	0.52
4:5:44:GLU:OE1	4:5:44:GLU:N	2.42	0.52
4:5:377:LEU:HD12	4:5:377:LEU:O	2.09	0.52
5:6:200:ILE:HD13	5:6:230:VAL:HG21	1.91	0.52
6:7:106:ARG:HH22	6:7:225:ARG:HB2	1.75	0.52
6:7:282:ARG:O	6:7:282:ARG:HD3	2.10	0.52
6:7:572:THR:N	6:7:623:ASP:OD2	2.21	0.52
2:3:388:LEU:HD12	2:3:389:GLU:N	2.25	0.52
4:5:41:PHE:O	4:5:49:LYS:HG3	2.09	0.52
6:7:160:LEU:CA	6:7:276:VAL:HG22	2.39	0.52
6:7:169:ARG:HG3	6:7:236:LYS:HD2	1.91	0.52
6:7:269:ASP:HB3	6:7:305:CYS:SG	2.50	0.52
6:7:565:LEU:HG	6:7:621:LEU:CD2	2.39	0.52
9:A:109:ILE:HG23	9:A:117:ILE:HD13	1.92	0.52
11:L:95:VAL:O	11:L:99:VAL:HG23	2.09	0.52
6:7:355:LEU:O	6:7:355:LEU:HD23	2.10	0.52
6:7:528:ASP:HA	6:7:531:LEU:HD12	1.92	0.52
6:7:586:VAL:HG12	6:7:590:ARG:HD3	1.92	0.52
11:L:93:MET:N	11:L:93:MET:SD	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:698:GLU:N	3:4:698:GLU:OE1	2.42	0.52
6:7:144:GLU:O	6:7:145:LYS:HD3	2.10	0.52
7:X:0:DG:H1'	7:X:1:DT:C5'	2.37	0.52
3:4:378:HIS:O	3:4:382:VAL:HG13	2.10	0.52
4:5:253:VAL:HG22	4:5:254:PRO:HD2	1.92	0.52
5:6:373:THR:OG1	5:6:374:GLU:N	2.43	0.52
6:7:205:ASP:HB2	6:7:219:ARG:HA	1.91	0.52
6:7:347:HIS:HE1	6:7:385:VAL:HG12	1.75	0.52
6:7:415:THR:HA	6:7:435:VAL:HG23	1.90	0.52
6:7:435:VAL:HG13	6:7:478:LEU:HD11	1.92	0.52
12:M:110:PRO:O	12:M:113:ARG:NH2	2.41	0.52
13:N:55:ILE:HD11	13:N:108:ARG:HH21	1.74	0.52
1:2:314:CYS:SG	1:2:343:THR:HG21	2.50	0.52
6:7:168:THR:O	6:7:235:VAL:HG12	2.10	0.52
6:7:319:LEU:HB2	6:7:322:GLU:CB	2.40	0.52
6:7:451:ALA:O	6:7:455:ARG:NE	2.43	0.52
9:A:93:VAL:N	9:A:114:GLN:OE1	2.43	0.52
1:2:297:VAL:HG23	1:2:397:LEU:HD11	1.92	0.51
1:2:648:VAL:HG23	1:2:648:VAL:O	2.10	0.51
2:3:109:THR:HG1	2:3:112:SER:HG	1.43	0.51
3:4:342:LEU:O	3:4:343:ILE:HD13	2.09	0.51
5:6:245:VAL:O	5:6:247:ASP:N	2.43	0.51
6:7:517:LEU:HB3	6:7:519:TRP:CE2	2.44	0.51
9:A:21:ILE:HG23	9:A:52:ILE:HD11	1.93	0.51
9:A:563:LEU:O	9:A:567:LEU:N	2.43	0.51
12:M:74:PRO:O	12:M:78:ARG:N	2.43	0.51
13:N:196:VAL:HG11	13:N:200:GLU:HB3	1.91	0.51
1:2:304:LEU:O	1:2:358:TYR:N	2.44	0.51
2:3:522:SER:OG	10:H:36:GLN:O	2.24	0.51
4:5:365:GLY:O	4:5:367:CYS:N	2.43	0.51
6:7:207:PRO:CD	6:7:220:LEU:HD21	2.40	0.51
6:7:340:LEU:HB2	6:7:351:LYS:HE2	1.92	0.51
6:7:381:GLY:HA2	6:7:490:PRO:CD	2.41	0.51
6:7:415:THR:HG21	6:7:469:ILE:CG1	2.40	0.51
9:A:53:MET:N	9:A:53:MET:SD	2.83	0.51
13:N:68:SER:OG	13:N:69:GLN:NE2	2.43	0.51
6:7:99:LEU:HD22	6:7:228:LYS:HA	1.92	0.51
6:7:164:ARG:CG	6:7:272:VAL:HG22	2.40	0.51
6:7:353:ALA:HA	6:7:356:LEU:HD11	1.93	0.51
6:7:505:ILE:CG2	6:7:507:LEU:HD13	2.40	0.51
6:7:566:CYS:HA	6:7:621:LEU:HG	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:111:SER:O	9:A:111:SER:OG	2.26	0.51
9:A:177:LEU:HD11	9:A:182:GLN:NE2	2.25	0.51
10:H:95:LEU:HD13	10:H:99:PHE:CZ	2.45	0.51
11:L:48:MET:O	11:L:52:LEU:N	2.43	0.51
13:N:112:ILE:HD12	13:N:119:ILE:CD1	2.40	0.51
1:2:252:VAL:O	1:2:256:PHE:N	2.32	0.51
1:2:579:ASP:O	1:2:583:THR:HG23	2.09	0.51
3:4:535:THR:O	3:4:536:SER:OG	2.26	0.51
4:5:27:LEU:O	4:5:31:LYS:N	2.43	0.51
6:7:83:GLU:O	6:7:84:LEU:HD23	2.10	0.51
6:7:266:GLN:NE2	6:7:267:PRO:O	2.43	0.51
6:7:315:LYS:HZ1	6:7:319:LEU:N	2.08	0.51
6:7:439:GLN:N	6:7:481:ARG:HG3	2.26	0.51
8:Y:12:DG:H2'	8:Y:13:DA:C8	2.45	0.51
10:H:95:LEU:HD13	10:H:99:PHE:HZ	1.76	0.51
1:2:731:SER:HB3	1:2:736:SER:HB3	1.92	0.51
4:5:108:PRO:CG	11:L:130:THR:HG21	2.40	0.51
4:5:383:ALA:HA	14:5:801:ATP:O2A	2.11	0.51
4:5:393:LYS:HG3	4:5:555:LEU:HD11	1.92	0.51
5:6:55:LEU:HD23	5:6:56:GLU:O	2.11	0.51
6:7:233:GLN:HG3	6:7:262:THR:HG23	1.91	0.51
6:7:455:ARG:HG2	6:7:508:PRO:HD3	1.91	0.51
6:7:468:SER:O	6:7:469:ILE:HD13	2.10	0.51
9:A:281:SER:O	9:A:376:LEU:HD11	2.11	0.51
11:L:27:HIS:O	13:N:86:ARG:NH2	2.42	0.51
12:M:23:VAL:O	12:M:53:ASN:ND2	2.40	0.51
13:N:187:VAL:HG11	13:N:224:GLN:CG	2.40	0.51
2:3:420:VAL:HG12	2:3:425:ARG:O	2.11	0.51
4:5:444:PHE:CE1	4:5:501:ILE:HD11	2.46	0.51
6:7:386:ALA:HA	15:7:801:ADP:H5'2	1.92	0.51
6:7:558:LEU:CD1	6:7:561:ARG:HD2	2.36	0.51
1:2:634:LEU:HB3	1:2:638:ILE:HD11	1.91	0.51
5:6:524:LEU:HD11	5:6:526:PHE:CE2	2.46	0.51
6:7:380:MET:HE2	6:7:520:LEU:CD1	2.39	0.51
6:7:421:ASP:HB2	6:7:425:GLY:N	2.22	0.51
10:H:47:GLU:OE1	10:H:47:GLU:N	2.43	0.51
10:H:97:TRP:CZ3	10:H:143:LEU:HD22	2.45	0.51
2:3:377:VAL:CG2	7:X:8:DT:H4'	2.35	0.51
5:6:447:GLY:N	5:6:489:THR:HG21	2.25	0.51
6:7:366:PRO:CG	6:7:371:ILE:HG23	2.38	0.51
12:M:14:GLU:OE1	12:M:100:TYR:OH	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:435:LYS:HG3	1:2:526:PRO:HB2	1.93	0.51
6:7:389:GLN:CD	15:7:801:ADP:H3'	2.31	0.51
9:A:243:GLN:NE2	9:A:249:ILE:HD12	2.26	0.51
11:L:150:LEU:HD12	11:L:153:ILE:CG2	2.40	0.51
12:M:103:GLU:OE1	12:M:103:GLU:N	2.44	0.51
2:3:91:MET:O	2:3:93:GLU:N	2.44	0.51
2:3:459:THR:OG1	2:3:461:MET:O	2.17	0.51
14:3:901:ATP:C8	4:5:609:VAL:HG21	2.46	0.51
5:6:363:GLN:NE2	5:6:491:ILE:O	2.44	0.51
6:7:458:ILE:O	6:7:462:MET:HE1	2.11	0.51
6:7:530:ASP:OD2	6:7:531:LEU:HD12	2.10	0.51
6:7:619:LEU:HD12	6:7:620:ARG:HG2	1.93	0.51
12:M:104:PHE:HE2	12:M:108:LEU:HD13	1.73	0.51
1:2:233:LEU:CD1	1:2:290:LEU:HD21	2.41	0.50
4:5:349:ALA:HB2	4:5:642:LEU:HD23	1.94	0.50
4:5:589:ARG:HG2	4:5:607:ILE:HD13	1.93	0.50
6:7:376:ASN:HB3	6:7:484:ILE:CG2	2.41	0.50
9:A:381:ARG:HG3	9:A:382:SER:H	1.76	0.50
11:L:84:PHE:CZ	11:L:148:LEU:HD12	2.45	0.50
1:2:518:LEU:HD22	1:2:572:ASP:OD1	2.12	0.50
1:2:707:ASN:O	1:2:709:ARG:NH2	2.44	0.50
2:3:338:LEU:HD11	2:3:478:PHE:CB	2.40	0.50
5:6:253:GLY:O	5:6:285:ASN:ND2	2.43	0.50
6:7:455:ARG:H	6:7:455:ARG:HD2	1.76	0.50
6:7:464:GLN:HG2	6:7:465:GLN:N	2.25	0.50
9:A:424:LEU:O	9:A:427:ALA:HB3	2.12	0.50
10:H:45:PHE:CE1	10:H:49:VAL:HG21	2.46	0.50
1:2:547:ARG:CZ	1:2:556:LEU:HD22	2.41	0.50
3:4:253:PRO:O	3:4:257:LEU:HD11	2.10	0.50
6:7:287:GLN:HG2	6:7:288:MET:N	2.25	0.50
6:7:459:HIS:CE1	6:7:511:LEU:HA	2.46	0.50
9:A:52:ILE:N	9:A:52:ILE:HD12	2.26	0.50
9:A:434:LEU:HD12	9:A:435:LEU:N	2.26	0.50
11:L:6:ILE:O	11:L:10:GLY:N	2.40	0.50
12:M:25:CYS:HB3	12:M:54:LEU:HD12	1.93	0.50
3:4:468:ILE:CD1	3:4:486:LEU:HD11	2.38	0.50
6:7:239:GLU:OE1	6:7:244:VAL:HG22	2.12	0.50
6:7:402:GLN:O	6:7:443:CYS:N	2.23	0.50
9:A:212:ARG:NH1	9:A:257:GLU:OE2	2.36	0.50
11:L:165:ASP:N	11:L:165:ASP:OD1	2.44	0.50
1:2:499:ARG:HG3	1:2:749:ARG:HE	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:257:LEU:C	2:3:258:LEU:HD23	2.32	0.50
2:3:375:ALA:HB1	7:X:9:DT:C5'	2.42	0.50
5:6:205:THR:HG22	5:6:207:ALA:N	2.26	0.50
6:7:149:ILE:CG2	6:7:239:GLU:HG3	2.41	0.50
6:7:153:LYS:HB2	6:7:155:GLN:HE22	1.77	0.50
6:7:261:VAL:HA	6:7:264:MET:HE2	1.91	0.50
6:7:575:ASP:O	6:7:578:THR:OG1	2.19	0.50
1:2:560:ALA:O	1:2:564:ALA:N	2.45	0.50
1:2:586:HIS:O	1:2:586:HIS:ND1	2.39	0.50
2:3:143:HIS:CE1	2:3:183:THR:HG22	2.47	0.50
4:5:436:GLY:N	4:5:478:ARG:O	2.44	0.50
6:7:171:THR:OG1	6:7:423:LEU:HD22	2.11	0.50
6:7:372:ARG:HH12	6:7:374:ASN:HB2	1.76	0.50
6:7:379:LEU:HB2	6:7:487:ALA:CA	2.41	0.50
6:7:528:ASP:HA	6:7:531:LEU:CD1	2.42	0.50
2:3:159:LEU:HD22	2:3:241:LEU:HD13	1.93	0.50
2:3:576:LEU:HD12	2:3:577:GLY:H	1.75	0.50
4:5:546:SER:OG	4:5:547:GLU:N	2.45	0.50
4:5:607:ILE:HA	4:5:611:GLN:HE22	1.76	0.50
5:6:187:LEU:CD2	5:6:189:VAL:HG13	2.42	0.50
5:6:204:GLU:O	5:6:206:GLN:NE2	2.44	0.50
6:7:93:VAL:HG11	6:7:96:LYS:CE	2.41	0.50
6:7:474:ILE:HB	6:7:475:MET:HE1	1.93	0.50
6:7:566:CYS:HB3	6:7:619:LEU:CA	2.33	0.50
11:L:127:LYS:HD2	11:L:128:LEU:HD12	1.94	0.50
12:M:151:ASN:N	12:M:151:ASN:OD1	2.44	0.50
1:2:389:ASP:OD1	4:5:238:ARG:NH2	2.43	0.50
1:2:513:ALA:HA	14:2:901:ATP:H5'1	1.93	0.50
1:2:640:SER:HB3	4:5:380:PRO:HB2	1.94	0.50
2:3:138:VAL:HB	6:7:292:LEU:HB3	1.94	0.50
2:3:501:ARG:O	2:3:503:ARG:N	2.43	0.50
5:6:236:TYR:HD2	5:6:295:VAL:HG13	1.76	0.50
6:7:269:ASP:HB2	6:7:271:ILE:CG2	2.42	0.50
6:7:310:ASP:HA	6:7:316:ASP:CB	2.34	0.50
6:7:499:ARG:HH21	6:7:499:ARG:HG2	1.77	0.50
10:H:136:ASN:ND2	13:N:64:GLU:OE2	2.45	0.50
2:3:470:LEU:H	2:3:470:LEU:HD12	1.76	0.50
2:3:471:LEU:HD23	2:3:477:LEU:CD2	2.41	0.50
3:4:301:GLU:O	3:4:350:THR:N	2.45	0.50
4:5:298:ASP:OD1	4:5:299:SER:N	2.44	0.50
4:5:595:GLN:O	4:5:603:LEU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:21:ALA:HB1	5:6:69:LEU:HD21	1.94	0.50
6:7:563:ILE:HG13	6:7:564:ASN:ND2	2.27	0.50
9:A:22:VAL:O	9:A:52:ILE:HD13	2.12	0.50
9:A:163:ASP:OD1	9:A:164:GLN:N	2.42	0.50
11:L:153:ILE:HG23	11:L:157:ARG:NH2	2.27	0.50
2:3:338:LEU:HD11	2:3:478:PHE:HB3	1.94	0.49
3:4:454:LEU:O	3:4:460:ILE:HD12	2.12	0.49
4:5:386:GLN:NE2	14:5:801:ATP:O3'	2.43	0.49
5:6:129:ILE:HG23	5:6:131:ILE:CD1	2.34	0.49
5:6:152:CYS:SG	5:6:180:SER:N	2.83	0.49
6:7:282:ARG:NH1	6:7:284:GLY:HA3	2.27	0.49
6:7:319:LEU:HD13	6:7:322:GLU:OE2	2.11	0.49
1:2:312:TYR:HB2	1:2:321:LEU:HD22	1.93	0.49
4:5:378:GLY:HA3	4:5:517:VAL:HB	1.94	0.49
5:6:568:VAL:O	5:6:572:ARG:NH1	2.45	0.49
2:3:43:ARG:HD3	2:3:222:LEU:HD21	1.95	0.49
2:3:377:VAL:HG13	7:X:8:DT:H4'	1.94	0.49
3:4:691:ASP:O	3:4:695:TYR:N	2.44	0.49
6:7:184:CYS:HA	6:7:220:LEU:HB3	1.94	0.49
6:7:382:ASP:CG	6:7:387:LYS:HG2	2.32	0.49
9:A:333:LEU:HD23	9:A:338:ALA:HB2	1.94	0.49
4:5:153:ALA:HB1	4:5:221:THR:O	2.13	0.49
5:6:64:LYS:O	5:6:67:GLN:NE2	2.45	0.49
6:7:5:ASP:OD1	6:7:6:TYR:N	2.45	0.49
6:7:286:ALA:HA	6:7:290:GLN:CD	2.32	0.49
6:7:546:GLN:O	6:7:548:PRO:HD3	2.13	0.49
6:7:160:LEU:CB	6:7:276:VAL:HG22	2.43	0.49
6:7:171:THR:OG1	6:7:423:LEU:HD13	2.12	0.49
6:7:284:GLY:H	6:7:290:GLN:HE22	1.60	0.49
6:7:467:ILE:CG2	6:7:478:LEU:HB3	2.42	0.49
7:X:10:DT:H2"	7:X:11:DT:C6	2.46	0.49
7:X:12:DT:H2"	7:X:13:DT:C5	2.48	0.49
9:A:266:SER:OG	9:A:267:ARG:NE	2.45	0.49
1:2:712:LEU:HD23	1:2:713:THR:H	1.76	0.49
2:3:377:VAL:CG2	7:X:9:DT:H5'	2.42	0.49
3:4:211:LEU:O	3:4:262:GLN:NE2	2.42	0.49
4:5:464:ILE:N	4:5:475:LEU:O	2.46	0.49
5:6:340:GLN:HA	5:6:343:ILE:HD12	1.94	0.49
6:7:74:THR:HG22	6:7:138:PHE:CE2	2.47	0.49
6:7:315:LYS:HZ1	6:7:319:LEU:H	1.60	0.49
6:7:385:VAL:HG23	6:7:387:LYS:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:29:ILE:HG23	11:L:33:VAL:CG1	2.42	0.49
2:3:130:LYS:O	2:3:132:SER:OG	2.28	0.49
3:4:267:ASN:ND2	3:4:267:ASN:O	2.45	0.49
3:4:650:PHE:CZ	3:4:766:LEU:HD22	2.47	0.49
6:7:462:MET:CE	6:7:514:ARG:HB3	2.43	0.49
1:2:440:SER:OG	1:2:441:LEU:N	2.46	0.49
1:2:545:VAL:HB	1:2:556:LEU:CD1	2.42	0.49
2:3:628:SER:O	2:3:630:SER:N	2.45	0.49
4:5:336:LEU:HD12	4:5:347:LYS:HE3	1.95	0.49
5:6:198:GLN:HE21	5:6:222:LEU:HD12	1.78	0.49
12:M:65:ASN:OD1	12:M:66:ASN:N	2.46	0.49
2:3:206:PRO:O	2:3:209:GLN:N	2.44	0.49
6:7:182:TYR:CE1	6:7:222:LEU:HB2	2.48	0.49
1:2:545:VAL:HG11	1:2:554:TRP:O	2.12	0.49
1:2:739:ILE:O	1:2:739:ILE:HG13	2.12	0.49
4:5:397:ILE:HG23	4:5:437:GLY:HA3	1.95	0.49
5:6:187:LEU:HD23	5:6:188:ASP:N	2.27	0.49
5:6:387:VAL:CB	5:6:527:ILE:HD12	2.39	0.49
6:7:215:LYS:O	6:7:215:LYS:NZ	2.31	0.49
6:7:337:ALA:O	6:7:351:LYS:HE2	2.13	0.49
6:7:344:ILE:HG21	15:7:801:ADP:N1	2.28	0.49
6:7:386:ALA:HB1	6:7:389:GLN:CB	2.40	0.49
9:A:347:LEU:HD22	9:A:351:LYS:HE3	1.95	0.49
9:A:457:SER:O	9:A:499:LEU:HD13	2.13	0.49
1:2:520:TYR:O	1:2:524:VAL:HG12	2.13	0.48
6:7:93:VAL:HG11	6:7:96:LYS:HE2	1.94	0.48
6:7:315:LYS:HZ3	6:7:318:GLU:H	1.59	0.48
6:7:566:CYS:HA	6:7:621:LEU:CG	2.43	0.48
9:A:27:ILE:HD12	9:A:393:LEU:HD13	1.95	0.48
1:2:512:THR:HG21	1:2:648:VAL:HG21	1.95	0.48
2:3:337:LEU:HD12	2:3:338:LEU:H	1.78	0.48
2:3:379:THR:HG23	7:X:5:DT:C2	2.48	0.48
6:7:421:ASP:OD2	6:7:426:GLU:N	2.47	0.48
6:7:435:VAL:HG22	6:7:478:LEU:HD13	1.94	0.48
6:7:455:ARG:NH1	6:7:508:PRO:HD3	2.28	0.48
6:7:517:LEU:HB3	6:7:519:TRP:CZ2	2.48	0.48
6:7:616:LEU:HD22	6:7:632:GLU:OE2	2.13	0.48
4:5:595:GLN:HE21	4:5:603:LEU:HD13	1.77	0.48
4:5:612:LEU:O	4:5:616:ILE:HG12	2.13	0.48
6:7:173:VAL:O	6:7:174:LYS:HD2	2.14	0.48
6:7:530:ASP:OD2	6:7:530:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:505:CYS:N	9:A:515:LEU:O	2.46	0.48
11:L:17:ILE:O	11:L:42:VAL:N	2.40	0.48
2:3:299:ALA:CB	2:3:302:ILE:HD11	2.42	0.48
2:3:407:ASP:N	2:3:407:ASP:OD1	2.47	0.48
6:7:266:GLN:HG3	6:7:269:ASP:CG	2.32	0.48
6:7:343:GLU:O	6:7:536:HIS:HB3	2.12	0.48
6:7:366:PRO:HD3	6:7:371:ILE:HG12	1.95	0.48
6:7:446:GLU:HA	6:7:488:ALA:HA	1.94	0.48
6:7:559:MET:HB3	6:7:560:ARG:HH21	1.78	0.48
6:7:631:ALA:O	6:7:635:ARG:HG2	2.14	0.48
1:2:218:SER:OG	1:2:272:GLU:OE1	2.20	0.48
1:2:545:VAL:HG21	1:2:554:TRP:O	2.13	0.48
2:3:190:TYR:CZ	6:7:154:ALA:HA	2.48	0.48
3:4:666:SER:HB3	6:7:582:VAL:HG21	1.95	0.48
4:5:245:ASP:OD2	4:5:246:ARG:NH1	2.46	0.48
5:6:189:VAL:N	5:6:190:GLU:OE2	2.47	0.48
6:7:207:PRO:HD2	6:7:220:LEU:CD2	2.42	0.48
6:7:214:ASN:ND2	6:7:216:ALA:H	2.12	0.48
6:7:317:ALA:HB2	6:7:561:ARG:HA	1.95	0.48
6:7:388:SER:OG	6:7:445:ASP:OD2	2.22	0.48
6:7:614:THR:HA	6:7:625:VAL:HG21	1.95	0.48
9:A:197:ARG:CG	9:A:200:ILE:HD12	2.43	0.48
13:N:104:TYR:HD1	13:N:105:LEU:HD22	1.79	0.48
13:N:107:CYS:SG	13:N:108:ARG:N	2.86	0.48
1:2:184:PHE:HD2	1:2:247:VAL:HG21	1.79	0.48
2:3:375:ALA:CB	7:X:9:DT:H5"	2.43	0.48
3:4:316:THR:HG21	3:4:331:CYS:HB2	1.94	0.48
4:5:444:PHE:HE1	4:5:501:ILE:HD11	1.78	0.48
6:7:38:VAL:HG22	6:7:42:HIS:CE1	2.49	0.48
6:7:387:LYS:NZ	6:7:388:SER:OG	2.40	0.48
1:2:487:GLY:O	1:2:756:ARG:NH2	2.47	0.48
3:4:200:LEU:HD11	3:4:248:PHE:HD1	1.79	0.48
5:6:253:GLY:O	5:6:257:ARG:NH2	2.46	0.48
5:6:436:ILE:HD13	5:6:479:ALA:HB3	1.96	0.48
6:7:464:GLN:HG2	6:7:465:GLN:HG2	1.96	0.48
6:7:588:LEU:HD11	6:7:637:LEU:HD21	1.94	0.48
14:3:901:ATP:C8	4:5:609:VAL:HG11	2.49	0.48
3:4:634:ASP:N	3:4:634:ASP:OD1	2.45	0.48
1:2:731:SER:CB	1:2:736:SER:HB3	2.44	0.48
1:2:755:ALA:HB1	1:2:760:ARG:HB3	1.95	0.48
2:3:301:SER:HB3	4:5:364:ASP:OD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:354:LEU:HD13	2:3:362:PRO:HD2	1.95	0.48
4:5:592:ALA:HB1	4:5:604:SER:CB	2.43	0.48
6:7:235:VAL:HG12	6:7:236:LYS:H	1.78	0.48
6:7:240:HIS:HB3	6:7:243:GLN:NE2	2.28	0.48
6:7:280:LEU:HB3	6:7:295:GLU:O	2.13	0.48
6:7:364:LYS:HD3	6:7:365:ARG:H	1.79	0.48
6:7:499:ARG:HA	6:7:499:ARG:NE	2.28	0.48
6:7:619:LEU:HD12	6:7:620:ARG:N	2.28	0.48
9:A:470:PHE:CD2	9:A:479:LEU:HD11	2.49	0.48
9:A:491:SER:O	9:A:491:SER:OG	2.27	0.48
2:3:432:GLY:C	2:3:433:ILE:HD12	2.34	0.48
6:7:569:LYS:HG2	6:7:621:LEU:HA	1.96	0.48
9:A:259:GLU:N	9:A:259:GLU:OE1	2.45	0.48
9:A:387:ALA:O	9:A:390:VAL:N	2.46	0.48
1:2:712:LEU:HD23	1:2:713:THR:O	2.13	0.47
2:3:20:LEU:HD23	2:3:30:ALA:HB2	1.96	0.47
3:4:368:GLN:OE1	6:7:400:ARG:NH2	2.37	0.47
5:6:448:ILE:HG23	5:6:490:SER:O	2.13	0.47
5:6:580:GLN:O	5:6:584:HIS:N	2.44	0.47
6:7:533:LEU:HA	6:7:536:HIS:ND1	2.29	0.47
6:7:604:ARG:NH1	6:7:607:LEU:HB2	2.29	0.47
9:A:21:ILE:HD12	9:A:21:ILE:N	2.29	0.47
12:M:16:ILE:O	12:M:16:ILE:HG22	2.13	0.47
2:3:342:PRO:HB3	14:3:901:ATP:O3G	2.13	0.47
2:3:385:GLU:OE1	2:3:385:GLU:HA	2.15	0.47
2:3:544:LEU:HD11	2:3:554:GLU:OE2	2.14	0.47
6:7:149:ILE:O	6:7:152:VAL:HG22	2.14	0.47
6:7:378:CYS:CB	6:7:486:ALA:HB3	2.44	0.47
6:7:555:ASP:O	6:7:559:MET:N	2.36	0.47
6:7:609:ILE:HA	6:7:612:LEU:HD21	1.94	0.47
6:7:613:SER:HA	6:7:629:ASP:OD1	2.14	0.47
10:H:103:ILE:HG13	10:H:192:LEU:HD21	1.95	0.47
11:L:164:LEU:HD12	11:L:167:ILE:CD1	2.41	0.47
1:2:199:THR:O	1:2:203:ARG:N	2.32	0.47
1:2:776:LEU:HA	1:2:790:LYS:NZ	2.29	0.47
2:3:333:ASP:OD1	2:3:333:ASP:N	2.47	0.47
2:3:533:LYS:HG2	12:M:100:TYR:HB2	1.97	0.47
3:4:509:LEU:CD1	3:4:617:ALA:HB3	2.44	0.47
4:5:310:ASN:OD1	12:M:141:GLN:NE2	2.46	0.47
5:6:91:TYR:O	5:6:95:ARG:NH2	2.47	0.47
5:6:471:GLN:O	5:6:473:THR:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:415:THR:CB	6:7:469:ILE:HG13	2.44	0.47
