Full wwPDB EM Validation Report (i)

Dec 11, 2022 – 12:58 am GMT

PDB ID	:	6RAW
EMDB ID	:	EMD-4785
Title	:	D. melanogaster CMG-DNA, State 1A
Authors	:	Eickhoff, P.; Martino, F.; Costa, A.
Deposited on	:	2019-04-08
Resolution	:	3.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

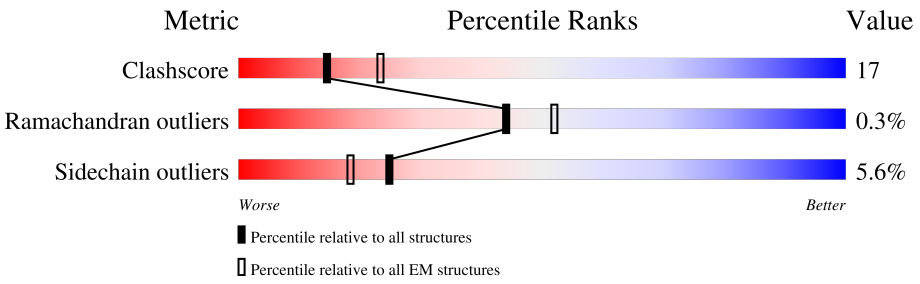
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.70 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	10% 46% 18% • 32%
2	3	819	11% 49% 19% • 29%
3	4	866	16% 49% 19% • 30%
4	5	733	10% 55% 21% • 21%
5	6	817	16% 49% 23% • 26%
6	7	720	16% 34% 51% • 12%
7	F	26	58% 23% 73% •
8	G	13	77% 62% 38%

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Mol	Chain	Length	Quality of chain
9	A	575	15% 68% 24% 6%
10	H	202	27% 67% 28%
11	L	203	5% 60% 22% 16%
12	M	212	17% 54% 22% 24%
13	N	228	14% 64% 24% 11%

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	2	902	-	-	X	-
15	ADP	7	801	-	-	X	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 39710 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	603	4769	3012	831	895	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	585	4551	2835	817	872	27	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	608	4863	3060	861	916	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	576	4532	2847	804	852	29	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	601	4777	2995	842	913	27	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	631	4923	3077	877	935	34	0	1

- Molecule 7 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	F	26	527	257	76	168	26	0	0

- Molecule 8 is a DNA chain called DNA (5'-D(P*TP*CP*GP*AP*TP*CP*GP*AP*TP*CP *GP*AP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	G	13	266	127	47	79	13	0	0

- Molecule 9 is a protein called CDC45L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	A	542	4362	2781	749	810	22	0	0

- Molecule 10 is a protein called IP07275p.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	171	1395	903	231	249	12	0	0

- Molecule 12 is a protein called AT18545p.

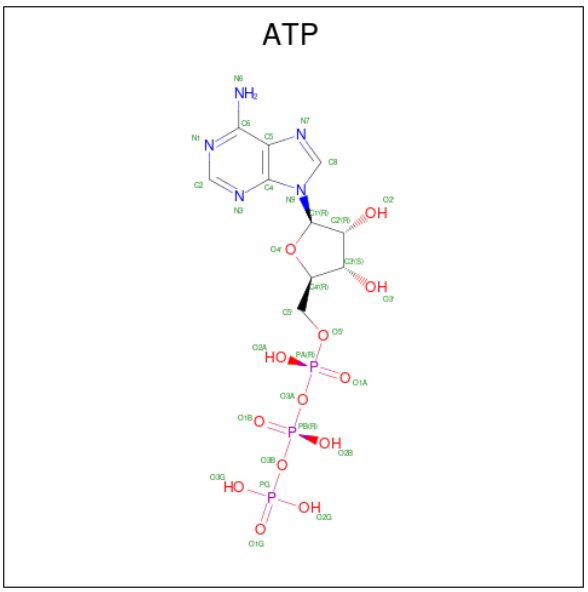
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	162	1349	860	240	245	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	203	1639	1021	276	329	13	0	0

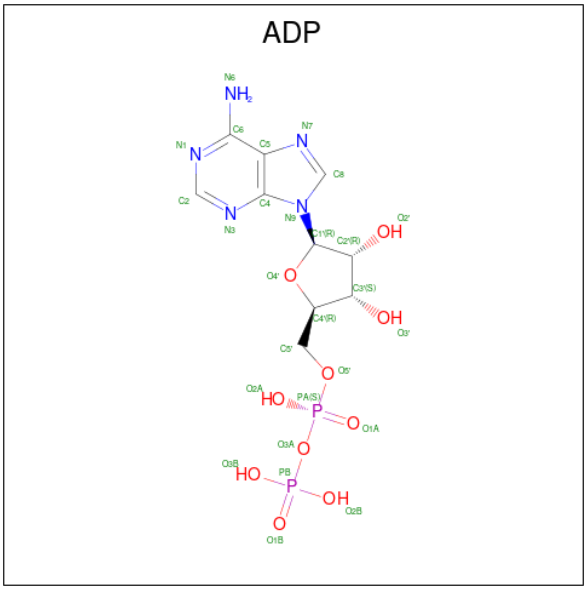
- Molecule 14 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

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



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
14	2	1	62	20	10	26	6	0
			Total	C	N	O	P	
14	2	1	62	20	10	26	6	0
			Total	C	N	O	P	
14	3	1	31	10	5	13	3	0

- 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).

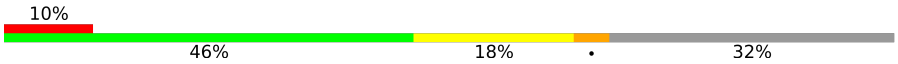


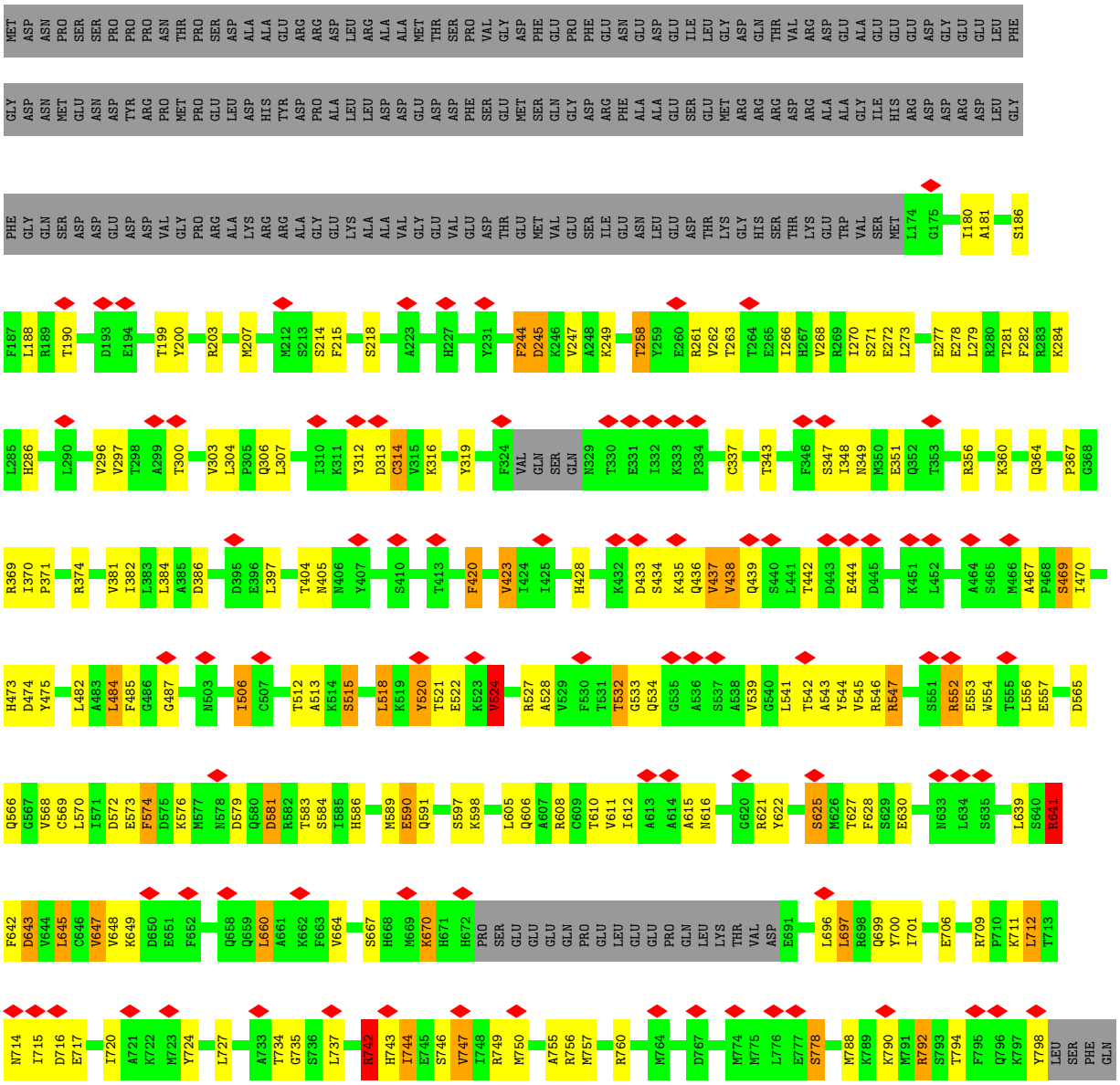
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
15	4	1	27	10	5	10	2	0
			Total	C	N	O	P	
15	6	1	27	10	5	10	2	0
			Total	C	N	O	P	
15	7	1	27	10	5	10	2	0

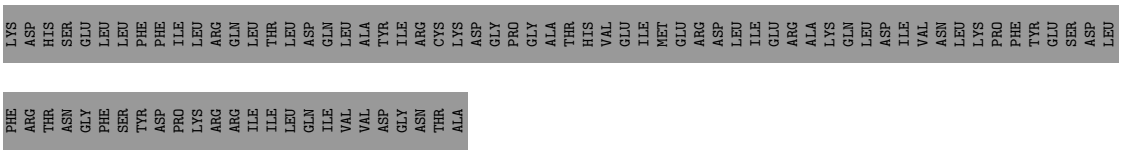
3 Residue-property plots (i)

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

- Molecule 1: DNA replication licensing factor Mcm2

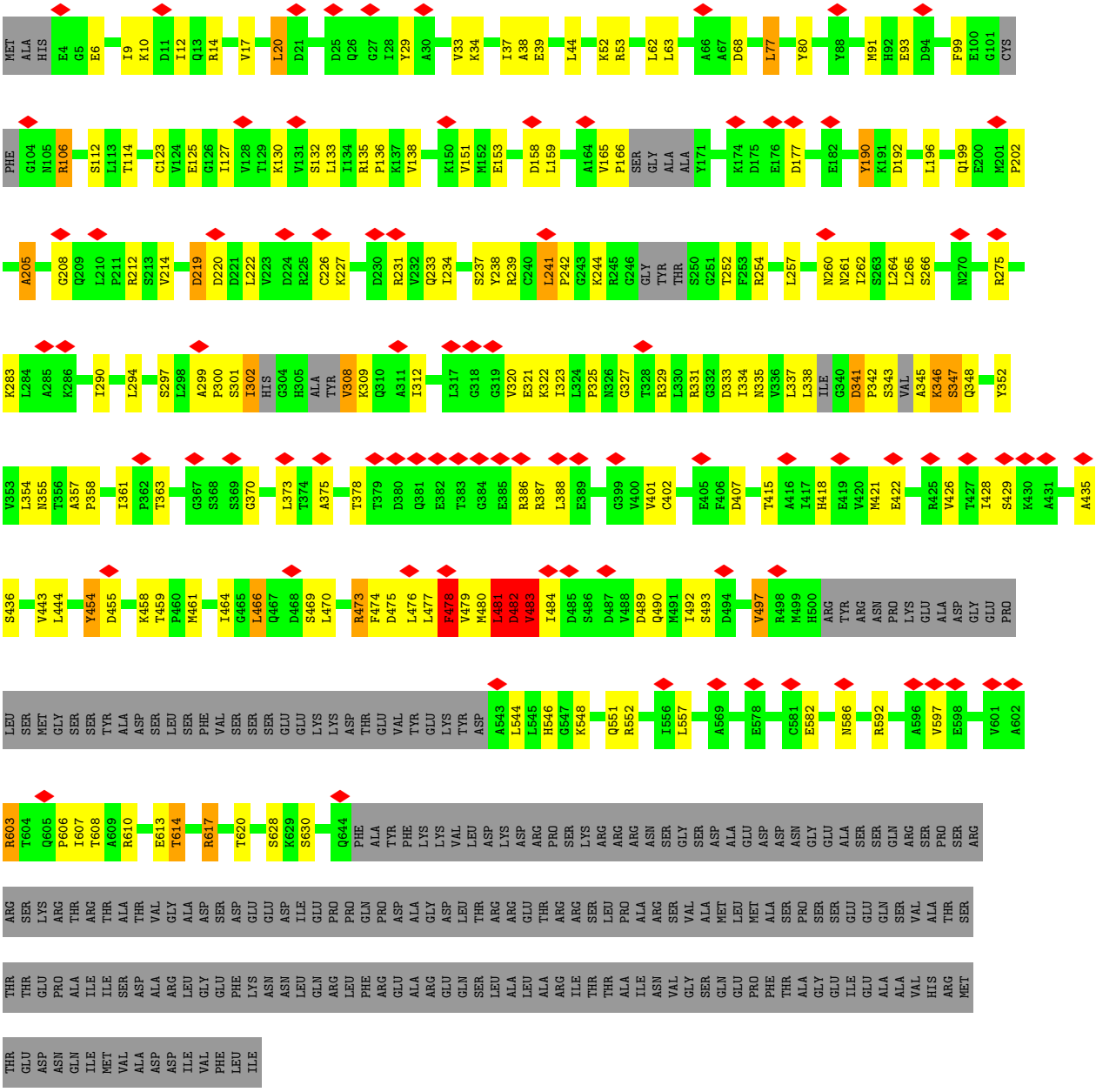
Chain 2: 





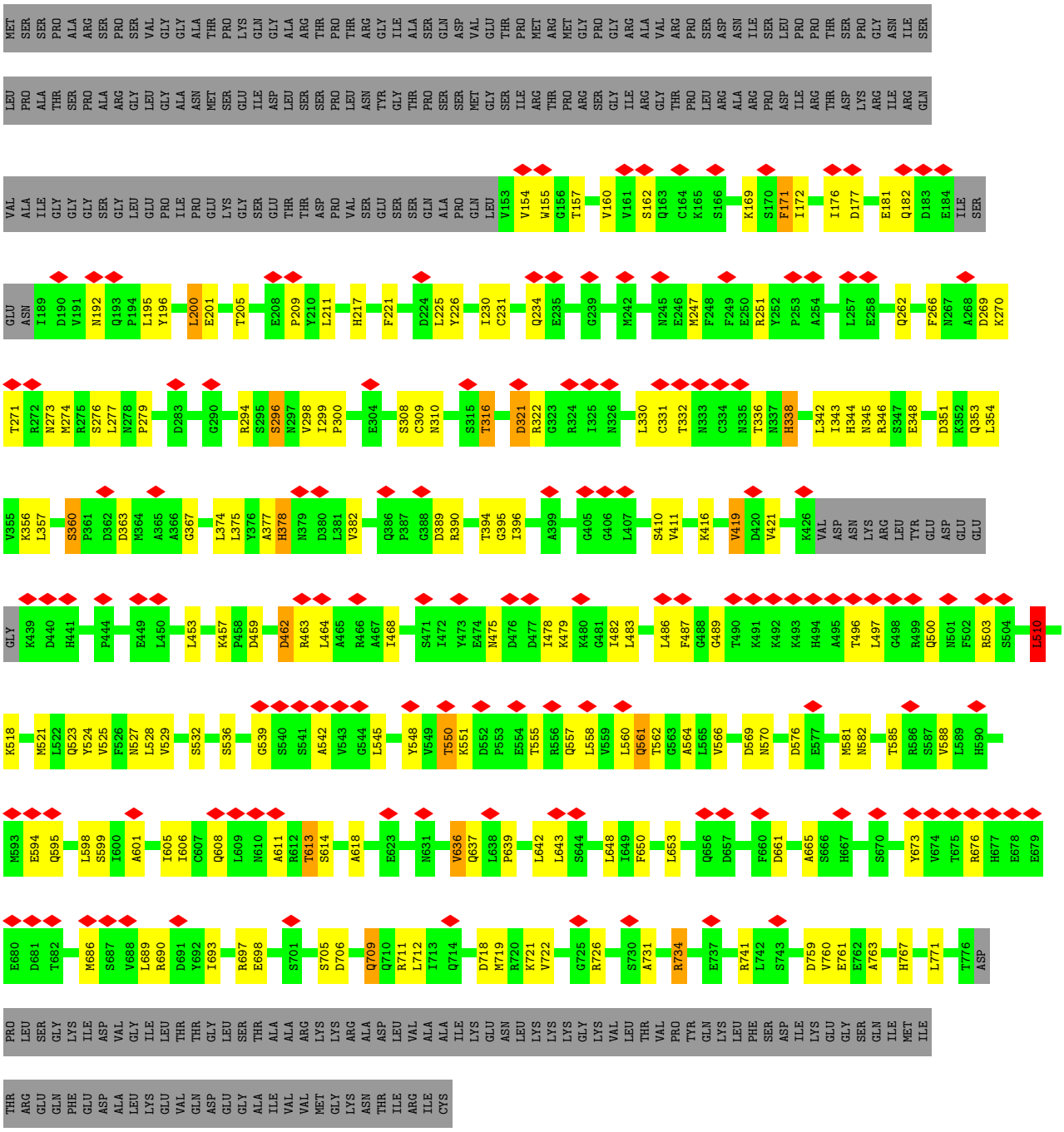
• Molecule 2: DNA replication licensing factor Mcm3