6:7:529:ASN:HB2	6:7:532:ARG:HH11	1.79	0.47
7:X:-5:DC:H2"	7:X:-4:DG:O4'	2.14	0.47
9:A:300:THR:OG1	9:A:338:ALA:HB1	2.14	0.47
1:2:398:GLU:N	1:2:430:VAL:O	2.38	0.47
3:4:369:THR:HG21	6:7:430:GLU:HA	1.96	0.47
3:4:454:LEU:C	3:4:460:ILE:HD12	2.35	0.47
4:5:20:GLN:C	4:5:25:ILE:HD13	2.35	0.47
4:5:49:LYS:HG2	4:5:51:ARG:HD3	1.95	0.47
5:6:542:ARG:HA	5:6:545:VAL:HG23	1.96	0.47
9:A:333:LEU:HD11	9:A:345:MET:CE	2.43	0.47
1:2:460:GLU:OE1	1:2:460:GLU:N	2.47	0.47
2:3:633:ILE:O	2:3:636:ALA:HB3	2.14	0.47
4:5:24:GLN:OE1	4:5:86:GLN:NE2	2.48	0.47
4:5:358:SER:N	4:5:620:GLU:OE2	2.47	0.47
6:7:206:CYS:CB	6:7:211:CYS:HB3	2.28	0.47
6:7:510:ALA:O	6:7:513:SER:OG	2.27	0.47
6:7:581:ILE:HG13	6:7:582:VAL:N	2.30	0.47
9:A:82:ASP:O	9:A:85:GLU:N	2.40	0.47
10:H:81:LEU:O	10:H:85:LEU:HD23	2.15	0.47
12:M:94:LEU:HD21	12:M:99:PRO:HA	1.96	0.47
1:2:479:ALA:CB	1:2:644:VAL:HG11	2.45	0.47
2:3:308:VAL:HG12	2:3:312:ILE:HD11	1.96	0.47
2:3:529:SER:OG	2:3:530:GLU:N	2.47	0.47
4:5:469:ALA:O	4:5:471:ILE:N	2.43	0.47
1:2:470:ILE:HD13	14:2:901:ATP:HN61	1.80	0.47
1:2:573:GLU:OE2	1:2:616:ASN:ND2	2.48	0.47
1:2:645:LEU:O	1:2:645:LEU:HG	2.14	0.47
2:3:464:ILE:HG22	2:3:466:LEU:HD21	1.96	0.47
2:3:477:LEU:HD11	2:3:606:PRO:CD	2.45	0.47
3:4:228:GLN:O	3:4:236:VAL:HG21	2.15	0.47
3:4:375:LEU:CD2	3:4:421:VAL:HG12	2.45	0.47
6:7:77:PHE:CZ	6:7:81:ILE:HD11	2.50	0.47
6:7:305:CYS:N	6:7:311:GLU:OE2	2.48	0.47
6:7:397:LEU:HD22	6:7:560:ARG:CZ	2.44	0.47
6:7:402:GLN:NE2	6:7:436:LEU:HD23	2.30	0.47
6:7:467:ILE:CG2	6:7:478:LEU:HD22	2.44	0.47
6:7:467:ILE:HG21	6:7:478:LEU:HD22	1.96	0.47
6:7:511:LEU:HD22	6:7:515:PHE:CZ	2.49	0.47
6:7:512:LEU:HB3	6:7:600:PHE:CZ	2.50	0.47
8:Y:12:DG:H2"	8:Y:13:DA:C5'	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:318:LEU:H	9:A:318:LEU:HD12	1.80	0.47
11:L:153:ILE:HG23	11:L:157:ARG:HH21	1.80	0.47
2:3:138:VAL:HB	6:7:292:LEU:HD23	1.95	0.47
3:4:168:PHE:HD2	3:4:225:LEU:HD21	1.79	0.47
6:7:14:LYS:HD3	6:7:80:VAL:HG13	1.97	0.47
6:7:337:ALA:CA	6:7:355:LEU:HD12	2.45	0.47
6:7:446:GLU:HA	6:7:446:GLU:OE1	2.15	0.47
6:7:566:CYS:O	6:7:618:ARG:HB3	2.14	0.47
7:X:-3:DA:C8	7:X:-2:DT:H72	2.50	0.47
9:A:187:GLN:OE1	9:A:191:ARG:NH1	2.47	0.47
10:H:16:LEU:HD21	10:H:19:LEU:HD23	1.96	0.47
10:H:23:SER:OG	10:H:24:GLN:N	2.47	0.47
10:H:98:GLU:O	10:H:145:ASN:ND2	2.47	0.47
11:L:103:ALA:C	11:L:107:VAL:HG23	2.35	0.47
1:2:534:GLN:HA	1:2:577:MET:HG3	1.97	0.47
2:3:29:TYR:O	2:3:33:VAL:HG11	2.15	0.47
2:3:33:VAL:O	2:3:37:ILE:HD11	2.14	0.47
2:3:348:GLN:HG2	14:3:901:ATP:O2'	2.14	0.47
4:5:382:THR:HG21	4:5:517:VAL:CG1	2.45	0.47
12:M:28:ASN:OD1	12:M:70:THR:HG22	2.15	0.47
1:2:627:THR:OG1	1:2:630:GLU:OE1	2.32	0.47
2:3:576:LEU:HD12	2:3:577:GLY:N	2.30	0.47
4:5:585:TYR:CB	4:5:612:LEU:HD11	2.45	0.47
5:6:387:VAL:HG22	5:6:495:ALA:HB3	1.97	0.47
6:7:52:LEU:HD12	6:7:141:LEU:HB3	1.97	0.47
6:7:76:ILE:O	6:7:80:VAL:HG23	2.15	0.47
6:7:208:SER:OG	6:7:209:ASP:N	2.48	0.47
9:A:99:ASP:OD1	9:A:100:SER:N	2.48	0.47
13:N:114:THR:O	13:N:117:GLN:NE2	2.48	0.47
3:4:658:GLU:HB2	6:7:593:ARG:HH11	1.80	0.46
3:4:722:VAL:HG11	3:4:731:ALA:HB3	1.97	0.46
4:5:132:ILE:HD12	4:5:226:GLU:CB	2.44	0.46
4:5:388:LEU:HD23	4:5:440:CYS:SG	2.55	0.46
4:5:456:HIS:O	4:5:510:ARG:NE	2.48	0.46
4:5:527:ILE:O	4:5:530:ALA:HB3	2.14	0.46
4:5:614:ALA:HA	4:5:617:ARG:NE	2.28	0.46
1:2:552:ARG:NH1	1:2:553:GLU:OE2	2.48	0.46
3:4:289:SER:OG	3:4:391:VAL:O	2.30	0.46
6:7:66:VAL:HG12	6:7:70:CYS:HA	1.97	0.46
6:7:337:ALA:HB2	6:7:355:LEU:HD12	1.96	0.46
6:7:415:THR:CG2	6:7:469:ILE:HG13	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:597:SER:OG	1:2:598:LYS:N	2.48	0.46
3:4:703:THR:O	3:4:755:VAL:N	2.48	0.46
4:5:585:TYR:CD1	4:5:612:LEU:HG	2.50	0.46
5:6:125:ILE:N	5:6:125:ILE:HD12	2.30	0.46
5:6:354:ASP:O	5:6:358:ARG:NE	2.48	0.46
3:4:331:CYS:HB3	3:4:340:PHE:CE2	2.49	0.46
5:6:381:ASP:O	5:6:618:ARG:NH1	2.47	0.46
6:7:28:LYS:NZ	6:7:32:VAL:HG22	2.31	0.46
6:7:467:ILE:HG22	6:7:478:LEU:HB3	1.96	0.46
6:7:575:ASP:HA	6:7:578:THR:CG2	2.44	0.46
10:H:29:PHE:O	10:H:109:GLN:NE2	2.48	0.46
2:3:192:ASP:CG	6:7:154:ALA:HB2	2.35	0.46
2:3:354:LEU:HD13	2:3:362:PRO:CD	2.46	0.46
2:3:593:SER:OG	2:3:594:GLN:N	2.48	0.46
3:4:172:ILE:HG22	3:4:196:TYR:CE2	2.51	0.46
3:4:316:THR:HG23	3:4:331:CYS:HB2	1.94	0.46
4:5:431:MET:HE1	4:5:439:VAL:HG21	1.96	0.46
6:7:173:VAL:C	6:7:174:LYS:HD2	2.36	0.46
6:7:244:VAL:HG13	6:7:245:PRO:HD2	1.98	0.46
6:7:366:PRO:CD	6:7:371:ILE:HG12	2.46	0.46
6:7:516:ASP:OD1	6:7:517:LEU:N	2.48	0.46
10:H:167:GLU:HG2	10:H:176:LEU:HD22	1.98	0.46
1:2:374:ARG:HG3	1:2:375:ILE:H	1.81	0.46
1:2:442:THR:HG21	1:2:445:ASP:HB2	1.98	0.46
1:2:776:LEU:HA	1:2:790:LYS:HE2	1.97	0.46
5:6:58:SER:OG	5:6:110:GLU:OE1	2.26	0.46
9:A:546:LEU:HD12	9:A:547:LEU:H	1.81	0.46
11:L:48:MET:O	11:L:51:HIS:N	2.48	0.46
1:2:605:LEU:HD12	1:2:606:GLN:H	1.80	0.46
2:3:338:LEU:HD21	2:3:478:PHE:HB3	1.98	0.46
5:6:93:LYS:N	5:6:98:LEU:HD13	2.31	0.46
5:6:198:GLN:NE2	5:6:222:LEU:HD12	2.31	0.46
6:7:340:LEU:HA	6:7:393:TYR:HE2	1.79	0.46
6:7:385:VAL:HG23	6:7:387:LYS:HB3	1.97	0.46
1:2:734:THR:OG1	1:2:735:GLY:N	2.48	0.46
3:4:436:GLU:OE1	3:4:436:GLU:N	2.49	0.46
6:7:308:LYS:N	6:7:308:LYS:HD2	2.30	0.46
9:A:83:ILE:O	9:A:87:LEU:N	2.42	0.46
9:A:462:VAL:HA	9:A:504:SER:HB3	1.97	0.46
11:L:16:SER:HA	11:L:43:PHE:HA	1.98	0.46
13:N:216:VAL:HG11	13:N:219:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:163:GLU:OE1	2:3:163:GLU:N	2.49	0.46
3:4:227:ARG:HA	3:4:230:ILE:HD12	1.96	0.46
3:4:256:LEU:HD12	3:4:258:GLU:OE2	2.15	0.46
4:5:131:ASN:O	4:5:134:GLN:NE2	2.49	0.46
4:5:397:ILE:HG23	4:5:437:GLY:CA	2.46	0.46
5:6:370:LYS:HB2	5:6:378:LEU:HD11	1.96	0.46
6:7:276:VAL:HG12	6:7:278:LEU:HD12	1.98	0.46
6:7:386:ALA:HB2	15:7:801:ADP:C2	2.51	0.46
6:7:495:TYR:OH	6:7:644:LEU:HB2	2.16	0.46
11:L:20:ASN:OD1	11:L:59:ARG:NH1	2.48	0.46
12:M:30:LYS:O	12:M:31:LEU:HD23	2.15	0.46
1:2:577:MET:H	1:2:582:ARG:HH22	1.64	0.46
1:2:602:VAL:HG21	4:5:408:SER:HA	1.97	0.46
3:4:285:LEU:C	3:4:286:ILE:HD12	2.36	0.46
3:4:407:LEU:CD2	7:X:3:DT:H5’	2.36	0.46
3:4:670:SER:O	3:4:674:VAL:HG22	2.16	0.46
5:6:190:GLU:OE2	5:6:190:GLU:N	2.48	0.46
5:6:451:ILE:HB	5:6:454:PHE:HE1	1.81	0.46
6:7:166:ILE:O	6:7:238:GLN:N	2.40	0.46
6:7:585:TYR:OH	6:7:605:ASN:HB2	2.16	0.46
9:A:17:LYS:HB2	10:H:155:ILE:HD11	1.98	0.46
12:M:127:GLN:O	12:M:131:HIS:N	2.49	0.46
2:3:322:LYS:HE2	2:3:330:LEU:HD22	1.97	0.45
6:7:172:GLU:O	6:7:423:LEU:HD21	2.16	0.45
6:7:443:CYS:O	6:7:444:ILE:HD13	2.17	0.45
6:7:509:ALA:CA	6:7:512:LEU:HD13	2.35	0.45
6:7:577:LEU:HB3	6:7:581:ILE:HG23	1.98	0.45
7:X:-7:DA:H2”	7:X:-6:DT:C6	2.51	0.45
7:X:9:DT:H2”	7:X:10:DT:OP2	2.16	0.45
9:A:19:ILE:HG22	9:A:21:ILE:HD11	1.98	0.45
9:A:36:LEU:HD22	9:A:39:LEU:HD12	1.98	0.45
9:A:318:LEU:O	9:A:321:GLU:N	2.48	0.45
9:A:568:ASP:HA	9:A:571:THR:HG23	1.97	0.45
12:M:150:ASP:OD1	12:M:151:ASN:N	2.49	0.45
1:2:269:ARG:NH2	1:2:387:LEU:HD21	2.30	0.45
1:2:383:LEU:HD23	1:2:383:LEU:N	2.31	0.45
2:3:499:MET:O	2:3:503:ARG:HG2	2.16	0.45
4:5:594:GLN:OE1	4:5:598:ALA:HB2	2.16	0.45
6:7:167:VAL:CG1	6:7:267:PRO:HA	2.46	0.45
6:7:361:GLY:O	6:7:618:ARG:NH1	2.47	0.45
6:7:460:GLU:OE1	6:7:466:THR:OG1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:506:ILE:HG22	1:2:646:CYS:HB2	1.99	0.45
5:6:92:VAL:HG12	5:6:98:LEU:HD12	1.98	0.45
6:7:337:ALA:CB	6:7:355:LEU:HD12	2.46	0.45
9:A:216:LEU:CD2	9:A:261:ILE:HD11	2.47	0.45
1:2:549:PRO:O	1:2:552:ARG:NH2	2.49	0.45
3:4:226:TYR:CZ	3:4:230:ILE:HD11	2.52	0.45
3:4:658:GLU:CB	6:7:593:ARG:HH11	2.29	0.45
4:5:580:LYS:NZ	4:5:633:ASP:OD1	2.49	0.45
6:7:160:LEU:HA	6:7:275:GLY:O	2.16	0.45
6:7:181:THR:HG22	6:7:191:THR:O	2.16	0.45
6:7:269:ASP:O	6:7:271:ILE:HG23	2.15	0.45
6:7:334:GLU:CD	6:7:337:ALA:HB3	2.37	0.45
6:7:556:MET:O	6:7:559:MET:HB2	2.16	0.45
9:A:91:ASP:OD1	9:A:92:ASP:N	2.45	0.45
4:5:348:LYS:CB	4:5:642:LEU:HD21	2.47	0.45
5:6:560:THR:O	5:6:564:VAL:HG23	2.16	0.45
6:7:469:ILE:CB	6:7:476:THR:HG21	2.47	0.45
10:H:49:VAL:HG12	10:H:52:ALA:HB2	1.99	0.45
1:2:307:LEU:HD12	1:2:307:LEU:N	2.31	0.45
1:2:629:SER:HB2	1:2:737:LEU:HD21	1.97	0.45
3:4:211:LEU:HD23	3:4:212:ASN:CA	2.46	0.45
3:4:309:CYS:SG	3:4:311:ILE:N	2.90	0.45
3:4:401:PRO:O	3:4:402:LEU:HD12	2.17	0.45
3:4:472:ILE:HG23	15:4:901:ADP:HN62	1.82	0.45
5:6:42:ARG:HA	5:6:45:ALA:HB3	1.99	0.45
5:6:117:VAL:O	5:6:120:LEU:HD11	2.17	0.45
6:7:159:LYS:HE3	6:7:159:LYS:HB2	1.72	0.45
6:7:235:VAL:HG12	6:7:236:LYS:N	2.32	0.45
6:7:386:ALA:HB2	15:7:801:ADP:N3	2.31	0.45
9:A:49:VAL:O	10:H:158:ARG:NH2	2.48	0.45
1:2:300:THR:HG21	1:2:360:LYS:O	2.17	0.45
1:2:435:LYS:HE3	1:2:527:ARG:HG3	1.99	0.45
2:3:123:CYS:HB2	2:3:235:VAL:HG22	1.99	0.45
3:4:513:ASP:O	3:4:518:LYS:NZ	2.49	0.45
6:7:22:LYS:NZ	6:7:53:ASP:OD1	2.49	0.45
6:7:478:LEU:HD23	6:7:480:ALA:N	2.31	0.45
6:7:645:ASN:ND2	6:7:646:GLN:HG2	2.32	0.45
2:3:591:LEU:HD21	2:3:607:ILE:HD12	1.98	0.45
3:4:545:LEU:O	3:4:564:ALA:N	2.45	0.45
4:5:52:ASP:N	4:5:52:ASP:OD1	2.50	0.45
4:5:451:ASP:N	4:5:451:ASP:OD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:366:PRO:HD2	6:7:370:LYS:HA	1.99	0.45
6:7:372:ARG:HE	6:7:464:GLN:CB	2.27	0.45
8:Y:9:DA:H2'	8:Y:10:DT:H72	1.98	0.45
9:A:546:LEU:C	9:A:547:LEU:HD12	2.37	0.45
10:H:148:ARG:HA	10:H:151:LYS:HZ1	1.81	0.45
1:2:512:THR:O	1:2:514:LYS:NZ	2.35	0.45
2:3:338:LEU:HD21	2:3:479:VAL:N	2.31	0.45
4:5:394:VAL:HG13	4:5:555:LEU:HB2	1.98	0.45
4:5:589:ARG:CB	4:5:607:ILE:HG21	2.26	0.45
5:6:130:ARG:C	5:6:131:ILE:HD12	2.37	0.45
5:6:544:ILE:HA	5:6:547:LEU:HD12	1.99	0.45
6:7:309:ASN:HB3	6:7:311:GLU:OE1	2.17	0.45
6:7:512:LEU:HA	6:7:515:PHE:CD1	2.52	0.45
7:X:6:DT:H2"	7:X:8:DT:C7	2.47	0.45
7:X:8:DT:C2'	7:X:9:DT:H71	2.40	0.45
2:3:342:PRO:O	2:3:343:SER:OG	2.27	0.45
5:6:373:THR:HG23	5:6:375:LYS:HB2	1.99	0.45
6:7:529:ASN:OD1	6:7:533:LEU:HG	2.17	0.45
9:A:244:LEU:O	9:A:246:LEU:N	2.50	0.45
12:M:15:ASP:O	12:M:18:VAL:HG21	2.17	0.45
13:N:55:ILE:HD11	13:N:108:ARG:NH2	2.32	0.45
1:2:657:ASP:O	1:2:660:LEU:HD23	2.17	0.44
2:3:521:ASP:O	10:H:36:GLN:NE2	2.50	0.44
4:5:416:MET:HG2	4:5:427:GLU:OE1	2.17	0.44
5:6:132:SER:OG	5:6:133:GLY:N	2.49	0.44
6:7:151:GLU:O	6:7:151:GLU:HG2	2.17	0.44
6:7:222:LEU:HD23	6:7:223:GLN:N	2.31	0.44
6:7:378:CYS:HA	6:7:486:ALA:C	2.37	0.44
6:7:386:ALA:C	6:7:390:LEU:HD12	2.38	0.44
6:7:518:LEU:HD23	6:7:518:LEU:H	1.83	0.44
7:X:10:DT:H6	7:X:10:DT:H2'	1.67	0.44
13:N:112:ILE:HG23	13:N:119:ILE:HD13	1.99	0.44
2:3:343:SER:HA	14:3:901:ATP:H5'1	1.99	0.44
3:4:213:LEU:HD11	3:4:218:LEU:CD1	2.47	0.44
4:5:165:ILE:HG23	4:5:208:PHE:O	2.17	0.44
4:5:355:PHE:CE2	4:5:625:ILE:HG12	2.52	0.44
5:6:156:GLN:OE1	5:6:156:GLN:N	2.47	0.44
5:6:157:THR:HG21	5:6:185:PHE:CD2	2.52	0.44
5:6:572:ARG:O	5:6:574:PHE:N	2.50	0.44
6:7:343:GLU:HB3	6:7:546:GLN:HB3	1.97	0.44
9:A:139:GLY:N	9:A:164:GLN:OE1	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:214:SER:OG	1:2:386:ASP:OD1	2.35	0.44
1:2:508:GLY:HA3	1:2:648:VAL:HG22	1.99	0.44
2:3:470:LEU:O	2:3:473:ARG:N	2.50	0.44
3:4:400:THR:N	3:4:416:LYS:O	2.51	0.44
3:4:673:TYR:CE1	6:7:573:ILE:HB	2.46	0.44
4:5:252:VAL:HA	4:5:307:ARG:HH11	1.83	0.44
6:7:152:VAL:HA	6:7:156:HIS:ND1	2.31	0.44
6:7:173:VAL:HB	6:7:262:THR:HG21	1.99	0.44
6:7:224:THR:HA	6:7:227:SER:HB3	1.99	0.44
6:7:287:GLN:N	6:7:287:GLN:OE1	2.50	0.44
6:7:359:VAL:HG13	6:7:360:GLY:H	1.83	0.44
6:7:634:LEU:HD12	6:7:635:ARG:N	2.33	0.44
13:N:24:ASP:N	13:N:24:ASP:OD1	2.50	0.44
2:3:357:ALA:HB1	2:3:358:PRO:HD2	2.00	0.44
2:3:492:ILE:O	2:3:496:VAL:HG23	2.17	0.44
3:4:323:GLY:HA2	5:6:258:ALA:HB2	2.00	0.44
3:4:713:ILE:HG22	3:4:713:ILE:O	2.17	0.44
5:6:386:ILE:CD1	5:6:398:LEU:HD21	2.47	0.44
6:7:164:ARG:HG2	6:7:272:VAL:HG22	1.99	0.44
6:7:402:GLN:OE1	6:7:437:ALA:N	2.51	0.44
6:7:435:VAL:HG22	6:7:478:LEU:CD1	2.47	0.44
9:A:313:LEU:HD21	9:A:365:ASP:HB3	1.98	0.44
9:A:347:LEU:HD23	9:A:350:ARG:NH1	2.31	0.44
9:A:457:SER:O	9:A:499:LEU:HD22	2.18	0.44
9:A:457:SER:C	9:A:499:LEU:HD13	2.38	0.44
12:M:103:GLU:OE2	12:M:152:ILE:HD13	2.16	0.44
1:2:776:LEU:HA	1:2:790:LYS:CE	2.47	0.44
2:3:313:LEU:O	2:3:316:LEU:N	2.51	0.44
6:7:84:LEU:C	6:7:85:LEU:HD12	2.38	0.44
6:7:261:VAL:O	6:7:264:MET:HB2	2.18	0.44
6:7:438:ASP:HB2	6:7:481:ARG:HG2	1.99	0.44
6:7:453:GLN:O	6:7:456:THR:OG1	2.26	0.44
6:7:591:GLU:O	6:7:594:ASN:ND2	2.51	0.44
9:A:81:VAL:O	9:A:108:ASN:ND2	2.49	0.44
13:N:171:ARG:O	13:N:172:ILE:HD12	2.17	0.44
2:3:127:ILE:O	2:3:198:ILE:HG23	2.18	0.44
2:3:262:ILE:HD12	2:3:262:ILE:N	2.33	0.44
2:3:565:TYR:CE1	2:3:569:ALA:HB2	2.52	0.44
3:4:411:VAL:HG22	6:7:201:THR:HA	1.98	0.44
3:4:710:GLN:HA	3:4:713:ILE:HD12	1.99	0.44
6:7:338:THR:O	6:7:342:PRO:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:359:VAL:HG13	6:7:360:GLY:N	2.33	0.44
9:A:443:VAL:HG22	9:A:483:LEU:HD12	2.00	0.44
13:N:58:SER:N	13:N:132:ARG:O	2.50	0.44
13:N:114:THR:HG22	13:N:173:VAL:CG1	2.48	0.44
13:N:122:GLN:O	13:N:125:SER:OG	2.09	0.44
1:2:763:VAL:HG21	1:2:767:ASP:CG	2.38	0.44
2:3:77:LEU:HD23	2:3:78:LYS:N	2.33	0.44
3:4:453:LEU:HD12	3:4:456:LYS:HE2	2.00	0.44
3:4:662:LYS:HG3	6:7:582:VAL:HG23	2.00	0.44
4:5:65:LEU:HD23	4:5:65:LEU:O	2.18	0.44
4:5:443:GLU:N	4:5:443:GLU:OE1	2.51	0.44
6:7:379:LEU:HB2	6:7:487:ALA:HB1	1.99	0.44
6:7:459:HIS:CD2	6:7:511:LEU:HG	2.53	0.44
11:L:45:PRO:C	11:L:46:LEU:HD12	2.38	0.44
12:M:8:PRO:HD3	13:N:171:ARG:HE	1.83	0.44
13:N:114:THR:O	13:N:173:VAL:HG11	2.18	0.44
2:3:309:LYS:HG2	2:3:312:ILE:HD12	1.99	0.44
4:5:420:GLN:O	4:5:421:THR:OG1	2.28	0.44
5:6:404:PHE:CE1	5:6:565:LEU:HD11	2.53	0.44
6:7:160:LEU:HB2	6:7:276:VAL:HG22	2.00	0.44
6:7:539:TYR:HB3	6:7:546:GLN:NE2	2.33	0.44
6:7:559:MET:O	6:7:563:ILE:HG23	2.18	0.44
10:H:175:HIS:O	10:H:177:LYS:N	2.51	0.44
11:L:69:ASP:N	11:L:69:ASP:OD1	2.50	0.44
3:4:343:ILE:HG22	3:4:344:HIS:H	1.82	0.44
5:6:34:GLU:N	5:6:37:GLU:O	2.46	0.44
5:6:351:TYR:H	15:6:901:ADP:HN62	1.65	0.44
5:6:375:LYS:O	5:6:376:THR:OG1	2.29	0.44
6:7:136:VAL:HG12	6:7:137:GLY:O	2.18	0.44
11:L:117:ILE:HG13	11:L:118:LYS:N	2.32	0.44
13:N:112:ILE:HD13	13:N:112:ILE:N	2.33	0.44
6:7:275:GLY:CA	6:7:300:ALA:HA	2.47	0.43
6:7:354:LEU:O	6:7:357:LEU:HB2	2.17	0.43
6:7:372:ARG:HE	6:7:464:GLN:CG	2.31	0.43
6:7:527:ARG:HG2	6:7:527:ARG:O	2.18	0.43
7:X:6:DT:C2'	7:X:8:DT:H72	2.48	0.43
4:5:473:THR:O	4:5:473:THR:OG1	2.30	0.43
5:6:84:LEU:O	5:6:88:VAL:HG23	2.18	0.43
6:7:132:LYS:HB2	6:7:228:LYS:HZ1	1.83	0.43
6:7:203:VAL:HG12	6:7:207:PRO:HG3	2.00	0.43
6:7:344:ILE:HG12	6:7:345:TYR:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:536:HIS:O	6:7:546:GLN:HG3	2.17	0.43
10:H:65:PRO:O	10:H:68:ASN:N	2.48	0.43
2:3:111:ARG:CD	2:3:212:ARG:HG3	2.48	0.43
4:5:369:ARG:NH2	4:5:610:ARG:HD3	2.33	0.43
6:7:261:VAL:HA	6:7:264:MET:HE3	1.99	0.43
6:7:299:GLN:HG3	6:7:300:ALA:N	2.34	0.43
9:A:23:VAL:HA	9:A:52:ILE:HD13	1.99	0.43
12:M:88:GLU:OE2	12:M:91:HIS:N	2.51	0.43
1:2:622:TYR:CZ	1:2:647:VAL:HG11	2.54	0.43
2:3:338:LEU:HD11	2:3:478:PHE:HD2	1.84	0.43
6:7:163:VAL:HG23	6:7:273:VAL:HG13	2.00	0.43
6:7:336:LEU:HD13	6:7:554:LEU:HB3	2.01	0.43
9:A:154:HIS:O	9:A:156:ASP:N	2.51	0.43
9:A:184:ILE:HD12	9:A:187:GLN:OE1	2.18	0.43
10:H:79:ARG:CZ	10:H:82:LEU:HD22	2.48	0.43
2:3:592:ARG:HG2	2:3:607:ILE:HG21	2.00	0.43
3:4:372:ASN:ND2	6:7:428:THR:OG1	2.52	0.43
4:5:349:ALA:CB	4:5:642:LEU:HD23	2.48	0.43
4:5:596:GLU:HA	4:5:603:LEU:H	1.82	0.43
6:7:266:GLN:HG3	6:7:269:ASP:OD2	2.18	0.43
6:7:344:ILE:HA	6:7:536:HIS:CG	2.54	0.43