Chain 3:



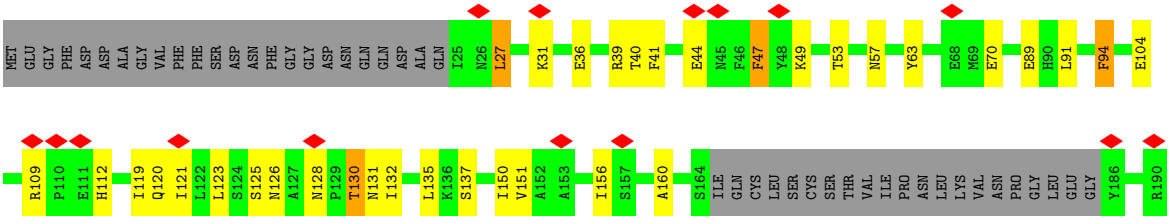
• Molecule 3: DNA replication licensing factor MCM4

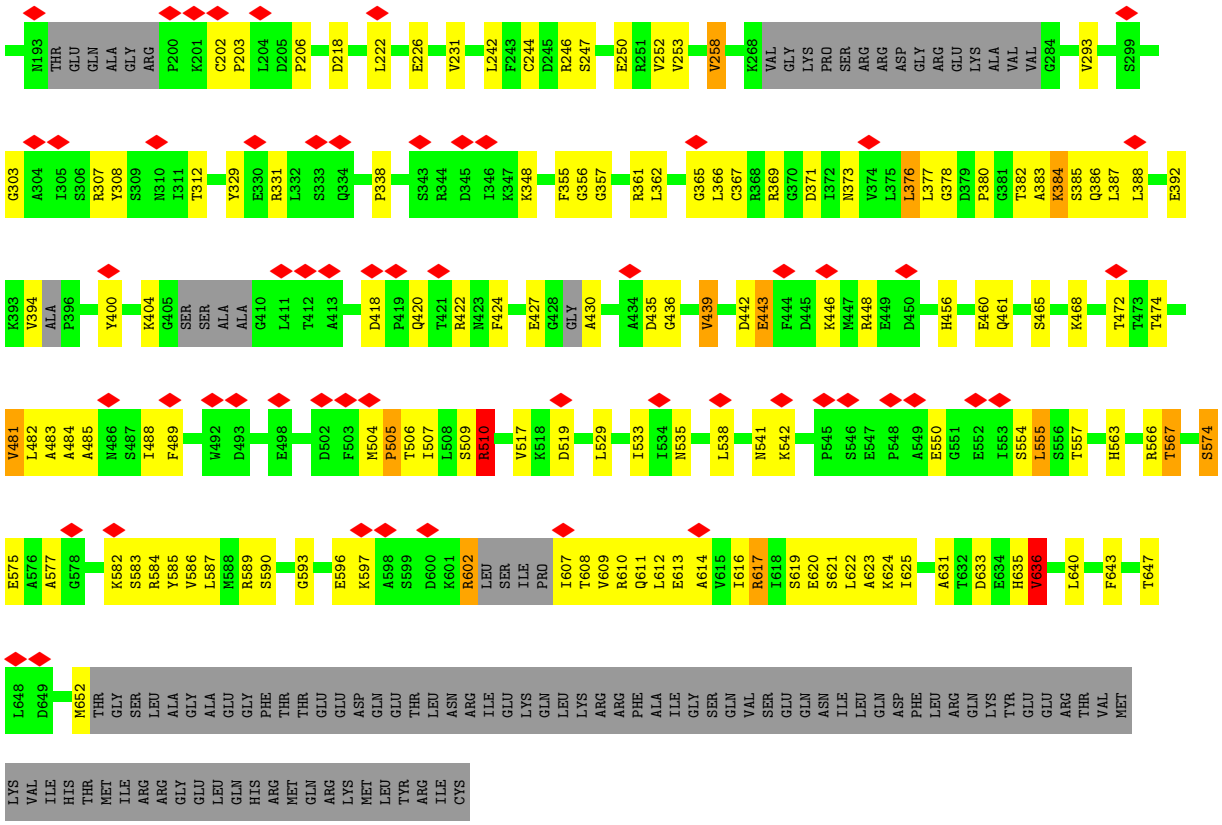
Chain 4:



• Molecule 4: DNA replication licensing factor Mcm5

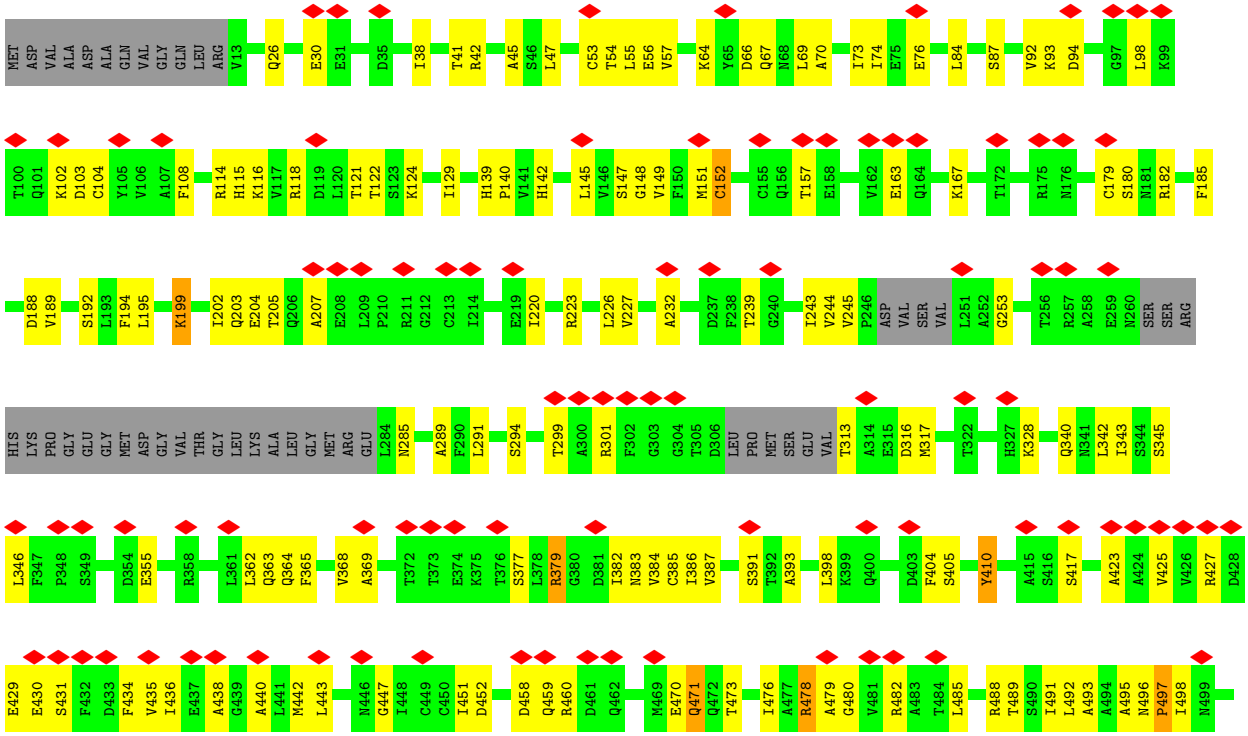
Chain 5:

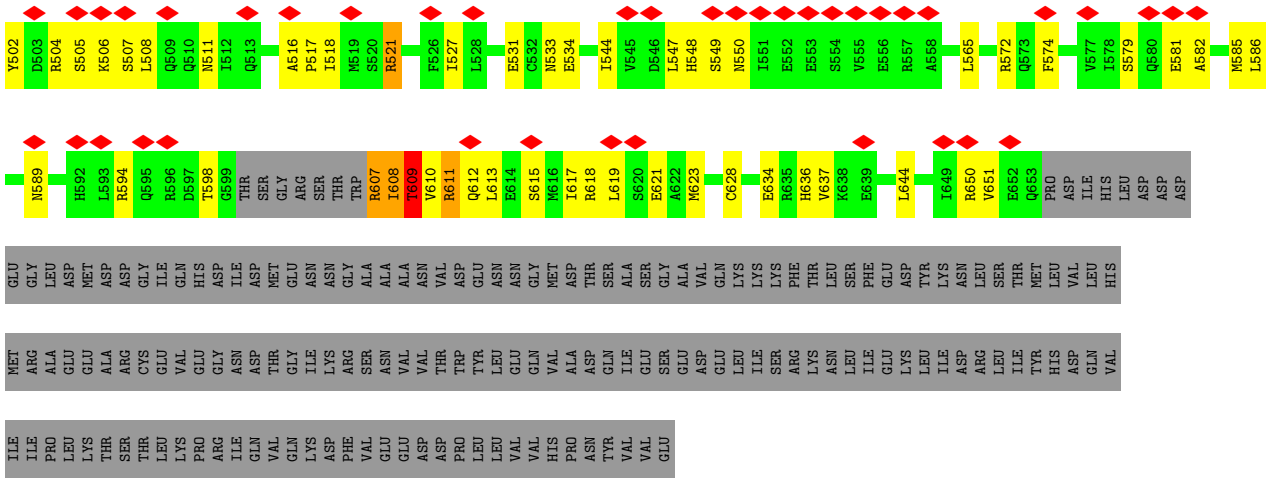




- Molecule 5: DNA replication licensing factor Mcm6

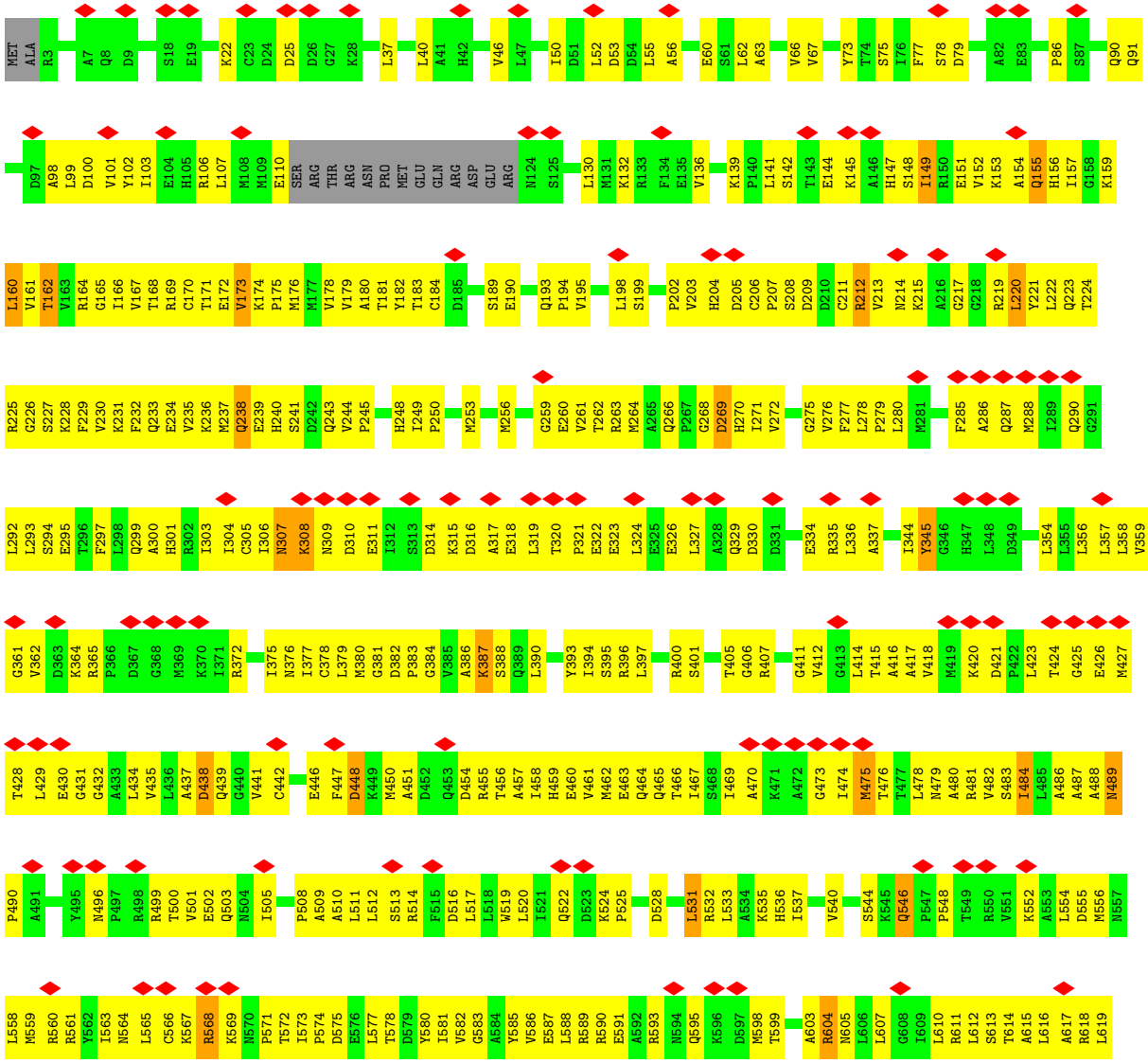
Chain 6:

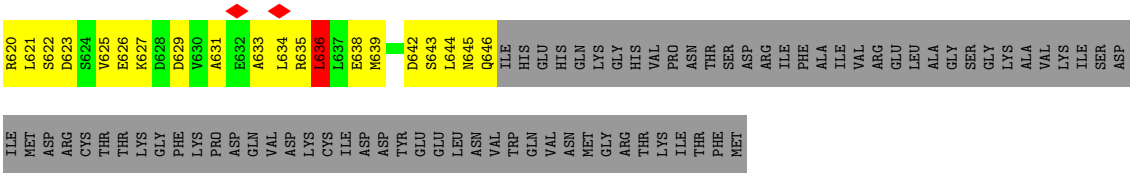




• Molecule 6: DNA replication licensing factor Mcm7

Chain 7:



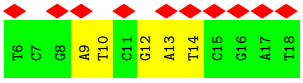


- Molecule 7: DNA

Chain F:

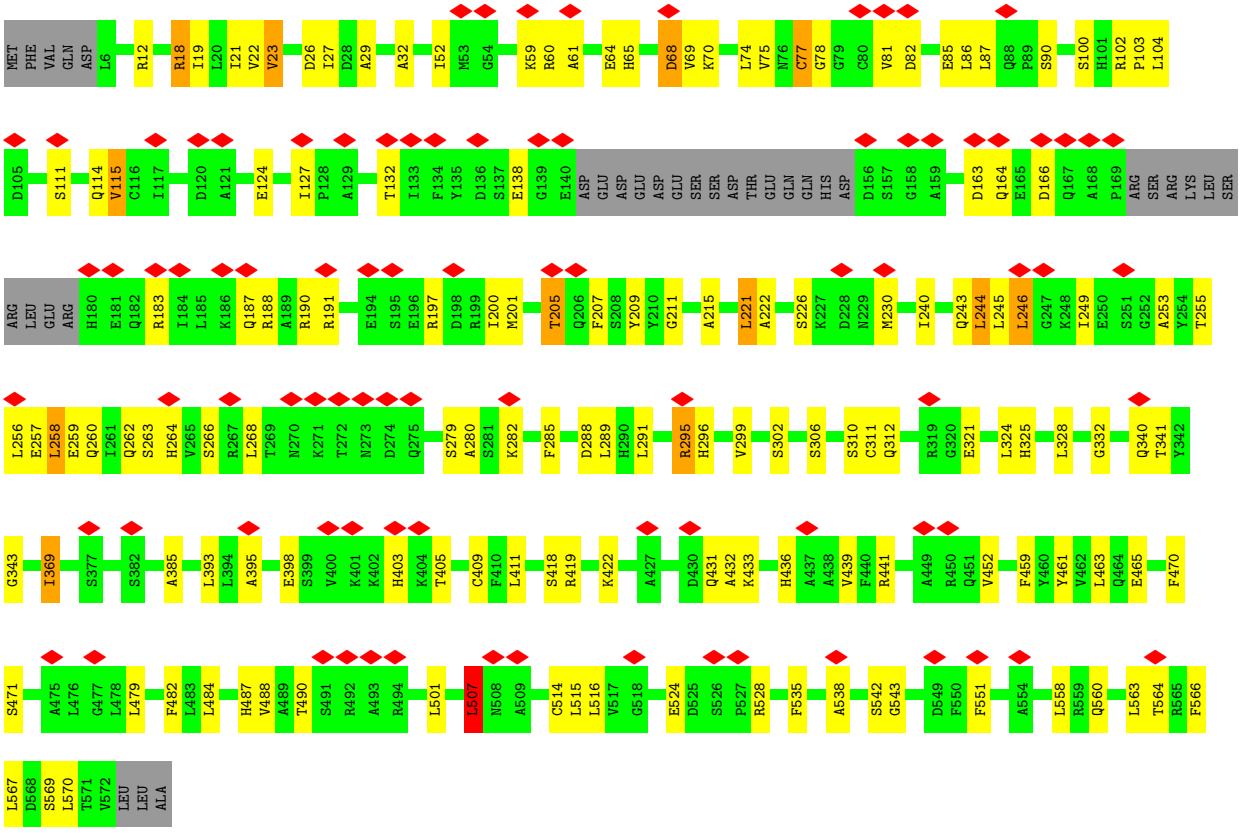
- Molecule 8: DNA (5'-D(P*TP*CP*GP*AP*TP*CP*GP*AP*TP*CP*GP*AP*T)-3')

Chain G:



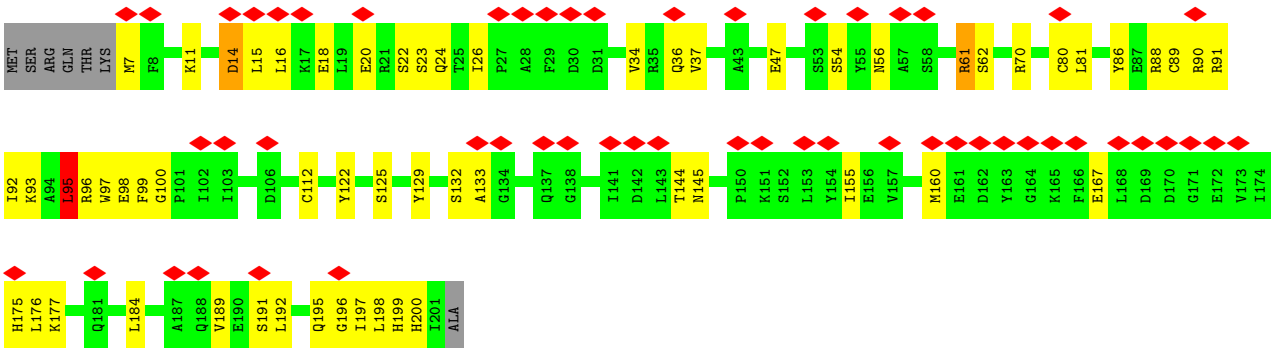
- Molecule 9: CDC45L

Chain A:



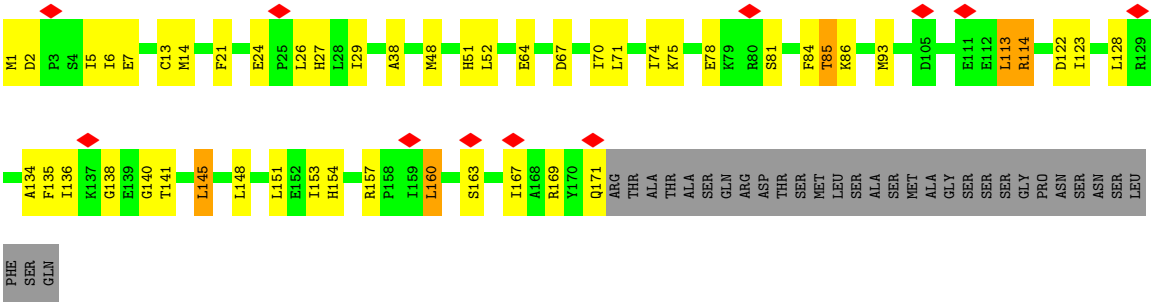
- Molecule 10: IP07275p

Chain H:



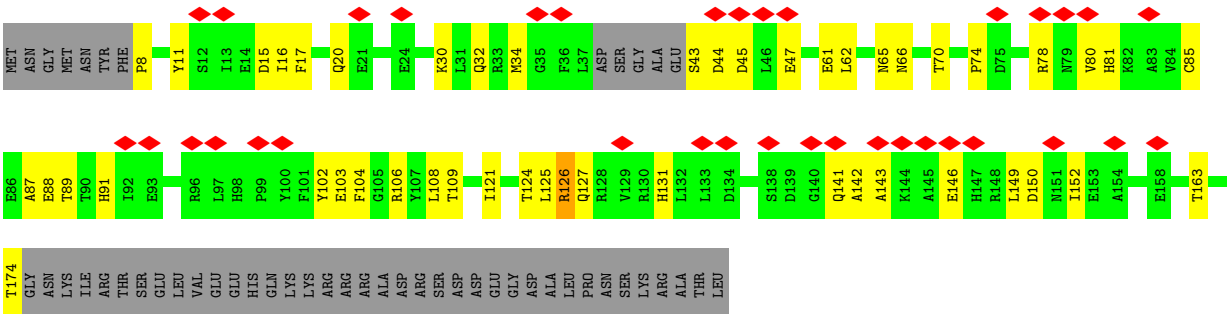
- Molecule 11: Probable DNA replication complex GINS protein PSF2

Chain L:



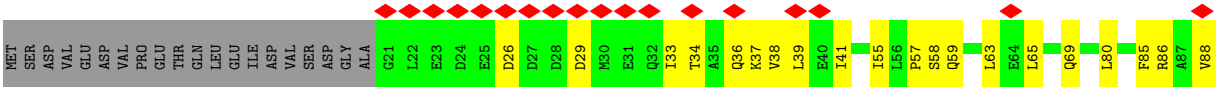
- Molecule 12: AT18545p

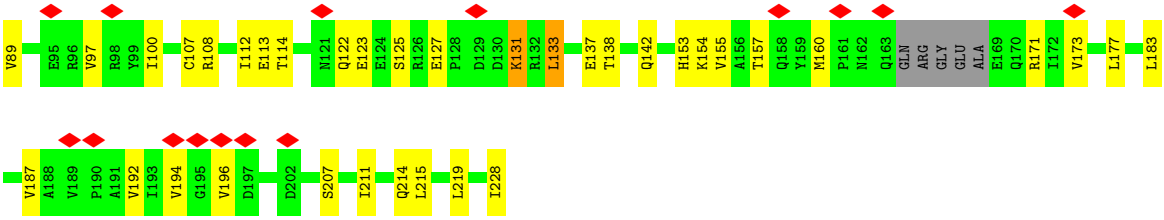
Chain M:



- Molecule 13: DNA replication complex GINS protein SLD5

Chain N:




V89
E95
R96
V97
R98
Y99
I100
C107
R108
I112
E113
T114
N121
Q122
E123
E124
S125
R126
E127
P128
D129
D130
K131
R132
L133
E137
T138
Q142
H153
K154
V155
A156
T157
Q158
Y159
M160
P161
N162
Q163
GLN
ARG
GLY
GLU
ALA
E169
Q170
R171
I172
V173
L177
L183
V187
A188
V189
P190
A191
V192
I193
V194
G195
V196
D197
D202
S207
I211
Q214
L215
L219
I228

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	170329	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	0.084	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	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 (i)

5.1 Standard geometry (i)

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	0.36	0/4855	0.86	22/6562 (0.3%)
2	3	0.36	1/4607 (0.0%)	0.81	13/6205 (0.2%)
3	4	0.33	0/4953	0.73	7/6703 (0.1%)
4	5	0.36	0/4602	0.77	7/6185 (0.1%)
5	6	0.34	0/4847	0.78	7/6536 (0.1%)
6	7	0.29	0/4988	0.63	7/6721 (0.1%)
7	F	0.59	1/585 (0.2%)	1.14	0/901
8	G	0.57	0/297	0.96	0/456
9	A	0.34	0/4453	0.74	7/6021 (0.1%)
10	H	0.38	0/1618	0.78	1/2184 (0.0%)
11	L	0.37	0/1431	0.71	1/1937 (0.1%)
12	M	0.41	0/1380	0.76	0/1868
13	N	0.35	0/1664	0.65	0/2251
All	All	0.35	2/40280 (0.0%)	0.77	72/54530 (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	0	7
2	3	0	7
3	4	0	8
4	5	0	9
5	6	1	5
6	7	0	1
9	A	0	2
10	H	0	2
11	L	0	1
12	M	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	1	46

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	454	TYR	CD1-CE1	-5.43	1.31	1.39
7	F	12	DT	C3'-O3'	-5.15	1.37	1.44