6:7:397:LEU:HD22	6:7:560:ARG:NE	2.33	0.43
6:7:484:ILE:HA	6:7:484:ILE:HD13	1.69	0.43
9:A:196:GLU:OE1	9:A:199:ARG:NH2	2.50	0.43
10:H:129:TYR:CZ	13:N:105:LEU:HD12	2.53	0.43
11:L:71:LEU:HB3	11:L:116:VAL:HG21	2.00	0.43
3:4:398:ARG:N	3:4:418:HIS:O	2.48	0.43
4:5:577:ALA:HA	4:5:633:ASP:HB2	2.00	0.43
5:6:306:ASP:OD1	5:6:320:GLN:N	2.51	0.43
5:6:447:GLY:C	5:6:489:THR:HG21	2.39	0.43
6:7:99:LEU:HD13	6:7:227:SER:O	2.19	0.43
6:7:184:CYS:HG	6:7:220:LEU:HD23	1.81	0.43
6:7:205:ASP:HB2	6:7:218:GLY:O	2.18	0.43
6:7:280:LEU:HD23	6:7:280:LEU:O	2.19	0.43
6:7:414:LEU:HD22	6:7:434:LEU:CD2	2.41	0.43
1:2:436:GLN:O	1:2:438:VAL:HG13	2.18	0.43
3:4:272:ARG:HH21	3:4:276:SER:HB3	1.84	0.43
4:5:150:ILE:HD11	4:5:258:VAL:HG13	2.00	0.43
4:5:476:ASN:O	4:5:477:SER:OG	2.31	0.43
5:6:206:GLN:HA	5:6:209:LEU:HD21	2.01	0.43
5:6:220:ILE:O	5:6:221:ILE:HD13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:261:VAL:O	6:7:261:VAL:HG12	2.18	0.43
6:7:327:LEU:HD23	6:7:328:ALA:N	2.34	0.43
9:A:177:LEU:HD11	9:A:182:GLN:HE21	1.82	0.43
10:H:174:ILE:HB	10:H:184:LEU:HD11	2.00	0.43
2:3:192:ASP:N	2:3:220:ASP:OD2	2.51	0.43
3:4:374:LEU:HD21	3:4:418:HIS:HA	2.01	0.43
3:4:746:HIS:NE2	3:4:762:GLU:OE2	2.52	0.43
4:5:302:ALA:HB2	4:5:560:LYS:NZ	2.34	0.43
4:5:606:PRO:O	4:5:608:THR:HG23	2.19	0.43
5:6:382:ILE:HD12	5:6:383:ASN:H	1.84	0.43
6:7:156:HIS:O	6:7:277:PHE:HB3	2.19	0.43
6:7:438:ASP:OD2	6:7:481:ARG:HG2	2.19	0.43
9:A:21:ILE:CG2	9:A:52:ILE:HD11	2.48	0.43
9:A:23:VAL:HG21	9:A:77:CYS:CB	2.48	0.43
9:A:312:GLN:C	9:A:313:LEU:HD23	2.39	0.43
12:M:27:VAL:HG21	12:M:31:LEU:HD11	2.01	0.43
1:2:192:VAL:HG13	1:2:198:TYR:HB2	1.99	0.43
2:3:569:ALA:HB1	2:3:624:ARG:HB3	2.00	0.43
4:5:371:ASP:N	4:5:371:ASP:OD1	2.51	0.43
4:5:519:ASP:OD1	4:5:519:ASP:N	2.51	0.43
6:7:376:ASN:HB3	6:7:484:ILE:CB	2.48	0.43
6:7:397:LEU:HB3	6:7:560:ARG:NH1	2.34	0.43
6:7:458:ILE:CG2	6:7:511:LEU:HD21	2.40	0.43
9:A:443:VAL:HG13	9:A:483:LEU:HD12	2.00	0.43
1:2:504:LEU:CB	1:2:644:VAL:HB	2.45	0.43
2:3:268:GLU:O	2:3:273:ILE:HD11	2.18	0.43
2:3:603:ARG:HD2	2:3:647:TYR:CE1	2.54	0.43
4:5:150:ILE:HD13	4:5:252:VAL:CG1	2.48	0.43
4:5:393:LYS:HG3	4:5:555:LEU:CD1	2.49	0.43
1:2:507:CYS:O	1:2:647:VAL:HG13	2.19	0.42
2:3:123:CYS:HA	2:3:235:VAL:HA	2.00	0.42
3:4:457:LYS:O	3:4:750:ARG:NH1	2.52	0.42
4:5:72:LEU:HD13	4:5:79:LEU:CB	2.45	0.42
4:5:125:SER:OG	4:5:126:ASN:N	2.52	0.42
6:7:293:LEU:O	6:7:293:LEU:HG	2.19	0.42
6:7:353:ALA:HA	6:7:356:LEU:CD1	2.49	0.42
6:7:499:ARG:HG2	6:7:499:ARG:NH2	2.34	0.42
6:7:509:ALA:O	6:7:512:LEU:HB2	2.19	0.42
9:A:102:ARG:N	9:A:103:PRO:HD2	2.34	0.42
9:A:197:ARG:HG3	9:A:200:ILE:HD12	2.01	0.42
1:2:437:VAL:HB	1:2:706:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:242:LEU:HD12	5:6:290:PHE:HD1	1.84	0.42
5:6:262:SER:OG	5:6:263:ARG:N	2.52	0.42
6:7:469:ILE:O	6:7:476:THR:OG1	2.31	0.42
6:7:500:THR:OG1	6:7:501:VAL:N	2.53	0.42
9:A:170:ARG:O	9:A:171:SER:OG	2.26	0.42
10:H:44:ILE:N	10:H:46:GLU:OE1	2.51	0.42
12:M:25:CYS:CB	12:M:54:LEU:HD12	2.50	0.42
3:4:396:ILE:N	3:4:420:ASP:OD1	2.46	0.42
3:4:759:ASP:OD1	3:4:760:VAL:N	2.52	0.42
4:5:136:LYS:O	4:5:139:CYS:N	2.44	0.42
4:5:589:ARG:CG	4:5:607:ILE:HD13	2.49	0.42
6:7:83:GLU:C	6:7:84:LEU:HD23	2.40	0.42
6:7:185:ASP:HB2	6:7:186:ARG:HH22	1.84	0.42
6:7:323:GLU:HG3	6:7:323:GLU:O	2.19	0.42
6:7:377:ILE:CG2	6:7:517:LEU:HB2	2.50	0.42
6:7:386:ALA:CA	6:7:389:GLN:HG3	2.49	0.42
6:7:495:TYR:OH	6:7:644:LEU:HD12	2.20	0.42
6:7:557:ASN:O	6:7:561:ARG:HG3	2.19	0.42
9:A:310:SER:O	9:A:314:LYS:N	2.41	0.42
1:2:398:GLU:O	1:2:430:VAL:N	2.44	0.42
1:2:435:LYS:HD2	1:2:527:ARG:HA	2.02	0.42
2:3:522:SER:HB2	10:H:40:GLU:HA	2.00	0.42
4:5:614:ALA:HA	4:5:617:ARG:HH21	1.85	0.42
5:6:318:LYS:HZ2	5:6:322:THR:HG21	1.84	0.42
6:7:174:LYS:CD	6:7:423:LEU:HD21	2.49	0.42
6:7:282:ARG:HH12	6:7:284:GLY:HA3	1.83	0.42
6:7:417:ALA:N	6:7:430:GLU:O	2.53	0.42
6:7:540:VAL:CG1	6:7:546:GLN:HG3	2.49	0.42
6:7:595:GLN:HB2	6:7:598:MET:CG	2.49	0.42
7:X:6:DT:H4'	7:X:8:DT:OP1	2.20	0.42
9:A:292:VAL:HG12	9:A:293:LEU:HB2	2.01	0.42
9:A:333:LEU:HD11	9:A:345:MET:HE1	2.01	0.42
12:M:27:VAL:HG13	12:M:31:LEU:HD21	2.01	0.42
1:2:192:VAL:HG13	1:2:198:TYR:N	2.34	0.42
1:2:408:ASP:OD1	1:2:411:LEU:N	2.43	0.42
2:3:81:ALA:O	2:3:85:ASP:N	2.46	0.42
2:3:353:VAL:HG12	2:3:360:ALA:HB1	2.02	0.42
2:3:476:LEU:CD2	2:3:643:VAL:HG22	2.50	0.42
2:3:620:THR:HG22	2:3:624:ARG:HE	1.83	0.42
3:4:329:THR:O	3:4:340:PHE:N	2.52	0.42
4:5:45:ASN:CA	12:M:172:GLN:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:589:ARG:HA	4:5:607:ILE:CG1	2.40	0.42
6:7:502:GLU:OE2	6:7:509:ALA:N	2.47	0.42
6:7:517:LEU:HA	6:7:517:LEU:HD23	1.58	0.42
9:A:539:ALA:HB2	9:A:546:LEU:CD2	2.49	0.42
11:L:173:THR:HG21	11:L:185:SER:C	2.40	0.42
2:3:175:ASP:OD1	2:3:176:GLU:N	2.52	0.42
3:4:602:LYS:NZ	5:6:424:ALA:HB2	2.33	0.42
4:5:323:ALA:HB1	4:5:627:LEU:HD12	2.01	0.42
6:7:168:THR:HG23	6:7:236:LYS:CB	2.48	0.42
6:7:251:ARG:HG3	6:7:252:SER:H	1.84	0.42
6:7:382:ASP:OD1	6:7:387:LYS:HG2	2.20	0.42
6:7:469:ILE:HG22	6:7:470:ALA:H	1.84	0.42
9:A:463:LEU:HD12	9:A:464:GLN:NE2	2.35	0.42
11:L:114:ARG:HA	11:L:117:ILE:HG12	2.01	0.42
12:M:46:LEU:HD23	12:M:47:GLU:HG2	2.02	0.42
12:M:173:MET:N	12:M:173:MET:SD	2.93	0.42
2:3:338:LEU:HD11	2:3:478:PHE:CD2	2.54	0.42
2:3:484:ILE:HG12	2:3:492:ILE:HD13	2.02	0.42
4:5:130:THR:HG22	4:5:131:ASN:H	1.85	0.42
4:5:518:LYS:CD	4:5:520:ILE:HD11	2.49	0.42
6:7:347:HIS:CE1	6:7:521:ILE:HG12	2.55	0.42
6:7:402:GLN:OE1	6:7:437:ALA:HB2	2.20	0.42
6:7:588:LEU:HD11	6:7:637:LEU:CD2	2.49	0.42
9:A:237:ILE:HD13	9:A:374:PHE:CD2	2.55	0.42
9:A:411:LEU:HD13	10:H:200:HIS:NE2	2.35	0.42
9:A:566:PHE:CZ	9:A:570:LEU:HD22	2.54	0.42
1:2:291:VAL:HG12	1:2:292:ARG:N	2.34	0.42
2:3:325:PRO:HD3	6:7:544:SER:HB3	2.02	0.42
3:4:601:ALA:HA	3:4:606:ILE:HG22	2.01	0.42
4:5:19:ASN:CG	4:5:25:ILE:HD11	2.40	0.42
4:5:299:SER:O	4:5:301:GLY:N	2.52	0.42
4:5:386:GLN:HE21	14:5:801:ATP:C3'	2.32	0.42
4:5:608:THR:OG1	4:5:611:GLN:HG3	2.20	0.42
4:5:613:GLU:OE1	4:5:617:ARG:NH2	2.53	0.42
5:6:223:ARG:HE	5:6:293:CYS:CB	2.33	0.42
6:7:347:HIS:CE1	6:7:385:VAL:HG12	2.53	0.42
6:7:485:LEU:HA	6:7:485:LEU:HD13	1.85	0.42
6:7:504:ASN:OD1	6:7:505:ILE:HG12	2.19	0.42
6:7:558:LEU:HD13	6:7:558:LEU:HA	1.84	0.42
9:A:536:GLU:O	9:A:539:ALA:HB3	2.20	0.42
2:3:244:LYS:NZ	4:5:160:ALA:O	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:596:GLU:HA	4:5:601:LYS:O	2.19	0.42
5:6:451:ILE:HB	5:6:454:PHE:CE1	2.54	0.42
5:6:578:ILE:HA	5:6:632:VAL:HG12	2.00	0.42
6:7:97:ASP:OD1	6:7:98:ALA:N	2.53	0.42
6:7:231:LYS:HE3	6:7:262:THR:HB	2.02	0.42
6:7:362:VAL:HG11	6:7:611:ARG:HB3	2.01	0.42
6:7:397:LEU:HD22	6:7:560:ARG:NH2	2.35	0.42
6:7:554:LEU:HD23	6:7:559:MET:CA	2.50	0.42
10:H:157:VAL:CG1	10:H:201:ILE:HD12	2.50	0.42
1:2:329:ASN:OD1	4:5:283:VAL:HG13	2.19	0.42
2:3:298:LEU:C	2:3:300:PRO:HD3	2.41	0.42
2:3:543:ALA:C	2:3:544:LEU:HD12	2.40	0.42
2:3:563:ARG:O	2:3:566:ILE:HG22	2.20	0.42
14:3:901:ATP:H8	4:5:609:VAL:HG11	1.85	0.42
3:4:346:ARG:NH1	5:6:76:GLU:OE1	2.53	0.42
4:5:104:GLU:HG2	4:5:105:ILE:HD12	2.01	0.42
4:5:165:ILE:O	4:5:169:SER:N	2.45	0.42
4:5:585:TYR:HB3	4:5:612:LEU:HD11	2.01	0.42
5:6:119:ASP:C	5:6:120:LEU:HD23	2.40	0.42
6:7:279:PRO:HA	6:7:296:THR:HG22	2.01	0.42
6:7:393:TYR:CE2	6:7:397:LEU:HD12	2.55	0.42
6:7:406:GLY:CA	6:7:450:MET:HA	2.39	0.42
10:H:50:ALA:HB3	10:H:51:GLN:NE2	2.34	0.42
10:H:136:ASN:CA	13:N:63:LEU:HD21	2.49	0.42
11:L:71:LEU:HA	11:L:74:ILE:HG22	2.00	0.42
11:L:111:GLU:HG2	11:L:112:GLU:H	1.84	0.42
12:M:15:ASP:N	12:M:15:ASP:OD1	2.41	0.42
13:N:188:ALA:HB3	13:N:192:VAL:CG1	2.50	0.42
2:3:34:LYS:O	2:3:38:ALA:N	2.53	0.41
2:3:377:VAL:HG13	7:X:8:DT:C4'	2.49	0.41
2:3:493:SER:OG	4:5:586:VAL:HG22	2.20	0.41
3:4:453:LEU:HD12	3:4:456:LYS:CE	2.50	0.41
3:4:468:ILE:HD12	3:4:479:LYS:HB3	2.02	0.41
3:4:592:VAL:O	3:4:596:GLN:N	2.53	0.41
4:5:555:LEU:HD23	4:5:556:SER:H	1.84	0.41
5:6:512:ILE:CG2	5:6:514:LEU:HD13	2.39	0.41
6:7:529:ASN:HB2	6:7:532:ARG:NH1	2.35	0.41
3:4:324:ARG:NH1	6:7:221:TYR:HB2	2.35	0.41
3:4:401:PRO:C	3:4:402:LEU:HD12	2.41	0.41
3:4:709:GLN:HG2	3:4:710:GLN:HG2	2.01	0.41
4:5:159:LYS:O	4:5:217:VAL:N	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:218:ASP:N	4:5:245:ASP:O	2.53	0.41
6:7:149:ILE:HD11	6:7:252:SER:C	2.40	0.41
6:7:282:ARG:NH1	6:7:283:THR:O	2.53	0.41
6:7:352:LYS:HZ2	6:7:356:LEU:HD21	1.86	0.41
6:7:366:PRO:HG2	6:7:369:MET:O	2.20	0.41
6:7:372:ARG:NE	6:7:464:GLN:HB2	2.31	0.41
6:7:402:GLN:CD	6:7:437:ALA:HB2	2.41	0.41
9:A:442:GLN:OE1	9:A:442:GLN:N	2.53	0.41
13:N:153:HIS:CA	13:N:157:THR:HG21	2.39	0.41
1:2:411:LEU:HD13	5:6:168:PHE:HB3	2.02	0.41
3:4:491:LYS:NZ	3:4:697:ARG:O	2.50	0.41
4:5:348:LYS:HE3	4:5:642:LEU:HD11	2.02	0.41
5:6:122:THR:O	5:6:125:ILE:HD13	2.21	0.41
5:6:264:HIS:HB2	6:7:215:LYS:HE3	2.02	0.41
6:7:336:LEU:HD11	6:7:559:MET:CG	2.30	0.41
6:7:379:LEU:CD1	6:7:387:LYS:HB2	2.47	0.41
6:7:588:LEU:CD1	6:7:637:LEU:HD21	2.49	0.41
13:N:49:GLU:OE2	13:N:108:ARG:NH1	2.46	0.41
1:2:436:GLN:HE21	1:2:438:VAL:HG12	1.84	0.41
1:2:480:LEU:O	1:2:480:LEU:HD23	2.19	0.41
1:2:502:ILE:HD11	1:2:643:ASP:OD1	2.20	0.41
2:3:406:PHE:HB2	2:3:445:ALA:HB1	2.02	0.41
2:3:565:TYR:HE1	2:3:569:ALA:HB2	1.85	0.41
4:5:121:ILE:O	4:5:122:LEU:HD12	2.19	0.41
5:6:163:GLU:OE1	5:6:164:GLN:NE2	2.53	0.41
6:7:569:LYS:NZ	6:7:623:ASP:HB2	2.35	0.41
1:2:668:HIS:HA	5:6:370:LYS:NZ	2.36	0.41
2:3:407:ASP:OD2	2:3:448:ASN:N	2.53	0.41
3:4:485:GLN:HE21	3:4:508:LEU:HD12	1.85	0.41
4:5:25:ILE:HG23	4:5:28:GLN:H	1.85	0.41
4:5:47:PHE:HZ	12:M:174:THR:HG1	1.63	0.41
4:5:502:ASP:OD1	4:5:502:ASP:N	2.53	0.41
5:6:335:ASP:OD1	5:6:335:ASP:N	2.51	0.41
6:7:155:GLN:HG2	6:7:156:HIS:CD2	2.55	0.41
6:7:174:LYS:O	6:7:232:PHE:N	2.53	0.41
6:7:375:ILE:HG12	6:7:516:ASP:CG	2.41	0.41
6:7:447:PHE:HZ	6:7:458:ILE:HG21	1.85	0.41
9:A:484:LEU:HD23	9:A:485:ARG:NH2	2.36	0.41
11:L:26:LEU:HD11	13:N:80:LEU:HD12	2.03	0.41
1:2:249:LYS:NZ	1:2:266:ILE:O	2.47	0.41
2:3:576:LEU:HD11	2:3:580:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:289:SER:OG	3:4:290:GLY:N	2.53	0.41
3:4:357:LEU:HD11	3:4:375:LEU:HB2	2.03	0.41
3:4:483:LEU:HD21	3:4:487:PHE:CE2	2.55	0.41
3:4:517:SER:O	3:4:521:MET:N	2.49	0.41
4:5:38:ILE:HG23	4:5:50:TYR:HD1	1.84	0.41
4:5:442:ASP:OD1	4:5:443:GLU:N	2.45	0.41
1:2:458:ILE:HG22	1:2:461:ARG:HH11	1.86	0.41
1:2:502:ILE:O	1:2:610:THR:HG22	2.20	0.41
2:3:476:LEU:HD22	2:3:478:PHE:CE1	2.55	0.41
3:4:276:SER:O	3:4:277:LEU:HD22	2.20	0.41
4:5:492:TRP:O	4:5:495:THR:OG1	2.33	0.41
4:5:533:ILE:O	4:5:537:HIS:N	2.51	0.41
5:6:92:VAL:HG21	5:6:102:LYS:HE3	2.02	0.41
5:6:223:ARG:H	5:6:226:LEU:HD13	1.85	0.41
6:7:60:GLU:O	6:7:63:ALA:HB3	2.20	0.41
6:7:244:VAL:HG12	6:7:245:PRO:O	2.21	0.41
6:7:352:LYS:HZ2	6:7:356:LEU:CD2	2.34	0.41
6:7:555:ASP:O	6:7:559:MET:HG3	2.19	0.41
6:7:628:ASP:O	6:7:632:GLU:HG2	2.21	0.41
7:X:-6:DT:H2'	7:X:-5:DC:C6	2.56	0.41
1:2:314:CYS:N	1:2:319:TYR:O	2.53	0.41
1:2:529:VAL:O	1:2:570:LEU:N	2.41	0.41
3:4:272:ARG:NE	3:4:276:SER:OG	2.32	0.41
4:5:194:THR:HB	4:5:202:CYS:SG	2.61	0.41
4:5:348:LYS:HB3	4:5:642:LEU:HD21	2.03	0.41
4:5:603:LEU:HD23	4:5:603:LEU:HA	1.82	0.41
6:7:132:LYS:HZ2	6:7:258:ARG:HH12	1.65	0.41
6:7:168:THR:O	6:7:236:LYS:HB2	2.21	0.41
9:A:292:VAL:HG23	9:A:306:SER:OG	2.20	0.41
9:A:546:LEU:O	9:A:547:LEU:HD12	2.21	0.41
12:M:24:GLU:OE1	12:M:24:GLU:N	2.54	0.41
1:2:529:VAL:H	1:2:569:CYS:HA	1.85	0.41
3:4:363:ASP:OD1	3:4:363:ASP:N	2.53	0.41
3:4:560:LEU:HD12	3:4:605:ILE:HG22	2.03	0.41
3:4:616:LEU:HD23	3:4:617:ALA:N	2.36	0.41
4:5:552:GLU:N	4:5:553:ILE:HG23	2.36	0.41
5:6:149:VAL:HG13	5:6:159:ILE:H	1.85	0.41
5:6:187:LEU:HD23	5:6:188:ASP:C	2.41	0.41
5:6:306:ASP:OD1	5:6:321:MET:N	2.50	0.41
6:7:160:LEU:HG	6:7:275:GLY:O	2.21	0.41
6:7:182:TYR:HA	6:7:221:TYR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:326:GLU:O	6:7:329:GLN:HB3	2.21	0.41
6:7:380:MET:O	6:7:520:LEU:HD12	2.21	0.41
6:7:401:SER:O	6:7:402:GLN:HG3	2.21	0.41
6:7:462:MET:HE2	6:7:514:ARG:HB3	2.02	0.41
6:7:508:PRO:O	6:7:511:LEU:N	2.53	0.41
6:7:556:MET:HE3	6:7:556:MET:HB2	1.96	0.41
6:7:568:ARG:HG2	6:7:568:ARG:O	2.21	0.41
6:7:640:SER:HB3	6:7:641:LYS:NZ	2.36	0.41
9:A:26:ASP:OD1	9:A:28:ASP:N	2.48	0.41
9:A:70:LYS:HA	9:A:93:VAL:HG13	2.02	0.41
10:H:157:VAL:HG11	10:H:201:ILE:HD12	2.03	0.41
1:2:256:PHE:CE2	9:A:329:LEU:HD21	2.56	0.41
2:3:151:VAL:HG23	2:3:151:VAL:O	2.21	0.41
3:4:522:LEU:CD1	3:4:616:LEU:HD21	2.37	0.41
4:5:259:LEU:HD12	4:5:259:LEU:N	2.36	0.41
4:5:622:LEU:HB3	4:5:635:HIS:NE2	2.36	0.41
5:6:325:GLU:OE1	5:6:566:ARG:NH1	2.54	0.41
6:7:14:LYS:CD	6:7:80:VAL:HG13	2.50	0.41
6:7:28:LYS:HZ1	6:7:32:VAL:HG22	1.85	0.41
6:7:139:LYS:NZ	6:7:302:ARG:HG2	2.35	0.41
6:7:215:LYS:HA	6:7:215:LYS:HD2	1.88	0.41
9:A:19:ILE:CG2	9:A:21:ILE:HD11	2.51	0.41
9:A:254:TYR:HD2	9:A:255:THR:HG23	1.86	0.41
10:H:13:PHE:O	10:H:17:LYS:HE3	2.20	0.41
13:N:70:VAL:CG2	13:N:94:LEU:HD13	2.51	0.41
1:2:219:TYR:N	1:2:272:GLU:OE1	2.54	0.40
4:5:108:PRO:HA	11:L:126:SER:HB2	2.03	0.40
4:5:544:ALA:HB3	4:5:545:PRO:HD3	2.03	0.40
4:5:596:GLU:HG3	4:5:603:LEU:H	1.85	0.40
4:5:619:SER:HB3	4:5:636:VAL:HG21	2.03	0.40
8:Y:9:DA:C2'	8:Y:10:DT:H72	2.51	0.40
1:2:414:ASP:O	5:6:248:VAL:HG23	2.21	0.40
1:2:727:LEU:HG	1:2:728:ARG:N	2.35	0.40
3:4:398:ARG:NH2	3:4:420:ASP:OD2	2.54	0.40
3:4:739:LEU:HA	3:4:742:LEU:HD12	2.02	0.40
6:7:364:LYS:O	6:7:370:LYS:HG2	2.21	0.40
9:A:46:LEU:HD21	10:H:148:ARG:HH21	1.86	0.40
9:A:138:GLU:CD	9:A:190:ARG:HE	2.20	0.40
11:L:70:ILE:O	11:L:74:ILE:HG22	2.21	0.40
2:3:134:ILE:HG22	2:3:135:ARG:N	2.36	0.40
2:3:298:LEU:HD23	2:3:298:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:458:LYS:HD2	2:3:459:THR:HG23	2.04	0.40
6:7:150:ARG:HG3	6:7:151:GLU:N	2.36	0.40
6:7:582:VAL:H	6:7:582:VAL:HG22	1.68	0.40
12:M:60:LYS:O	12:M:107:TYR:OH	2.35	0.40
13:N:61:ASP:OD1	13:N:62:MET:N	2.53	0.40
1:2:277:GLU:O	1:2:293:THR:HG23	2.21	0.40
1:2:297:VAL:CG1	1:2:361:ILE:HD11	2.51	0.40
2:3:443:VAL:O	2:3:444:LEU:HD23	2.22	0.40
3:4:355:VAL:HG12	3:4:356:LYS:N	2.36	0.40
6:7:391:LEU:HA	6:7:394:ILE:HD11	2.03	0.40
6:7:417:ALA:HA	6:7:471:LYS:NZ	2.37	0.40
10:H:93:LYS:NZ	10:H:122:TYR:OH	2.47	0.40
11:L:48:MET:O	11:L:52:LEU:HD23	2.21	0.40
4:5:464:ILE:O	4:5:475:LEU:N	2.54	0.40
5:6:139:HIS:HB3	5:6:140:PRO:CD	2.51	0.40
6:7:51:ASP:OD1	6:7:52:LEU:N	2.55	0.40
6:7:206:CYS:HB2	6:7:211:CYS:O	2.22	0.40
6:7:315:LYS:HD3	6:7:315:LYS:HA	1.72	0.40
6:7:464:GLN:NE2	6:7:465:GLN:HE21	2.19	0.40
6:7:467:ILE:O	6:7:467:ILE:HG23	2.22	0.40
9:A:123:LEU:HD23	9:A:123:LEU:O	2.21	0.40
9:A:326:GLU:O	9:A:329:LEU:HB3	2.21	0.40
10:H:157:VAL:HG21	10:H:198:LEU:HD11	2.04	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	2	599/887 (68%)	445 (74%)	148 (25%)	6 (1%)	15 53
2	3	611/819 (75%)	492 (80%)	116 (19%)	3 (0%)	29 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	4	624/866 (72%)	520 (83%)	101 (16%)	3 (0%)	29	67
4	5	608/733 (83%)	471 (78%)	134 (22%)	3 (0%)	29	67
5	6	624/817 (76%)	511 (82%)	111 (18%)	2 (0%)	41	75
6	7	623/720 (86%)	537 (86%)	85 (14%)	1 (0%)	47	79
9	A	565/575 (98%)	465 (82%)	99 (18%)	1 (0%)	47	79
10	H	193/202 (96%)	147 (76%)	46 (24%)	0	100	100
11	L	183/203 (90%)	145 (79%)	35 (19%)	3 (2%)	9	44
12	M	165/212 (78%)	122 (74%)	41 (25%)	2 (1%)	13	49
13	N	206/228 (90%)	160 (78%)	46 (22%)	0	100	100
All	All	5001/6262 (80%)	4015 (80%)	962 (19%)	24 (0%)	32	67