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	7	604	ARG	NE-CZ-NH2	-13.43	113.59	120.30
3	4	734	ARG	CD-NE-CZ	12.95	141.73	123.60
1	2	641	ARG	NE-CZ-NH2	-11.47	114.56	120.30
2	3	481	LEU	CB-CG-CD1	10.03	128.05	111.00
3	4	171	PHE	CB-CG-CD1	-9.51	114.14	120.80
2	3	482	ASP	CB-CG-OD1	9.10	126.49	118.30
6	7	636	LEU	CB-CG-CD2	9.01	126.32	111.00
4	5	510	ARG	NE-CZ-NH2	-8.86	115.87	120.30
3	4	171	PHE	CB-CG-CD2	8.63	126.84	120.80
5	6	609	THR	CA-CB-CG2	8.27	123.98	112.40
1	2	712	LEU	CB-CG-CD2	8.02	124.63	111.00
2	3	239	ARG	NE-CZ-NH1	-8.00	116.30	120.30
2	3	238	TYR	CB-CG-CD2	-7.79	116.33	121.00
1	2	484	LEU	CB-CG-CD2	7.70	124.09	111.00
3	4	734	ARG	NE-CZ-NH1	-7.69	116.46	120.30
5	6	518	ILE	CG1-CB-CG2	7.63	128.19	111.40
6	7	604	ARG	CD-NE-CZ	7.47	134.05	123.60
5	6	382	ILE	CG1-CB-CG2	7.38	127.64	111.40
2	3	492	ILE	CG1-CB-CG2	7.36	127.59	111.40
1	2	518	LEU	CA-CB-CG	7.17	131.78	115.30
4	5	481	VAL	CG1-CB-CG2	7.13	122.32	110.90
2	3	238	TYR	CB-CG-CD1	7.07	125.24	121.00
1	2	568	VAL	CG1-CB-CG2	7.03	122.15	110.90
5	6	482	ARG	NE-CZ-NH1	-7.01	116.80	120.30
3	4	734	ARG	NE-CZ-NH2	-6.96	116.82	120.30
2	3	483	VAL	CG1-CB-CG2	6.92	121.97	110.90
1	2	641	ARG	NH1-CZ-NH2	-6.88	111.84	119.40
1	2	524	VAL	CG1-CB-CG2	6.87	121.90	110.90
1	2	647	VAL	CG1-CB-CG2	6.69	121.61	110.90
1	2	612	ILE	CG1-CB-CG2	6.69	126.12	111.40
9	A	558	LEU	CB-CG-CD1	6.52	122.08	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	469	SER	C-N-CA	6.45	137.83	121.70
11	L	160	LEU	CA-CB-CG	6.44	130.12	115.30
1	2	506	ILE	CG1-CB-CG2	6.42	125.53	111.40
4	5	529	LEU	CB-CG-CD2	6.40	121.89	111.00
2	3	497	VAL	CG1-CB-CG2	6.31	121.00	110.90
4	5	636	VAL	CG1-CB-CG2	6.30	120.98	110.90
2	3	484	ILE	CG1-CB-CG2	6.27	125.19	111.40
5	6	613	LEU	CB-CG-CD2	6.25	121.62	111.00
1	2	747	VAL	CG1-CB-CG2	6.18	120.79	110.90
2	3	478	PHE	CB-CG-CD1	6.17	125.12	120.80
6	7	55	LEU	CB-CG-CD1	6.11	121.39	111.00
1	2	515	SER	C-N-CA	6.04	136.81	121.70
10	H	95	LEU	CA-CB-CG	6.02	129.15	115.30
1	2	697	LEU	CB-CG-CD2	6.01	121.22	111.00
1	2	641	ARG	CD-NE-CZ	6.01	132.01	123.60
3	4	225	LEU	CB-CG-CD1	5.91	121.05	111.00
6	7	636	LEU	CB-CG-CD1	-5.89	100.98	111.00
1	2	552	ARG	CG-CD-NE	5.71	123.80	111.80
1	2	712	LEU	CA-CB-CG	5.57	128.12	115.30
3	4	510	LEU	CB-CG-CD2	5.56	120.45	111.00
6	7	55	LEU	CB-CG-CD2	-5.55	101.57	111.00
2	3	497	VAL	CA-CB-CG1	5.54	119.21	110.90
1	2	641	ARG	NE-CZ-NH1	5.53	123.06	120.30
9	A	558	LEU	CB-CG-CD2	-5.51	101.63	111.00
6	7	345	TYR	C-N-CA	-5.44	110.87	122.30
4	5	529	LEU	CB-CG-CD1	5.43	120.23	111.00
5	6	619	LEU	CB-CG-CD1	5.42	120.21	111.00
9	A	507	LEU	CB-CG-CD1	5.31	120.02	111.00
9	A	244	LEU	CA-CB-CG	5.30	127.48	115.30
9	A	18	ARG	CG-CD-NE	5.24	122.80	111.80
9	A	246	LEU	CB-CG-CD2	5.21	119.86	111.00
1	2	628	PHE	CB-CG-CD2	-5.20	117.16	120.80
1	2	697	LEU	CA-CB-CG	5.11	127.05	115.30
1	2	747	VAL	CA-CB-CG1	5.10	118.55	110.90
2	3	614	THR	OG1-CB-CG2	5.10	121.73	110.00
4	5	41	PHE	CB-CG-CD2	-5.10	117.23	120.80
9	A	18	ARG	NE-CZ-NH1	-5.04	117.78	120.30
5	6	517	PRO	C-N-CA	5.03	134.26	121.70
2	3	106	ARG	CG-CD-NE	-5.02	101.26	111.80
4	5	636	VAL	CA-CB-CG1	5.02	118.42	110.90
1	2	569	CYS	C-N-CA	5.01	134.23	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	6	609	THR	CB

All (46) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	266	ILE	Peptide
1	2	384	LEU	Peptide
1	2	437	VAL	Peptide
1	2	528	ALA	Peptide
1	2	641	ARG	Sidechain
1	2	742	ARG	Sidechain
1	2	744	ILE	Peptide
2	3	205	ALA	Peptide
2	3	219	ASP	Peptide
2	3	222	LEU	Peptide
2	3	241	LEU	Peptide
2	3	252	THR	Peptide
2	3	482	ASP	Peptide
2	3	546	HIS	Peptide
3	4	271	THR	Peptide
3	4	321	ASP	Peptide
3	4	360	SER	Peptide
3	4	378	HIS	Peptide
3	4	561	GLN	Peptide
3	4	636	VAL	Peptide
3	4	709	GLN	Peptide
3	4	734	ARG	Sidechain
4	5	112	HIS	Peptide
4	5	203	PRO	Peptide
4	5	231	VAL	Peptide
4	5	258	VAL	Peptide
4	5	430	ALA	Peptide
4	5	44	GLU	Peptide
4	5	443	GLU	Peptide
4	5	47	PHE	Peptide
4	5	510	ARG	Sidechain
5	6	488	ARG	Peptide
5	6	549	SER	Peptide
5	6	607	ARG	Peptide
5	6	608	ILE	Peptide
5	6	609	THR	Peptide
6	7	604	ARG	Sidechain
9	A	23	VAL	Peptide

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Mol	Chain	Res	Type	Group
9	A	490	THR	Peptide
10	H	198	LEU	Peptide
10	H	7	MET	Peptide
11	L	145	LEU	Peptide
12	M	106	ARG	Peptide
12	M	149	LEU	Peptide
12	M	17	PHE	Peptide
12	M	62	LEU	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	4769	0	4808	158	0
2	3	4551	0	4615	138	0
3	4	4863	0	4860	124	0
4	5	4532	0	4571	130	0
5	6	4777	0	4774	151	0
6	7	4923	0	4960	492	0
7	F	527	0	303	32	0
8	G	266	0	148	5	0
9	A	4362	0	4304	88	0
10	H	1583	0	1567	32	0
11	L	1395	0	1415	31	0
12	M	1349	0	1328	29	0
13	N	1639	0	1587	33	0
14	2	62	0	24	18	0
14	3	31	0	11	5	0
15	4	27	0	12	1	0
15	6	27	0	11	3	0
15	7	27	0	11	9	0
All	All	39710	0	39309	1349	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 17.

All (1349) 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)
1:2:541:LEU:HD13	5:6:479:ALA:CA	1.30	1.57
1:2:541:LEU:CD1	5:6:479:ALA:HA	1.10	1.53
1:2:541:LEU:HD13	5:6:479:ALA:N	1.41	1.31
1:2:541:LEU:HD22	5:6:480:GLY:N	1.49	1.28
1:2:541:LEU:CD1	5:6:479:ALA:CA	1.93	1.27
5:6:498:ILE:HD12	5:6:511:ASN:O	1.29	1.25
1:2:545:VAL:HG11	1:2:554:TRP:O	1.36	1.20
1:2:541:LEU:HD13	5:6:478:ARG:C	1.64	1.15
5:6:498:ILE:CD1	5:6:511:ASN:O	2.00	1.09
6:7:182:TYR:HB3	6:7:220:LEU:HB2	1.33	1.08
6:7:387:LYS:HB2	6:7:387:LYS:HZ2	1.18	1.05
1:2:543:ALA:CB	1:2:557:GLU:O	2.05	1.04
6:7:416:ALA:HA	6:7:431:GLY:HA2	1.36	1.03
1:2:541:LEU:HD11	5:6:479:ALA:HA	1.04	1.00
6:7:387:LYS:CB	6:7:387:LYS:NZ	2.23	0.99
6:7:615:ALA:HA	6:7:618:ARG:HG2	1.43	0.99
4:5:589:ARG:HB2	4:5:607:ILE:HD13	1.44	0.99
6:7:462:MET:HG2	6:7:514:ARG:HB3	1.44	0.97
2:3:346:LYS:NZ	2:3:346:LYS:HB3	1.78	0.97
1:2:543:ALA:HA	1:2:557:GLU:O	1.64	0.96
1:2:541:LEU:HD22	5:6:479:ALA:C	1.85	0.95
1:2:543:ALA:CA	1:2:557:GLU:O	2.16	0.93
6:7:317:ALA:HB3	6:7:564:ASN:HB2	1.49	0.92
6:7:441:VAL:HG22	6:7:483:SER:HB3	1.51	0.92
1:2:545:VAL:CG2	1:2:554:TRP:CD1	2.53	0.91
6:7:438:ASP:HB2	6:7:481:ARG:H	1.36	0.91
1:2:541:LEU:HD22	5:6:480:GLY:H	1.31	0.91
1:2:541:LEU:CD1	5:6:478:ARG:O	2.19	0.90
1:2:541:LEU:CD2	5:6:479:ALA:C	2.40	0.90
1:2:541:LEU:CD1	5:6:478:ARG:C	2.40	0.90
6:7:207:PRO:HD2	6:7:220:LEU:HD21	1.52	0.90
1:2:541:LEU:CG	5:6:479:ALA:HA	2.02	0.90
3:4:357:LEU:HD13	3:4:375:LEU:HD13	1.53	0.89
6:7:354:LEU:HD21	6:7:394:ILE:HD12	1.55	0.89
6:7:397:LEU:HD11	6:7:556:MET:HB2	1.55	0.89
1:2:541:LEU:CD2	5:6:480:GLY:N	2.35	0.89
1:2:543:ALA:HB1	1:2:557:GLU:O	1.71	0.89
3:4:518:LYS:HE2	3:4:618:ALA:HB1	1.53	0.89
6:7:358:LEU:HD11	6:7:394:ILE:HD11	1.55	0.89
10:H:81:LEU:HD21	13:N:155:VAL:HG21	1.56	0.88
6:7:321:PRO:HA	6:7:324:LEU:HD23	1.56	0.87
1:2:543:ALA:O	1:2:556:LEU:HD12	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:180:ALA:HB1	6:7:222:LEU:HD11	1.56	0.86
6:7:387:LYS:HZ2	6:7:387:LYS:CB	1.84	0.86
4:5:614:ALA:HA	4:5:617:ARG:HE	1.40	0.86
6:7:386:ALA:HA	15:7:801:ADP:H5'1	1.56	0.85
6:7:587:GLU:HG3	6:7:590:ARG:HE	1.41	0.85
4:5:619:SER:HB3	4:5:636:VAL:HG21	1.58	0.85
4:5:377:LEU:HB3	4:5:485:ALA:HB3	1.58	0.84
6:7:414:LEU:HD11	6:7:450:MET:HE2	1.60	0.83
1:2:545:VAL:HG21	1:2:554:TRP:CD1	2.12	0.83
2:3:454:TYR:OH	2:3:458:LYS:N	2.10	0.83
1:2:545:VAL:HG22	1:2:554:TRP:CD1	2.12	0.83
6:7:499:ARG:HG3	6:7:503:GLN:HG2	1.60	0.83
2:3:422:GLU:HG3	2:3:610:ARG:HH22	1.44	0.82
6:7:421:ASP:HB2	6:7:425:GLY:H	1.44	0.82
10:H:176:LEU:HD11	10:H:192:LEU:HD11	1.62	0.82
3:4:486:LEU:O	3:4:697:ARG:NH1	2.13	0.81
10:H:122:TYR:O	10:H:125:SER:OG	1.98	0.81
1:2:541:LEU:HD13	5:6:478:ARG:O	1.77	0.81
6:7:533:LEU:HD12	15:7:801:ADP:HN62	1.46	0.80
3:4:594:GLU:OE1	3:4:595:GLN:OE1	1.99	0.80
6:7:571:PRO:HB3	6:7:623:ASP:HA	1.62	0.79
6:7:531:LEU:HB3	6:7:535:LYS:HZ3	1.47	0.79
7:F:9:DT:H2"	7:F:10:DT:H72	1.65	0.79
2:3:342:PRO:HG3	4:5:506:THR:HG22	1.65	0.79
4:5:109:ARG:NH1	11:L:78:GLU:O	2.16	0.79
6:7:613:SER:OG	6:7:629:ASP:OD1	2.01	0.79
10:H:96:ARG:NH1	10:H:100:GLY:O	2.16	0.78
12:M:8:PRO:N	12:M:11:TYR:HH	1.81	0.78
6:7:315:LYS:HE2	6:7:317:ALA:HA	1.64	0.78
1:2:515:SER:OG	14:2:901:ATP:O1B	2.01	0.78
3:4:594:GLU:OE1	3:4:595:GLN:CD	2.22	0.78
1:2:520:TYR:O	1:2:524:VAL:HB	1.84	0.77
5:6:102:LYS:NZ	5:6:103:ASP:O	2.18	0.77
6:7:356:LEU:HD21	6:7:616:LEU:HD12	1.66	0.77
6:7:501:VAL:HG11	6:7:599:THR:HG23	1.66	0.76
7:F:-11:DA:H2"	7:F:-10:DT:H71	1.66	0.76
6:7:263:ARG:NH1	6:7:266:GLN:OE1	2.19	0.76
6:7:500:THR:HG22	6:7:503:GLN:HE21	1.50	0.76
6:7:170:CYS:HA	6:7:235:VAL:HG13	1.67	0.76
6:7:270:HIS:HB2	6:7:307:ASN:HB3	1.67	0.76
4:5:554:SER:O	4:5:557:THR:OG1	2.03	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:541:LEU:HD12	5:6:478:ARG:O	1.85	0.75
3:4:296:SER:OG	3:4:353:GLN:NE2	2.20	0.75
6:7:52:LEU:O	6:7:56:ALA:N	2.18	0.75
5:6:363:GLN:NE2	5:6:491:ILE:O	2.20	0.75
9:A:398:GLU:OE2	9:A:431:GLN:NE2	2.20	0.75
4:5:36:GLU:O	4:5:40:THR:OG1	2.02	0.75
1:2:278:GLU:O	1:2:281:THR:OG1	2.05	0.74
6:7:387:LYS:HB2	6:7:387:LYS:NZ	1.86	0.74
2:3:331:ARG:NE	2:3:421:MET:O	2.21	0.74
2:3:346:LYS:HB3	2:3:346:LYS:HZ1	1.50	0.74
4:5:371:ASP:O	4:5:617:ARG:NH1	2.20	0.74
4:5:613:GLU:O	4:5:617:ARG:NE	2.20	0.74
1:2:706:GLU:O	1:2:709:ARG:NH2	2.21	0.74
6:7:335:ARG:HH12	6:7:552:LYS:HB2	1.52	0.74
14:2:902:ATP:H3'	4:5:386:GLN:HG3	1.69	0.74
6:7:431:GLY:HA3	6:7:435:VAL:HG11	1.68	0.74
6:7:387:LYS:NZ	6:7:387:LYS:HB3	2.03	0.74
1:2:186:SER:O	1:2:190:THR:OG1	2.04	0.73
9:A:77:CYS:SG	9:A:78:GLY:N	2.61	0.73
10:H:90:ARG:NH2	13:N:113:GLU:OE2	2.21	0.73
1:2:547:ARG:NH2	1:2:554:TRP:O	2.22	0.73
6:7:178:VAL:HG21	6:7:228:LYS:HD2	1.70	0.73
6:7:151:GLU:HA	6:7:153:LYS:HE3	1.69	0.73
11:L:135:PHE:O	12:M:126:ARG:NH2	2.22	0.73
13:N:65:LEU:O	13:N:69:GLN:NE2	2.22	0.73
6:7:587:GLU:HA	6:7:590:ARG:HG2	1.70	0.73
6:7:467:ILE:HD11	6:7:480:ALA:HB3	1.69	0.72
3:4:353:GLN:NE2	3:4:354:LEU:O	2.22	0.72
3:4:561:GLN:OE1	5:6:203:GLN:NE2	2.22	0.72
6:7:387:LYS:HB3	6:7:387:LYS:HZ3	1.52	0.72
6:7:388:SER:N	15:7:801:ADP:O1A	2.15	0.72
6:7:612:LEU:HD11	6:7:633:ALA:HB2	1.71	0.72
6:7:435:VAL:HG13	6:7:478:LEU:HD21	1.72	0.72
6:7:459:HIS:O	6:7:514:ARG:NH1	2.23	0.72
6:7:387:LYS:CB	6:7:387:LYS:HZ3	2.03	0.71