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	611	VAL
1	2	644	VAL
1	2	738	PRO
1	2	740	THR
1	2	575	ASP
1	2	736	SER
2	3	419	GLU
3	4	211	LEU
2	3	503	ARG
4	5	300	GLU
5	6	549	SER
11	L	81	SER
9	A	245	LEU
12	M	38	ASP
12	M	142	ALA
2	3	245	ARG
3	4	271	THR
4	5	135	LEU
6	7	383	PRO
11	L	30	TYR
4	5	206	PRO
5	6	112	PRO
3	4	639	PRO
11	L	167	ILE

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	2	534/781 (68%)	494 (92%)	40 (8%)	13 41
2	3	537/699 (77%)	503 (94%)	34 (6%)	18 46
3	4	562/759 (74%)	530 (94%)	32 (6%)	20 49
4	5	535/630 (85%)	483 (90%)	52 (10%)	8 30
5	6	551/718 (77%)	521 (95%)	30 (5%)	22 50
6	7	544/630 (86%)	512 (94%)	32 (6%)	19 48
9	A	494/501 (99%)	472 (96%)	22 (4%)	27 55
10	H	170/176 (97%)	160 (94%)	10 (6%)	19 48
11	L	170/184 (92%)	158 (93%)	12 (7%)	14 42
12	M	149/188 (79%)	141 (95%)	8 (5%)	22 50
13	N	187/205 (91%)	177 (95%)	10 (5%)	22 51
All	All	4433/5471 (81%)	4151 (94%)	282 (6%)	21 45

All (282) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	195	ARG
1	2	269	ARG
1	2	271	SER
1	2	284	LYS
1	2	290	LEU
1	2	294	LEU
1	2	314	CYS
1	2	337	CYS
1	2	383	LEU
1	2	399	VAL
1	2	423	VAL
1	2	438	VAL
1	2	442	THR
1	2	463	VAL
1	2	484	LEU

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Mol	Chain	Res	Type
1	2	488	GLU
1	2	518	LEU
1	2	531	THR
1	2	532	THR
1	2	550	VAL
1	2	561	LEU
1	2	562	VAL
1	2	565	ASP
1	2	568	VAL
1	2	585	ILE
1	2	605	LEU
1	2	608	ARG
1	2	640	SER
1	2	641	ARG
1	2	642	PHE
1	2	660	LEU
1	2	663	PHE
1	2	698	ARG
1	2	727	LEU
1	2	731	SER
1	2	743	HIS
1	2	747	VAL
1	2	768	VAL
1	2	792	ARG
1	2	793	SER
2	3	14	ARG
2	3	33	VAL
2	3	45	ILE
2	3	55	ASN
2	3	77	LEU
2	3	112	SER
2	3	123	CYS
2	3	124	VAL
2	3	129	THR
2	3	140	ARG
2	3	214	VAL
2	3	218	CYS
2	3	232	VAL
2	3	254	ARG
2	3	256	VAL
2	3	258	LEU
2	3	260	ASN

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Mol	Chain	Res	Type
2	3	275	ARG
2	3	283	LYS
2	3	301	SER
2	3	341	ASP
2	3	348	GLN
2	3	350	LEU
2	3	361	ILE
2	3	363	THR
2	3	374	THR
2	3	400	VAL
2	3	464	ILE
2	3	466	LEU
2	3	476	LEU
2	3	503	ARG
2	3	528	SER
2	3	545	LEU
2	3	578	GLU
3	4	171	PHE
3	4	200	LEU
3	4	278	ASN
3	4	303	ARG
3	4	309	CYS
3	4	331	CYS
3	4	352	LYS
3	4	354	LEU
3	4	357	LEU
3	4	363	ASP
3	4	384	LYS
3	4	419	VAL
3	4	510	LEU
3	4	516	THR
3	4	550	THR
3	4	558	LEU
3	4	576	ASP
3	4	590	HIS
3	4	593	MET
3	4	599	SER
3	4	600	ILE
3	4	607	CYS
3	4	612	ARG
3	4	638	LEU
3	4	645	ARG

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Mol	Chain	Res	Type
3	4	647	ASP
3	4	653	LEU
3	4	664	LEU
3	4	671	LEU
3	4	676	ARG
3	4	726	ARG
3	4	740	ILE
4	5	38	ILE
4	5	53	THR
4	5	65	LEU
4	5	94	PHE
4	5	112	HIS
4	5	119	ILE
4	5	130	THR
4	5	134	GLN
4	5	137	SER
4	5	143	LEU
4	5	144	VAL
4	5	151	VAL
4	5	163	MET
4	5	164	SER
4	5	172	THR
4	5	204	LEU
4	5	216	CYS
4	5	236	ILE
4	5	244	CYS
4	5	245	ASP
4	5	253	VAL
4	5	263	ILE
4	5	307	ARG
4	5	313	SER
4	5	336	LEU
4	5	344	ARG
4	5	352	CYS
4	5	385	SER
4	5	387	LEU
4	5	402	SER
4	5	432	VAL
4	5	441	ILE
4	5	443	GLU
4	5	444	PHE
4	5	448	ARG

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Mol	Chain	Res	Type
4	5	463	THR
4	5	464	ILE
4	5	466	ILE
4	5	481	VAL
4	5	502	ASP
4	5	546	SER
4	5	555	LEU
4	5	556	SER
4	5	561	TYR
4	5	565	CYS
4	5	567	THR
4	5	573	LEU
4	5	580	LYS
4	5	602	ARG
4	5	617	ARG
4	5	636	VAL
4	5	652	MET
5	6	55	LEU
5	6	62	VAL
5	6	85	CYS
5	6	100	THR
5	6	114	ARG
5	6	123	SER
5	6	132	SER
5	6	145	LEU
5	6	160	ARG
5	6	174	CYS
5	6	182	ARG
5	6	193	LEU
5	6	194	PHE
5	6	195	LEU
5	6	199	LYS
5	6	243	ILE
5	6	284	LEU
5	6	346	LEU
5	6	374	GLU
5	6	378	LEU
5	6	389	ASP
5	6	398	LEU
5	6	410	TYR
5	6	441	LEU
5	6	451	ILE

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Mol	Chain	Res	Type
5	6	476	ILE
5	6	519	MET
5	6	546	ASP
5	6	607	ARG
5	6	609	THR
6	7	43	ARG
6	7	49	THR
6	7	125	SER
6	7	163	VAL
6	7	196	ASN
6	7	198	LEU
6	7	220	LEU
6	7	257	CYS
6	7	269	ASP
6	7	277	PHE
6	7	282	ARG
6	7	319	LEU
6	7	327	LEU
6	7	343	GLU
6	7	356	LEU
6	7	365	ARG
6	7	370	LYS
6	7	372	ARG
6	7	376	ASN
6	7	380	MET
6	7	387	LYS
6	7	390	LEU
6	7	420	LYS
6	7	461	VAL
6	7	484	ILE
6	7	503	GLN
6	7	511	LEU
6	7	552	LYS
6	7	605	ASN
6	7	634	LEU
6	7	641	LYS
6	7	644	LEU
9	A	19	ILE
9	A	74	LEU
9	A	101	HIS
9	A	115	VAL
9	A	190	ARG

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Mol	Chain	Res	Type
9	A	206	GLN
9	A	207	PHE
9	A	216	LEU
9	A	234	TRP
9	A	241	THR
9	A	279	SER
9	A	289	LEU
9	A	293	LEU
9	A	312	GLN
9	A	350	ARG
9	A	369	ILE
9	A	460	TYR
9	A	492	ARG
9	A	514	CYS
9	A	529	ASN
9	A	530	PHE
9	A	551	PHE
10	H	8	PHE
10	H	16	LEU
10	H	17	LYS
10	H	61	ARG
10	H	68	ASN
10	H	79	ARG
10	H	89	CYS
10	H	143	LEU
10	H	153	LEU
10	H	195	GLN
11	L	2	ASP
11	L	29	ILE
11	L	61	VAL
11	L	75	LYS
11	L	80	ARG
11	L	106	ASP
11	L	113	LEU
11	L	114	ARG
11	L	120	ILE
11	L	127	LYS
11	L	148	LEU
11	L	164	LEU
12	M	11	TYR
12	M	15	ASP
12	M	30	LYS

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Mol	Chain	Res	Type
12	M	81	HIS
12	M	85	CYS
12	M	115	HIS
12	M	148	ARG
12	M	151	ASN
13	N	44	THR
13	N	58	SER
13	N	100	ILE
13	N	107	CYS
13	N	114	THR
13	N	148	VAL
13	N	154	LYS
13	N	174	THR
13	N	215	LEU
13	N	228	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	352	GLN
1	2	390	GLN
1	2	412	ASN
1	2	439	GLN
1	2	534	GLN
1	2	548	ASN
1	2	631	ASN
1	2	694	GLN
1	2	699	GLN
1	2	754	HIS
2	3	13	GLN
2	3	57	GLN
2	3	233	GLN
2	3	288	ASN
2	3	348	GLN
2	3	448	ASN
2	3	504	ASN
2	3	551	GLN
2	3	586	ASN
3	4	182	GLN
3	4	192	ASN
3	4	214	ASN
3	4	267	ASN

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Mol	Chain	Res	Type
3	4	326	ASN
3	4	337	ASN
3	4	344	HIS
3	4	353	GLN
3	4	378	HIS
3	4	485	GLN
3	4	527	ASN
3	4	557	GLN
3	4	561	GLN
3	4	570	ASN
3	4	620	ASN
3	4	699	HIS
3	4	714	GLN
3	4	728	GLN
3	4	735	GLN
4	5	21	GLN
4	5	60	ASN
4	5	120	GLN
4	5	131	ASN
4	5	134	GLN
4	5	334	GLN
4	5	373	ASN
4	5	386	GLN
4	5	423	ASN
4	5	595	GLN
4	5	611	GLN
5	6	198	GLN
5	6	203	GLN
5	6	364	GLN
5	6	471	GLN
5	6	533	ASN
5	6	548	HIS
5	6	550	ASN
5	6	584	HIS
6	7	193	GLN
6	7	214	ASN
6	7	243	GLN
6	7	347	HIS
6	7	374	ASN
6	7	439	GLN
6	7	453	GLN
6	7	465	GLN

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Mol	Chain	Res	Type
6	7	506	GLN
6	7	564	ASN
6	7	570	ASN
6	7	645	ASN
9	A	182	GLN
9	A	262	GLN
9	A	273	ASN
9	A	312	GLN
9	A	464	GLN
9	A	467	HIS
9	A	508	ASN
9	A	529	ASN
9	A	540	GLN
10	H	36	GLN
10	H	48	ASN
10	H	71	HIS
10	H	182	HIS
10	H	195	GLN
11	L	91	HIS
11	L	147	ASN
12	M	127	GLN
12	M	131	HIS
12	M	141	GLN
12	M	172	GLN
13	N	36	GLN
13	N	142	GLN
13	N	164	GLN
13	N	180	HIS
13	N	208	GLN
13	N	214	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)

6 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	3	901	-	26,33,33	0.94	1 (3%)	31,52,52	1.73	5 (16%)
14	ATP	2	901	-	26,33,33	0.88	1 (3%)	31,52,52	1.69	7 (22%)
15	ADP	4	901	-	24,29,29	0.90	1 (4%)	29,45,45	1.63	5 (17%)
15	ADP	6	901	-	24,29,29	0.91	1 (4%)	29,45,45	1.53	3 (10%)
15	ADP	7	801	-	24,29,29	0.93	1 (4%)	29,45,45	1.55	5 (17%)
14	ATP	5	801	-	26,33,33	0.93	1 (3%)	31,52,52	1.72	8 (25%)

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	3	901	-	-	5/18/38/38	0/3/3/3
14	ATP	2	901	-	-	7/18/38/38	0/3/3/3
15	ADP	4	901	-	-	5/12/32/32	0/3/3/3
15	ADP	6	901	-	-	4/12/32/32	0/3/3/3
15	ADP	7	801	-	-	0/12/32/32	0/3/3/3
14	ATP	5	801	-	-	3/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	7	801	ADP	C5-C4	2.55	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	3	901	ATP	C5-C4	2.46	1.47	1.40
14	5	801	ATP	C5-C4	2.44	1.47	1.40
15	6	901	ADP	C5-C4	2.30	1.47	1.40
15	4	901	ADP	C5-C4	2.26	1.46	1.40
14	2	901	ATP	C5-C4	2.06	1.46	1.40

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	4	901	ADP	PA-O3A-PB	-5.09	115.34	132.83
14	2	901	ATP	PA-O3A-PB	-4.51	117.36	132.83
14	5	801	ATP	PA-O3A-PB	-4.50	117.38	132.83
15	6	901	ADP	PA-O3A-PB	-4.44	117.58	132.83
14	3	901	ATP	PB-O3B-PG	-4.38	117.79	132.83
14	3	901	ATP	PA-O3A-PB	-4.22	118.33	132.83
14	5	801	ATP	PB-O3B-PG	-4.15	118.58	132.83
15	7	801	ADP	PA-O3A-PB	-3.93	119.36	132.83
14	2	901	ATP	N3-C2-N1	-3.87	122.62	128.68
14	3	901	ATP	N3-C2-N1	-3.67	122.95	128.68
15	4	901	ADP	C3'-C2'-C1'	3.40	106.09	100.98
15	7	801	ADP	N3-C2-N1	-3.30	123.52	128.68
15	4	901	ADP	N3-C2-N1	-3.24	123.62	128.68
15	6	901	ADP	N3-C2-N1	-3.19	123.70	128.68
15	7	801	ADP	O4'-C1'-C2'	2.94	111.23	106.93
14	2	901	ATP	C3'-C2'-C1'	2.72	105.07	100.98
14	3	901	ATP	C2-N1-C6	2.70	123.38	118.75
15	6	901	ADP	C3'-C2'-C1'	2.66	104.99	100.98
14	5	801	ATP	N3-C2-N1	-2.50	124.77	128.68
14	3	901	ATP	C3'-C2'-C1'	2.45	104.67	100.98
14	5	801	ATP	C4-C5-N7	-2.42	106.88	109.40
14	2	901	ATP	PB-O3B-PG	-2.39	124.64	132.83
14	5	801	ATP	O2A-PA-O1A	2.36	123.89	112.24
15	4	901	ADP	O4'-C4'-C3'	2.29	109.65	105.11
14	2	901	ATP	C2-N1-C6	2.18	122.48	118.75
15	7	801	ADP	O2A-PA-O1A	2.17	122.99	112.24
14	2	901	ATP	C1'-N9-C4	-2.17	122.83	126.64
15	7	801	ADP	C1'-N9-C4	2.16	130.44	126.64
14	5	801	ATP	C3'-C2'-C1'	2.15	104.22	100.98
14	5	801	ATP	C1'-N9-C4	2.08	130.29	126.64
15	4	901	ADP	C5'-C4'-C3'	-2.04	107.52	115.18
14	2	901	ATP	O2A-PA-O1A	2.04	122.32	112.24
14	5	801	ATP	O4'-C4'-C3'	2.02	109.10	105.11

There are no chirality outliers.

All (24) 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	901	ATP	C5'-O5'-PA-O1A
14	3	901	ATP	C5'-O5'-PA-O2A
15	6	901	ADP	C5'-O5'-PA-O3A
14	3	901	ATP	O4'-C4'-C5'-O5'
15	4	901	ADP	O4'-C4'-C5'-O5'
15	6	901	ADP	O4'-C4'-C5'-O5'
14	3	901	ATP	C5'-O5'-PA-O3A
15	4	901	ADP	C5'-O5'-PA-O3A
14	5	801	ATP	PG-O3B-PB-O1B
15	4	901	ADP	C5'-O5'-PA-O1A
15	6	901	ADP	C5'-O5'-PA-O1A
14	5	801	ATP	O4'-C4'-C5'-O5'
14	2	901	ATP	C4'-C5'-O5'-PA
14	3	901	ATP	C4'-C5'-O5'-PA
14	2	901	ATP	PG-O3B-PB-O1B
15	4	901	ADP	C3'-C4'-C5'-O5'
15	6	901	ADP	C3'-C4'-C5'-O5'
14	2	901	ATP	PB-O3B-PG-O3G
14	2	901	ATP	C5'-O5'-PA-O3A
14	2	901	ATP	O4'-C4'-C5'-O5'
14	5	801	ATP	PG-O3B-PB-O2B
15	4	901	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

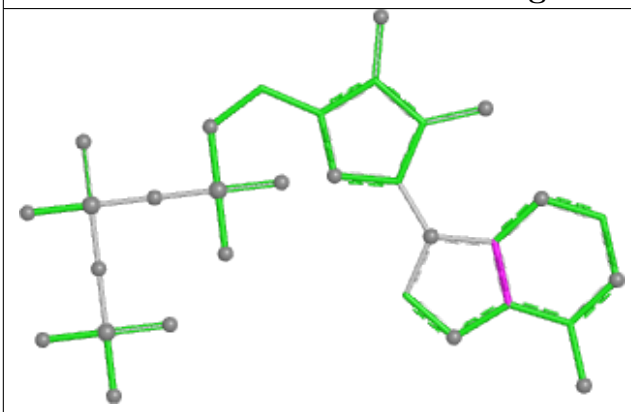
6 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	3	901	ATP	10	0
14	2	901	ATP	2	0
15	4	901	ADP	2	0
15	6	901	ADP	3	0
15	7	801	ADP	8	0
14	5	801	ATP	5	0

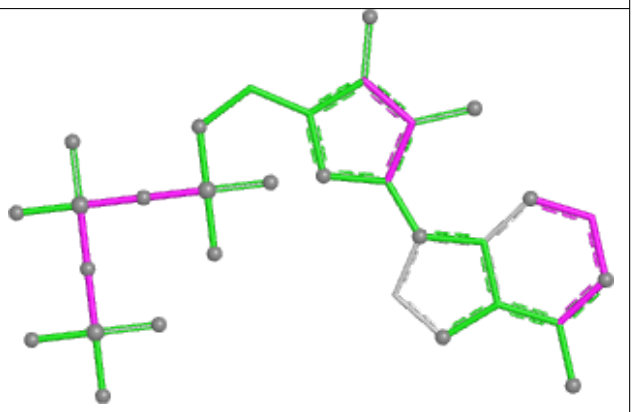
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

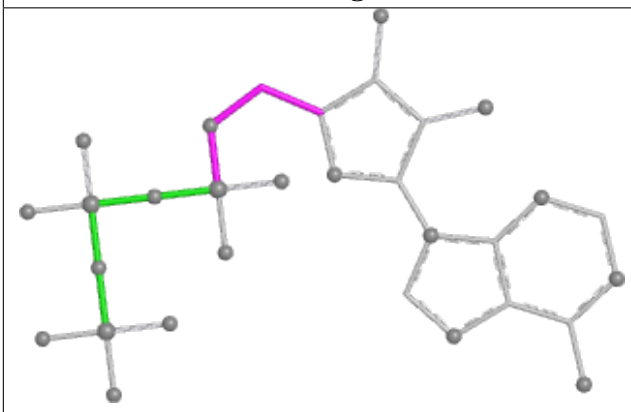
Ligand ATP 3 901



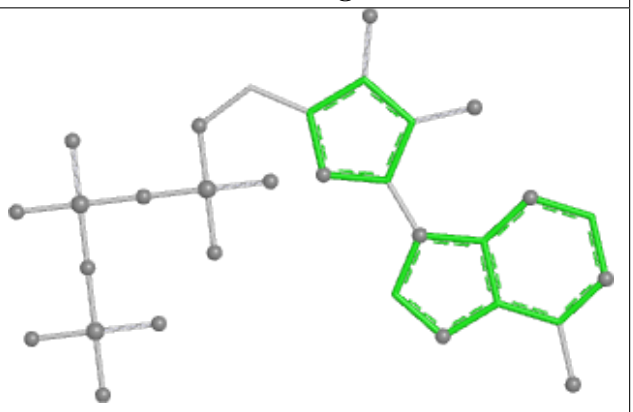
Bond lengths



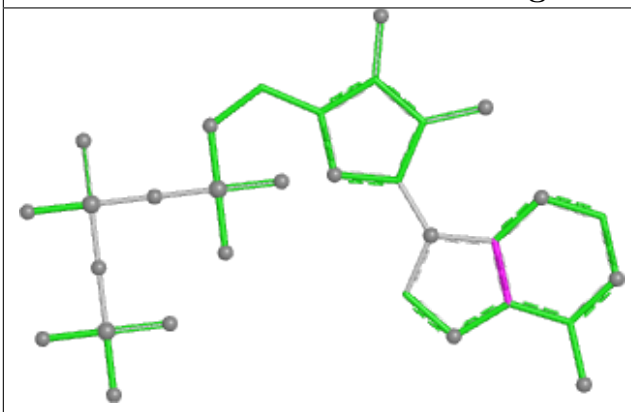
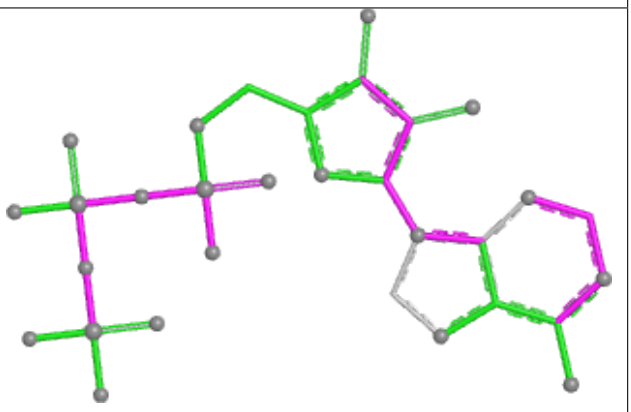
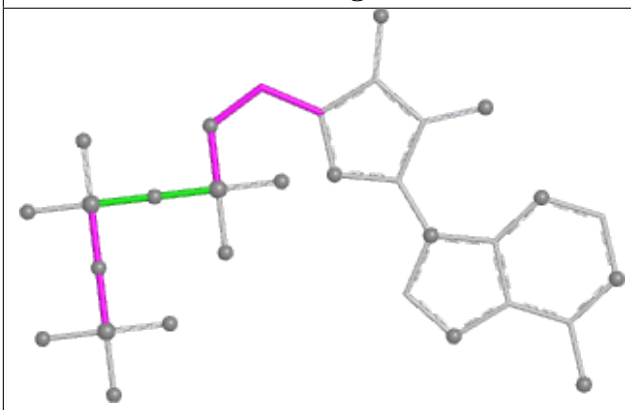
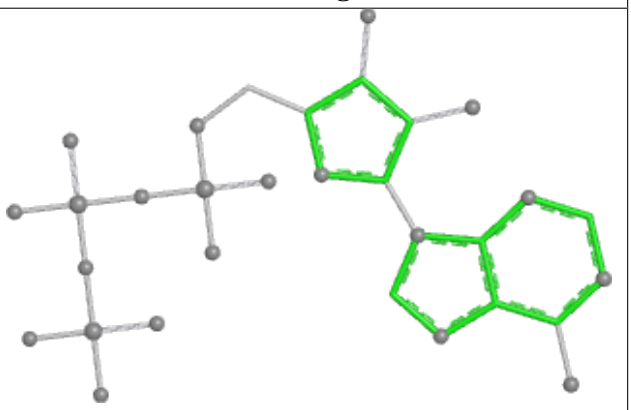
Bond angles

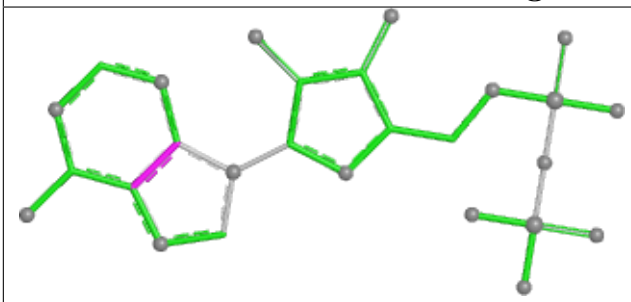
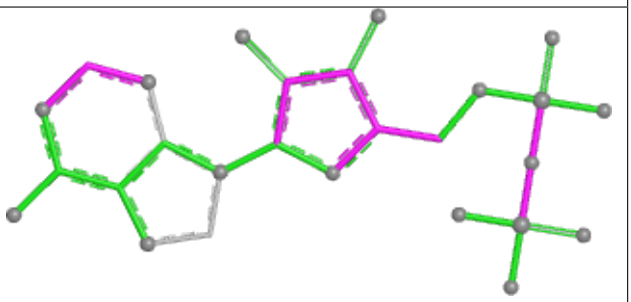
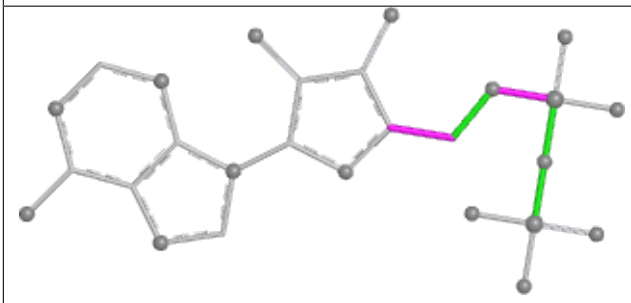
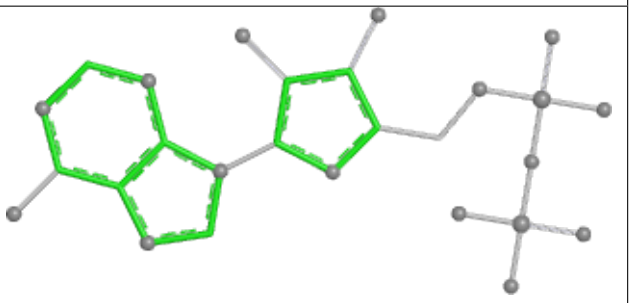


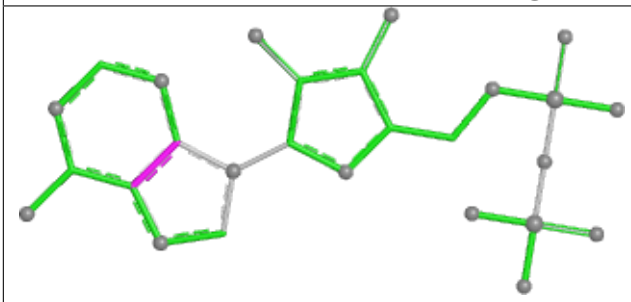
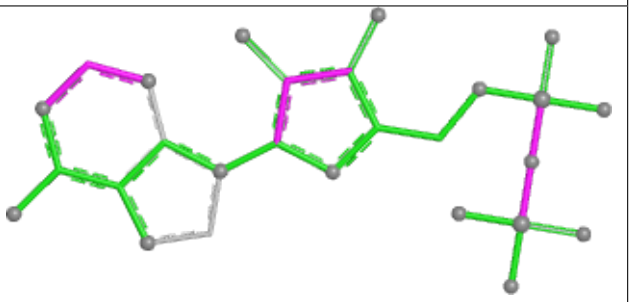
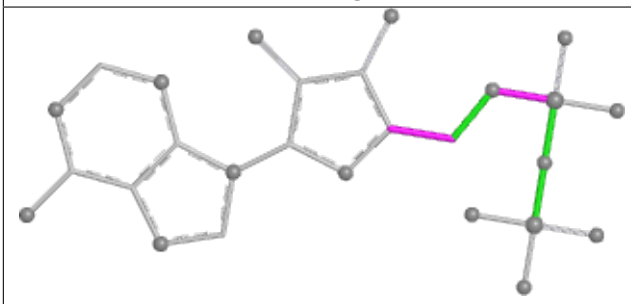
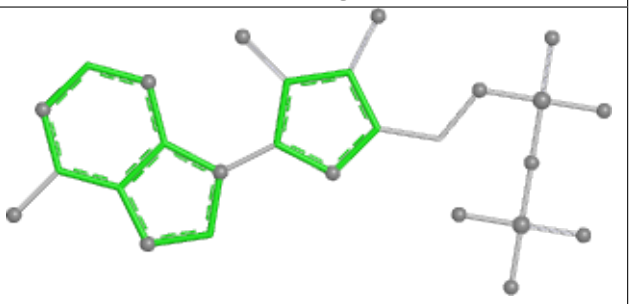
Torsions

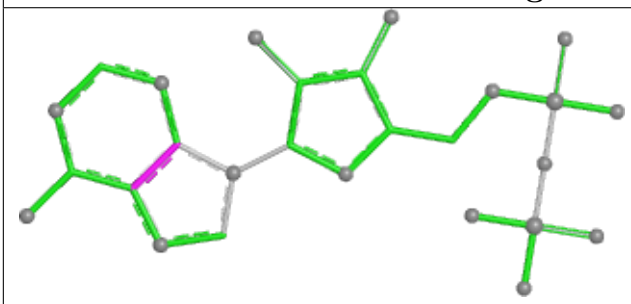
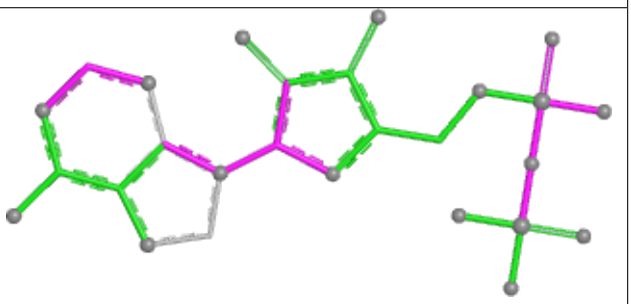
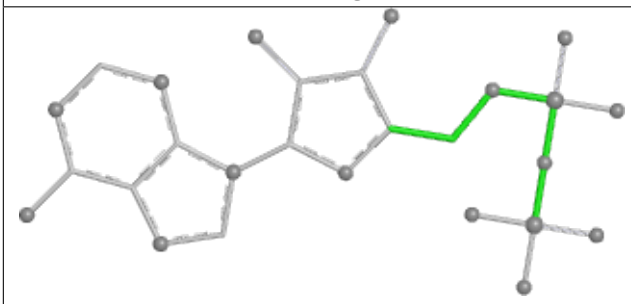
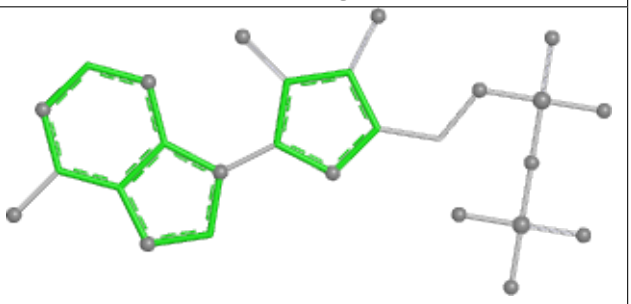


Rings

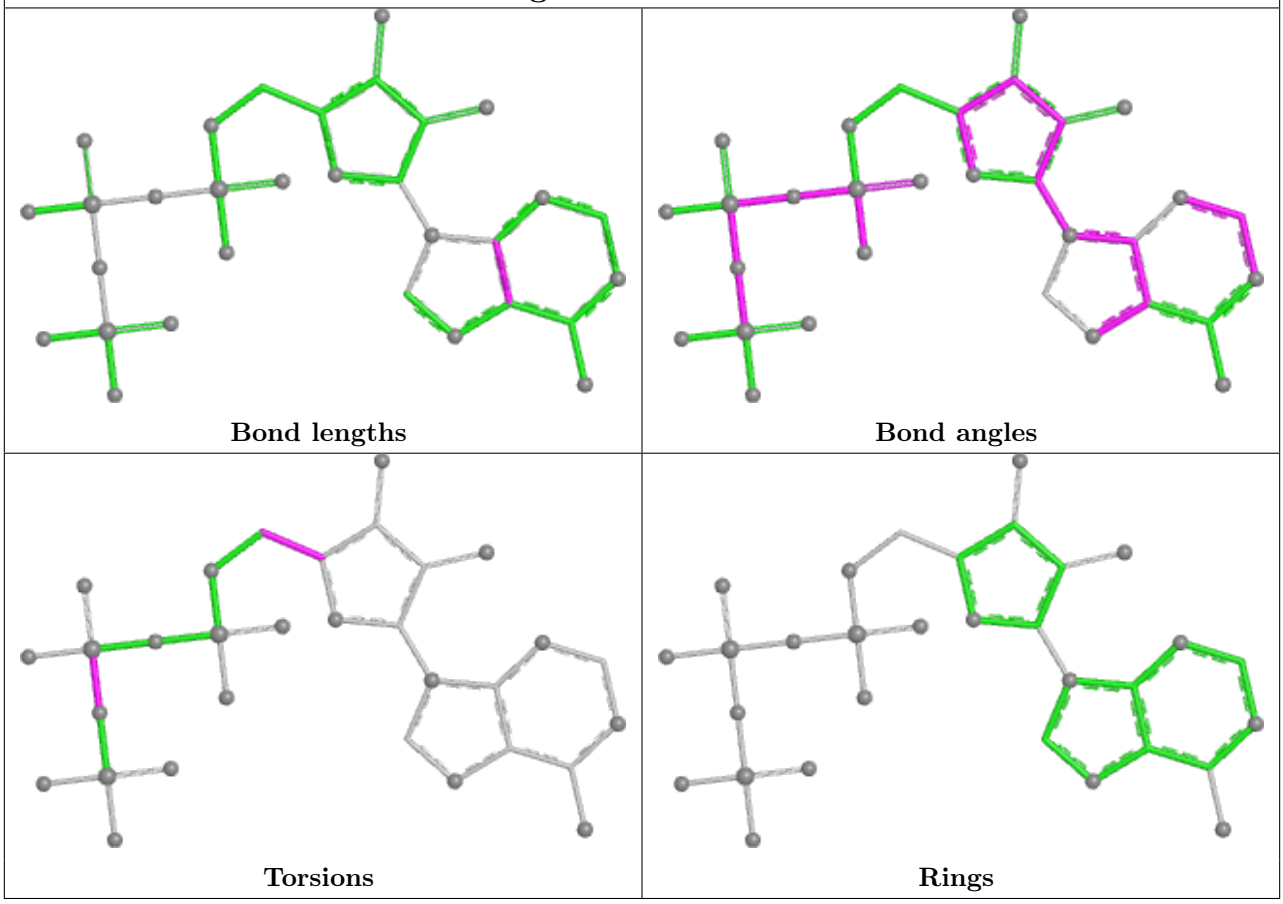
Ligand ATP 2 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP 4 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP 6 901	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand ADP 7 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand ATP 5 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	7	2
4	5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	7	316:ASP	C	317:ALA	N	11.10
1	5	405:GLY	C	408:SER	N	5.76
1	7	142:SER	C	143:THR	N	5.51

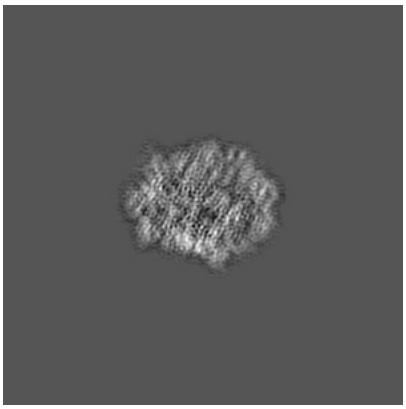
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4786. These allow visual inspection of the internal detail of the map and identification of artifacts.

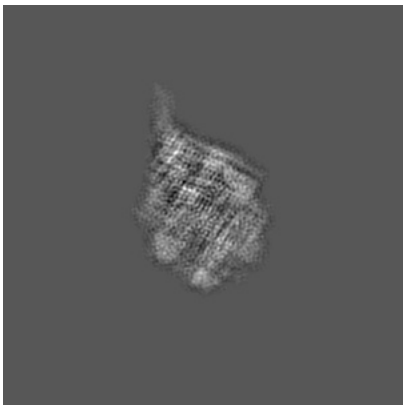
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

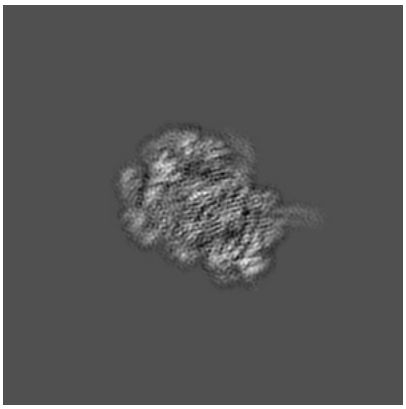
6.1.1 Primary map



X

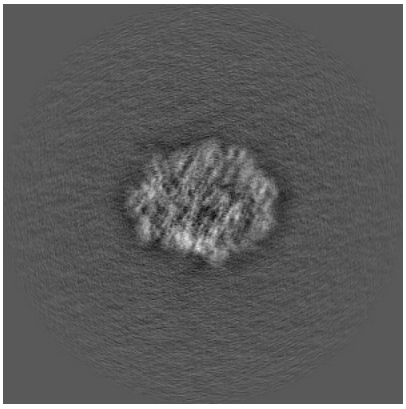


Y

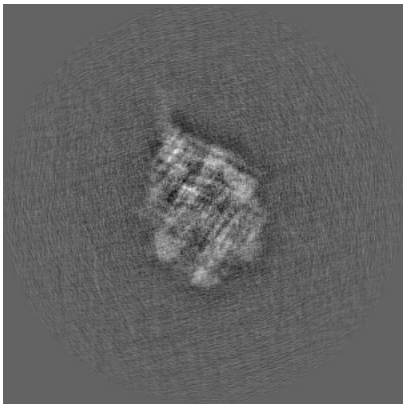


Z

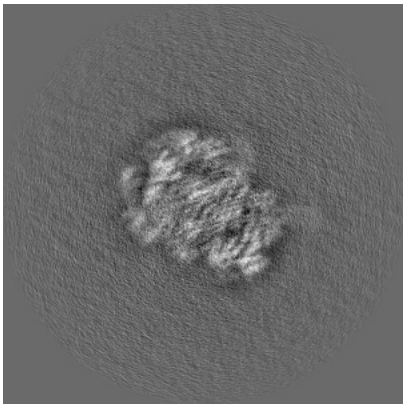
6.1.2 Raw map



X



Y

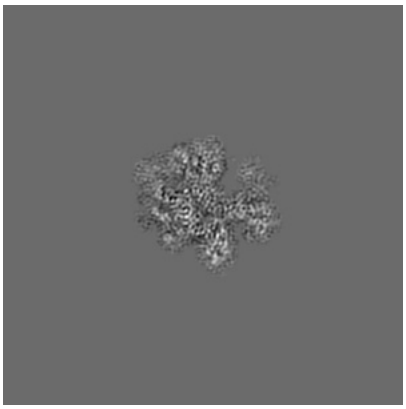


Z

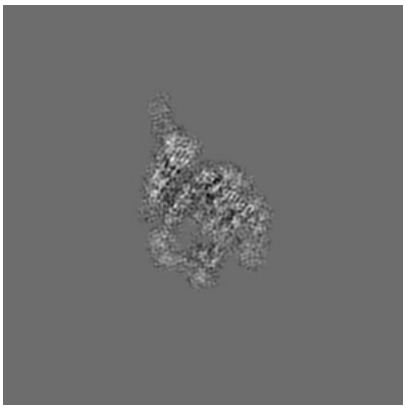
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

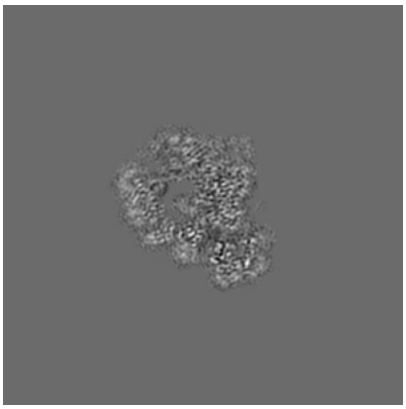
6.2.1 Primary map



X Index: 192

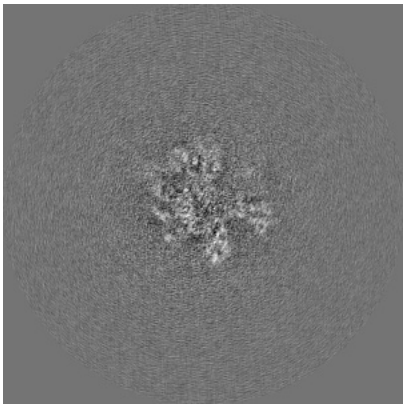


Y Index: 192

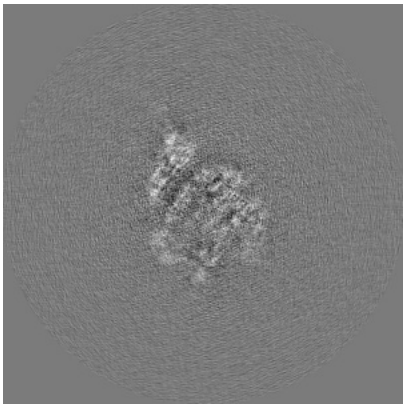


Z Index: 192

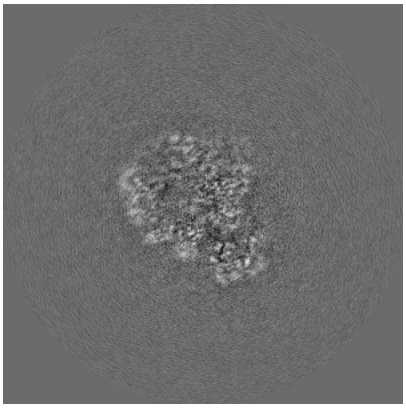
6.2.2 Raw map



X Index: 192



Y Index: 192

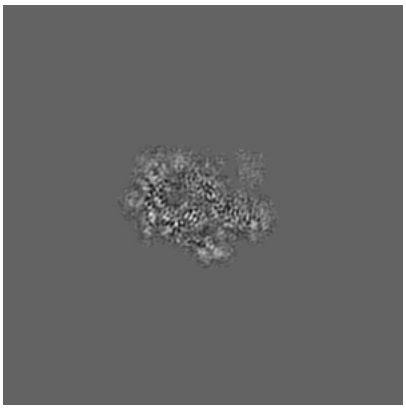


Z Index: 192

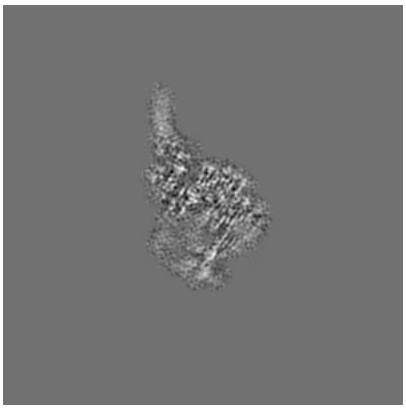
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

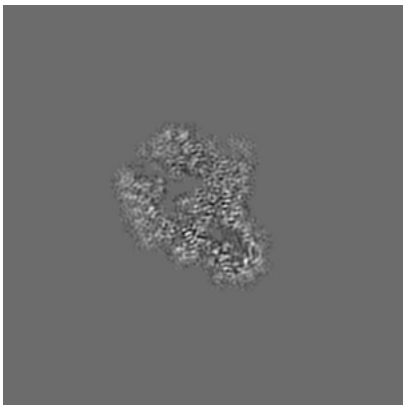
6.3.1 Primary map



X Index: 205

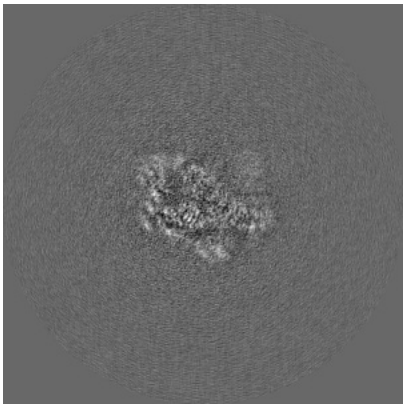


Y Index: 185

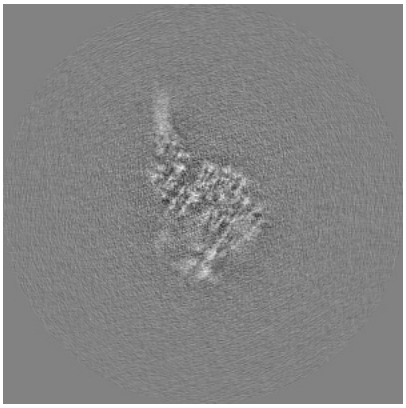


Z Index: 197

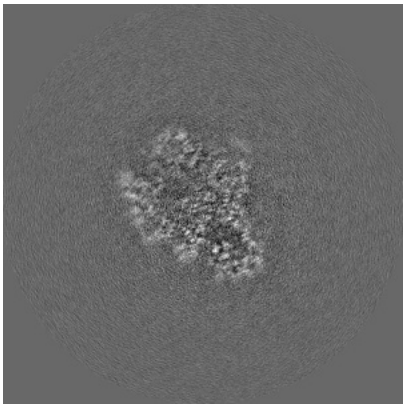
6.3.2 Raw map



X Index: 202



Y Index: 185



Z Index: 196

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 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

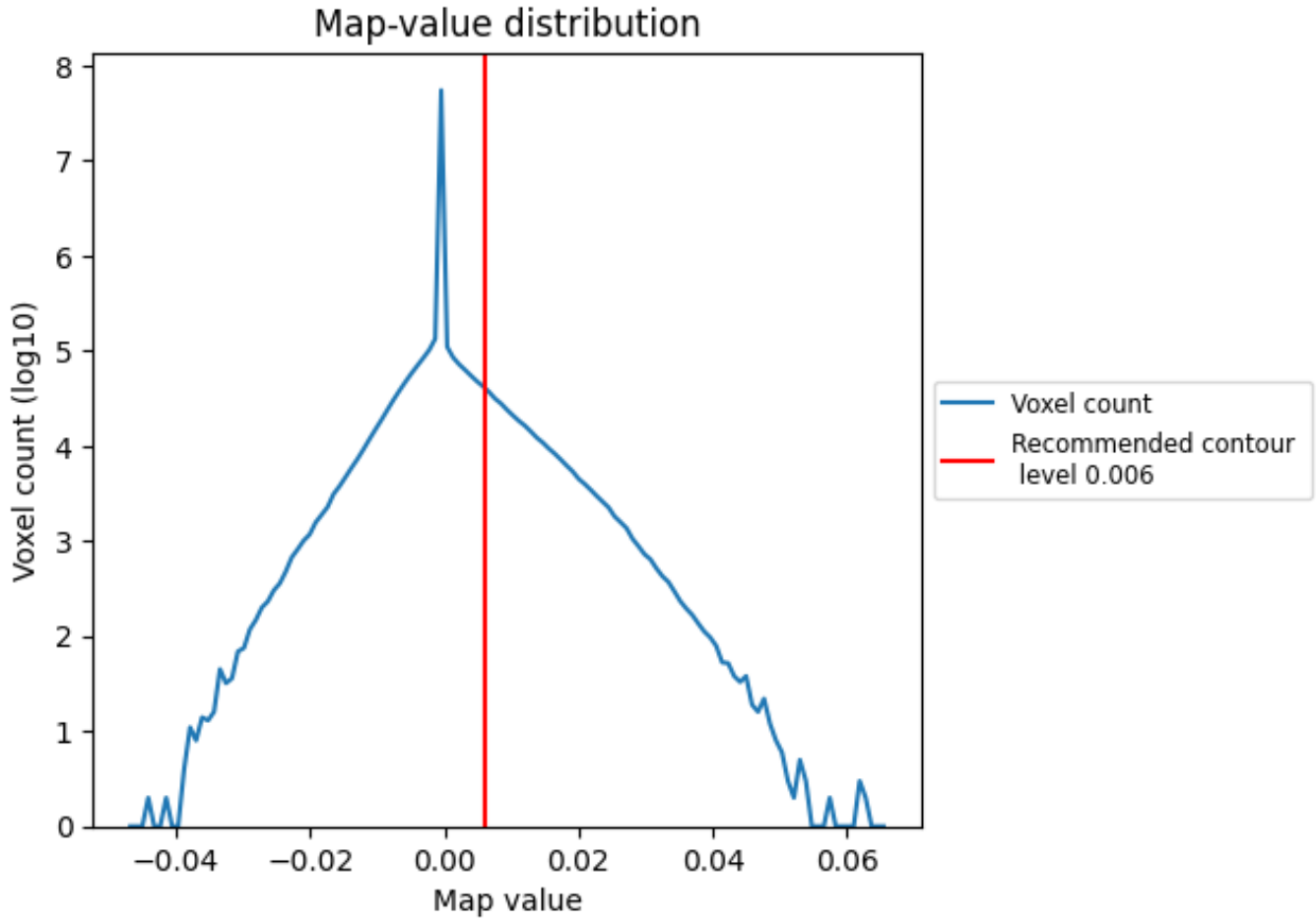
6.5 Mask visualisation (i)

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

7 Map analysis

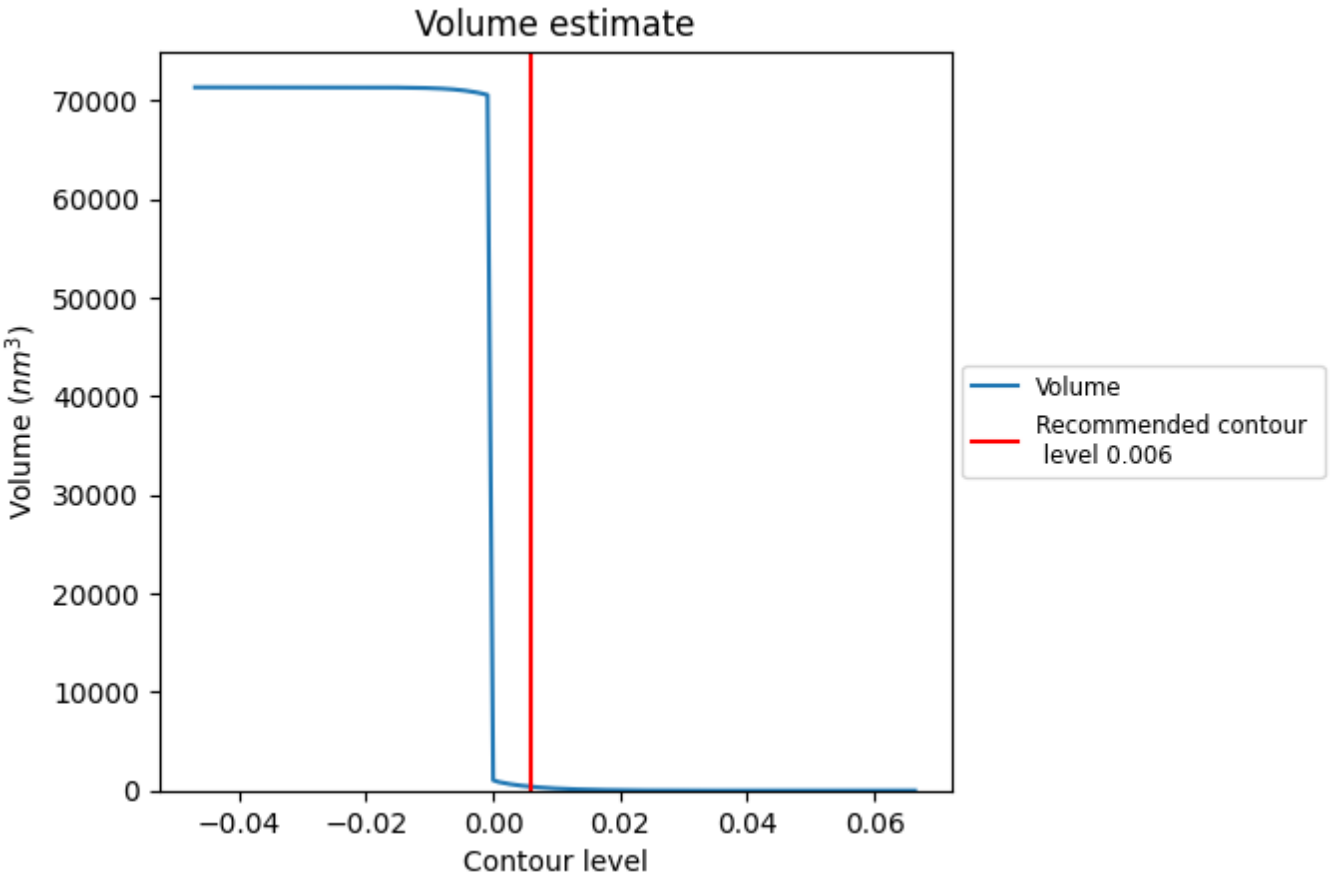
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

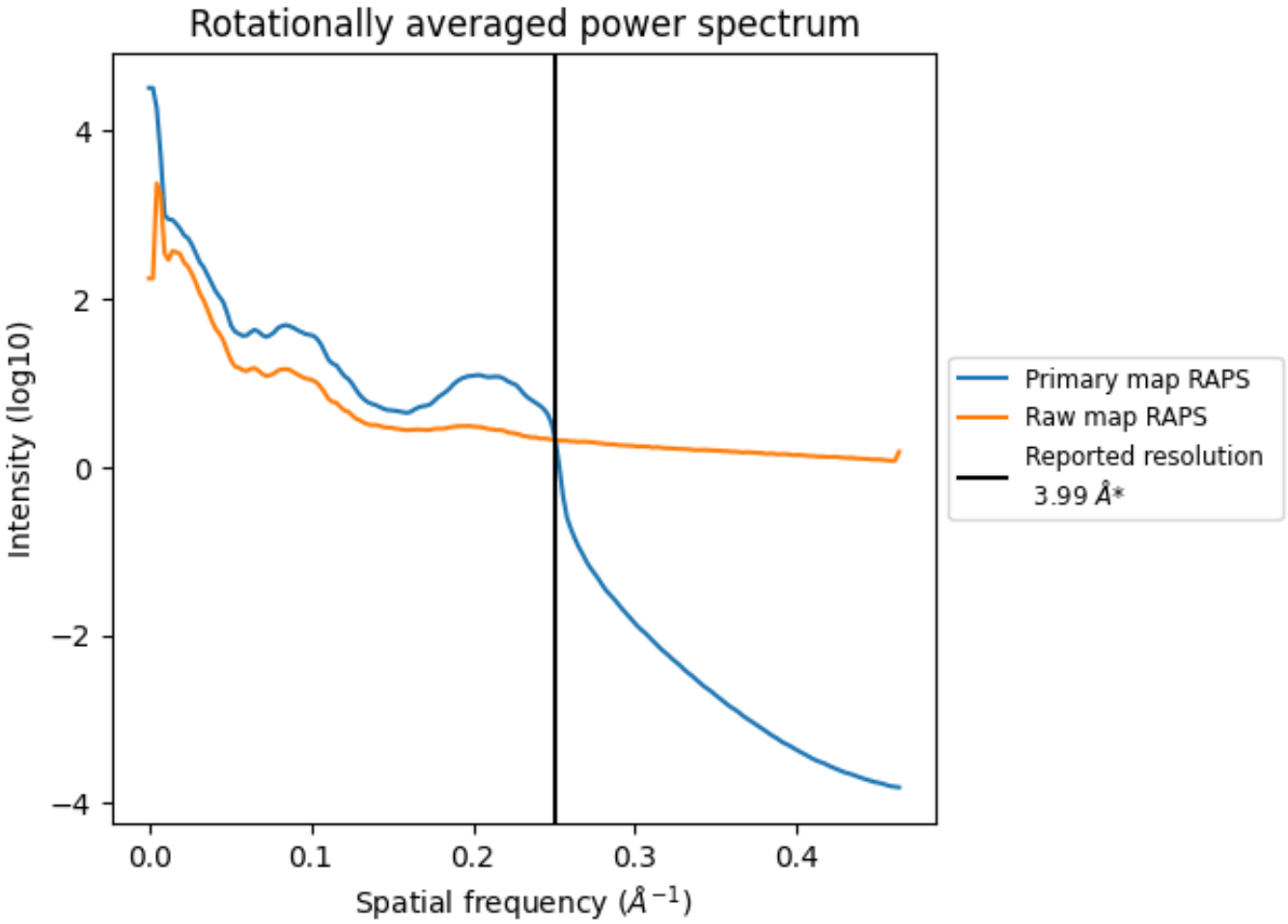
7.2 Volume estimate (i)



The volume at the recommended contour level is 393 nm^3; this corresponds to an approximate mass of 355 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)

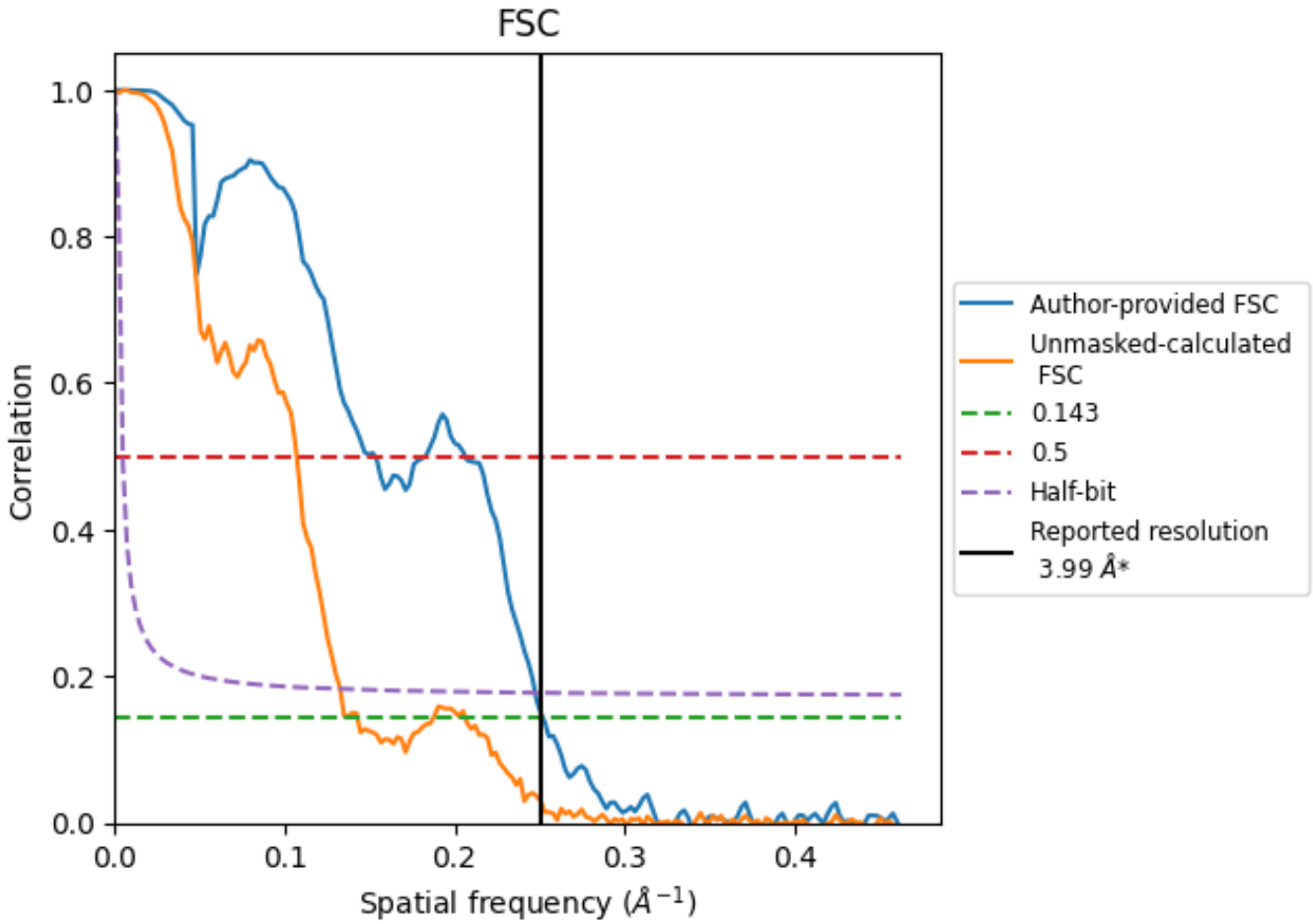


*Reported resolution corresponds to spatial frequency of 0.251 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.251 Å^{-1}

8.2 Resolution estimates (i)

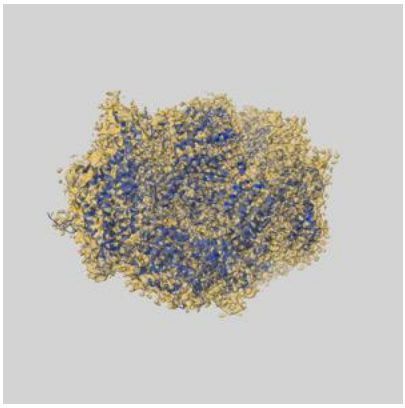
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.99	-	-
Author-provided FSC curve	3.97	6.54	4.04
Unmasked-calculated*	7.00	9.34	7.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.00 differs from the reported value 3.99 by more than 10 %

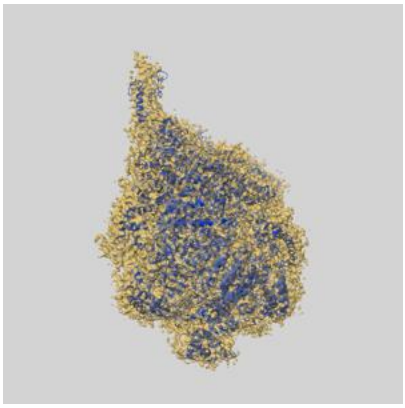
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4786 and PDB model 6RAX. Per-residue inclusion information can be found in section 3 on page 8.

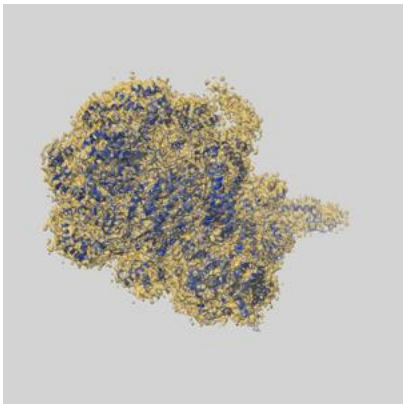
9.1 Map-model overlay



X



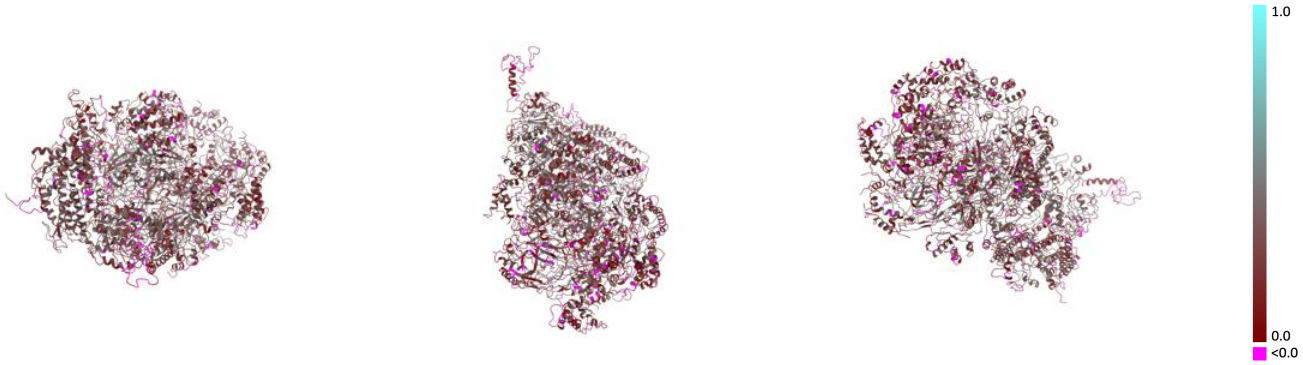
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 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.

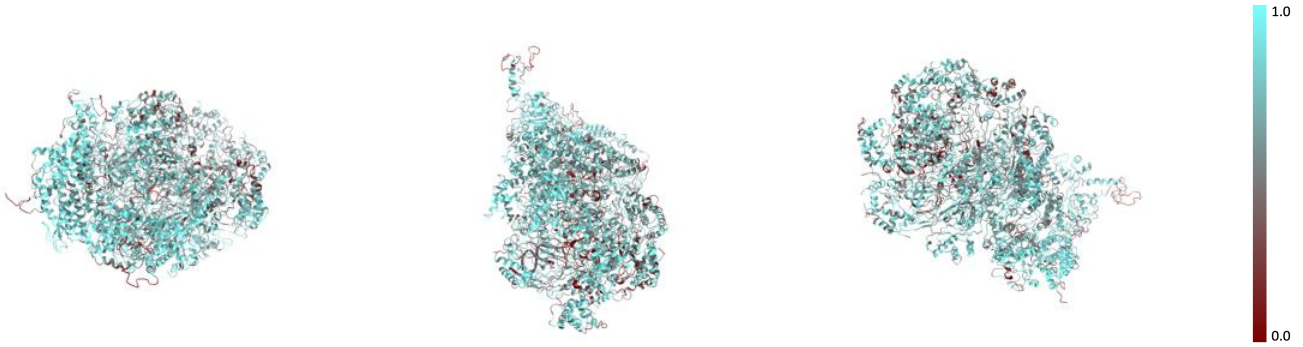
9.2 Q-score mapped to coordinate model (i)



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.

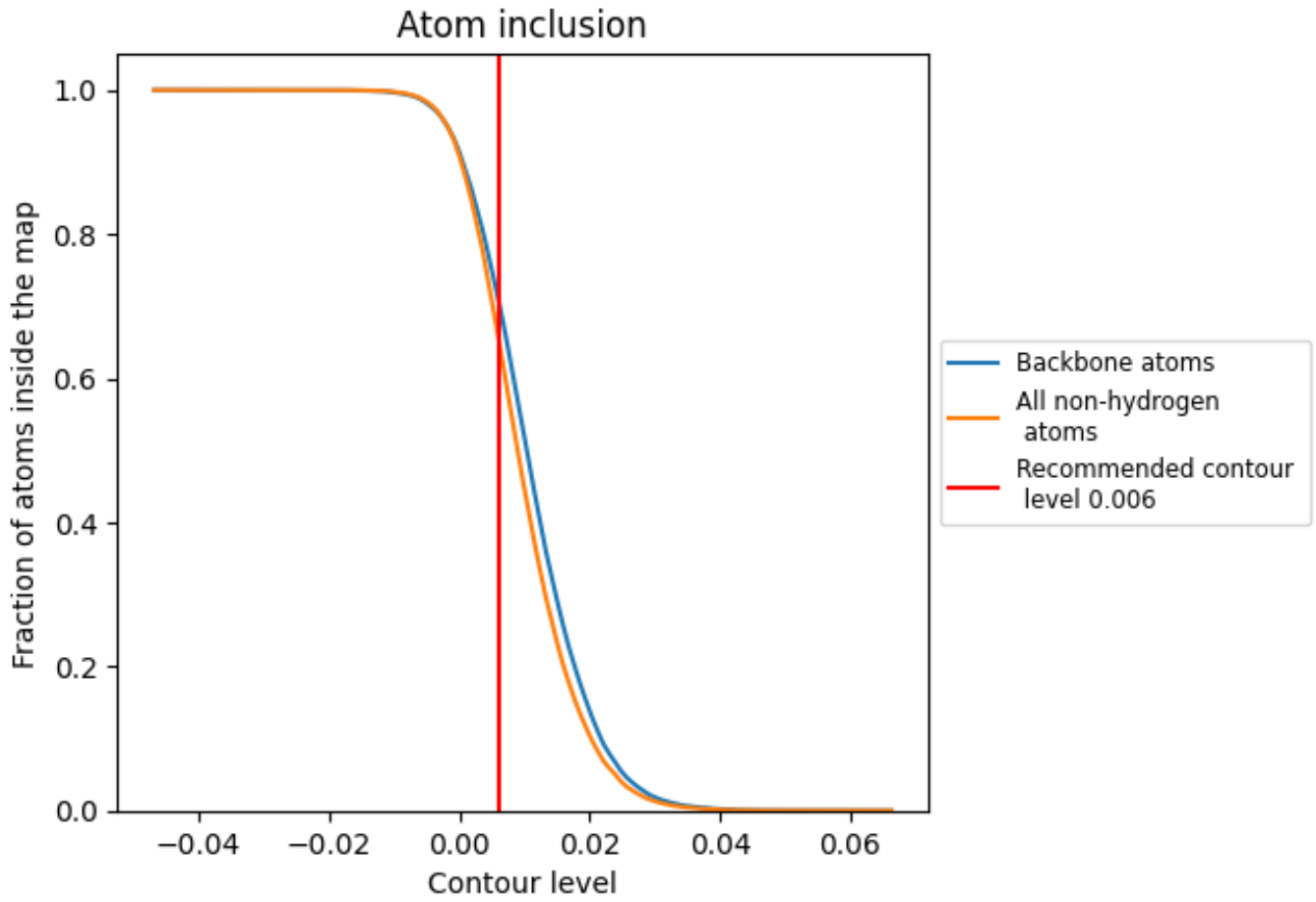
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 66% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6579	0.2550
2	0.6825	0.2740
3	0.6622	0.2570
4	0.6004	0.2010
5	0.6875	0.3080
6	0.6190	0.2340
7	0.6067	0.2310
A	0.7185	0.2900
H	0.6496	0.2090
L	0.7839	0.3110
M	0.6791	0.2560
N	0.7456	0.2750
X	0.3915	0.1550
Y	0.3232	0.0670