7:F:1:DA:H2"	7:F:2:DT:H71	1.72	0.71
9:A:68:ASP:O	9:A:70:LYS:NZ	2.22	0.71
6:7:554:LEU:HD21	6:7:558:LEU:HB2	1.73	0.71
13:N:26:ASP:OD2	13:N:37:LYS:NZ	2.22	0.71
4:5:436:GLY:O	4:5:566:ARG:NH1	2.22	0.71
1:2:245:ASP:OD2	1:2:249:LYS:NZ	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:206:CYS:HB3	6:7:211:CYS:HB3	1.71	0.71
3:4:605:ILE:HG13	5:6:232:ALA:HB1	1.73	0.70
5:6:410:TYR:OH	5:6:452:ASP:OD2	2.07	0.70
3:4:453:LEU:O	3:4:457:LYS:NZ	2.23	0.70
5:6:118:ARG:NH1	5:6:204:GLU:OE2	2.23	0.70
11:L:48:MET:O	11:L:52:LEU:N	2.25	0.70
2:3:233:GLN:NE2	2:3:234:ILE:O	2.24	0.70
5:6:355:GLU:OE1	5:6:650:ARG:NH2	2.25	0.70
6:7:501:VAL:HG23	6:7:505:ILE:HD11	1.74	0.70
2:3:190:TYR:OH	6:7:156:HIS:N	2.24	0.70
5:6:498:ILE:CD1	5:6:511:ASN:C	2.59	0.69
2:3:341:ASP:OD1	2:3:341:ASP:N	2.20	0.69
9:A:268:LEU:O	9:A:282:LYS:NZ	2.25	0.69
9:A:302:SER:OG	9:A:433:LYS:NZ	2.24	0.69
6:7:589:ARG:O	6:7:593:ARG:NH2	2.25	0.69
4:5:535:ASN:O	4:5:541:ASN:ND2	2.25	0.69
5:6:121:THR:OG1	5:6:124:LYS:NZ	2.26	0.69
3:4:273:ASN:ND2	3:4:363:ASP:O	2.26	0.69
1:2:444:GLU:N	1:2:444:GLU:OE1	2.25	0.69
1:2:545:VAL:CG1	1:2:554:TRP:O	2.28	0.69
1:2:545:VAL:HG22	1:2:554:TRP:NE1	2.07	0.69
1:2:700:TYR:OH	1:2:757:MET:O	2.10	0.69
3:4:181:GLU:OE2	3:4:192:ASN:ND2	2.25	0.69
6:7:520:LEU:HD21	6:7:643:SER:HB2	1.73	0.69
1:2:262:VAL:HG12	1:2:263:THR:HG23	1.74	0.68
6:7:372:ARG:HH12	6:7:376:ASN:HD21	1.41	0.68
6:7:378:CYS:SG	6:7:379:LEU:N	2.67	0.68
9:A:470:PHE:CE2	9:A:479:LEU:HD21	2.29	0.68
2:3:387:ARG:NH2	7:F:7:DT:OP1	2.26	0.68
4:5:329:TYR:OH	4:5:348:LYS:O	2.11	0.68
6:7:144:GLU:H	6:7:162:THR:HG21	1.58	0.68
6:7:516:ASP:OD1	6:7:517:LEU:HD12	1.93	0.68
12:M:61:GLU:N	12:M:61:GLU:OE1	2.27	0.68
2:3:346:LYS:NZ	2:3:346:LYS:CB	2.56	0.68
2:3:375:ALA:HB1	7:F:8:DT:H5"	1.76	0.68
6:7:446:GLU:N	6:7:487:ALA:O	2.26	0.68
6:7:595:GLN:HB2	6:7:598:MET:HG2	1.75	0.68
12:M:16:ILE:O	12:M:20:GLN:NE2	2.26	0.68
1:2:541:LEU:HD11	5:6:479:ALA:CA	1.94	0.68
4:5:538:LEU:O	4:5:541:ASN:ND2	2.27	0.67
1:2:349:ASN:ND2	1:2:351:GLU:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:123:CYS:SG	2:3:233:GLN:NE2	2.67	0.67
2:3:548:LYS:O	2:3:551:GLN:NE2	2.28	0.67
4:5:589:ARG:HA	4:5:607:ILE:HG21	1.76	0.67
3:4:410:SER:OG	6:7:199:SER:OG	2.09	0.67
6:7:130:LEU:O	6:7:228:LYS:NZ	2.22	0.67
6:7:393:TYR:HA	6:7:396:ARG:HH22	1.60	0.67
6:7:406:GLY:HA2	6:7:450:MET:HA	1.77	0.67
10:H:93:LYS:NZ	10:H:122:TYR:OH	2.18	0.67
6:7:261:VAL:HG13	6:7:264:MET:HG3	1.76	0.67
6:7:462:MET:HE2	6:7:514:ARG:HD2	1.75	0.67
13:N:85:PHE:O	13:N:89:VAL:HG23	1.95	0.67
4:5:584:ARG:HG2	4:5:640:LEU:HD23	1.77	0.67
1:2:541:LEU:CD2	5:6:479:ALA:CA	2.71	0.66
1:2:545:VAL:HG21	1:2:554:TRP:HD1	1.59	0.66
3:4:686:MET:O	3:4:690:ARG:NH2	2.27	0.66
6:7:564:ASN:O	6:7:567:LYS:HG2	1.96	0.66
1:2:541:LEU:CD1	5:6:479:ALA:N	2.35	0.66
6:7:308:LYS:HZ1	6:7:560:ARG:HH22	1.42	0.66
2:3:613:GLU:O	2:3:617:ARG:HD3	1.96	0.66
3:4:196:TYR:OH	3:4:217:HIS:ND1	2.29	0.66
6:7:496:ASN:HD22	6:7:499:ARG:HG2	1.59	0.66
1:2:270:ILE:O	1:2:428:HIS:ND1	2.28	0.66
1:2:513:ALA:HA	14:2:901:ATP:PA	2.36	0.66
1:2:590:GLU:HG2	1:2:742:ARG:HD3	1.76	0.66
3:4:510:LEU:HD12	3:4:518:LYS:HD2	1.76	0.66
10:H:145:ASN:ND2	10:H:191:SER:O	2.29	0.66
1:2:790:LYS:O	1:2:794:THR:OG1	2.04	0.66
3:4:693:ILE:O	3:4:697:ARG:NH2	2.28	0.66
5:6:152:CYS:SG	5:6:180:SER:OG	2.49	0.66
6:7:393:TYR:HA	6:7:396:ARG:NH2	2.11	0.66
11:L:171:GLN:N	11:L:171:GLN:OE1	2.29	0.66
6:7:90:GLN:NE2	6:7:91:GLN:O	2.29	0.66
6:7:522:GLN:OE1	6:7:524:LYS:HG3	1.96	0.66
9:A:87:LEU:O	9:A:90:SER:OG	2.13	0.66
11:L:7:GLU:OE2	11:L:7:GLU:N	2.28	0.66
13:N:183:LEU:HD11	13:N:211:ILE:HD11	1.76	0.66
3:4:711:ARG:NH2	3:4:761:GLU:OE1	2.29	0.66
5:6:386:ILE:HD12	5:6:492:LEU:HD21	1.78	0.66
4:5:378:GLY:HA3	4:5:517:VAL:HB	1.78	0.66
4:5:394:VAL:HG22	4:5:555:LEU:HD12	1.77	0.66
5:6:458:ASP:OD1	5:6:460:ARG:NH2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:625:SER:OG	1:2:649:LYS:NZ	2.29	0.65
1:2:788:MET:O	1:2:792:ARG:NE	2.28	0.65
2:3:477:LEU:HD12	2:3:606:PRO:HG3	1.78	0.65
12:M:74:PRO:O	12:M:78:ARG:N	2.29	0.65
6:7:326:GLU:HA	6:7:329:GLN:HB3	1.77	0.65
6:7:555:ASP:HB3	6:7:558:LEU:HD23	1.78	0.65
9:A:432:ALA:O	9:A:436:HIS:ND1	2.26	0.65
1:2:278:GLU:OE2	1:2:369:ARG:NH1	2.29	0.65
1:2:534:GLN:NE2	1:2:576:LYS:O	2.29	0.65
2:3:331:ARG:O	2:3:617:ARG:NH2	2.16	0.65
4:5:593:GLY:O	4:5:597:LYS:HD2	1.96	0.65
6:7:166:ILE:HD11	6:7:240:HIS:HD2	1.60	0.65
6:7:286:ALA:HA	6:7:290:GLN:HB2	1.79	0.65
6:7:589:ARG:HB3	6:7:593:ARG:HH22	1.61	0.65
12:M:32:GLN:NE2	12:M:44:ASP:O	2.29	0.65
1:2:541:LEU:CD2	5:6:479:ALA:HA	2.26	0.65
2:3:68:ASP:OD1	2:3:68:ASP:N	2.30	0.65
2:3:346:LYS:HB3	2:3:346:LYS:HZ2	1.60	0.65
4:5:622:LEU:HB3	4:5:635:HIS:CE1	2.31	0.65
6:7:375:ILE:O	6:7:483:SER:OG	2.13	0.65
13:N:58:SER:N	13:N:131:LYS:O	2.30	0.65
1:2:643:ASP:N	1:2:643:ASP:OD1	2.28	0.64
2:3:52:LYS:NZ	12:M:87:ALA:O	2.27	0.64
6:7:517:LEU:HD21	6:7:636:LEU:HD21	1.79	0.64
11:L:13:CYS:SG	11:L:14:MET:N	2.69	0.64
13:N:194:VAL:HG21	13:N:219:LEU:HD21	1.78	0.64
9:A:258:LEU:O	9:A:262:GLN:NE2	2.31	0.64
6:7:631:ALA:HA	6:7:634:LEU:HD21	1.79	0.64
6:7:275:GLY:HA3	6:7:300:ALA:HA	1.78	0.64
2:3:321:GLU:OE2	2:3:322:LYS:N	2.30	0.64
6:7:170:CYS:SG	6:7:233:GLN:NE2	2.70	0.64
2:3:455:ASP:HB3	2:3:481:LEU:HD21	1.80	0.64
5:6:151:MET:SD	5:6:152:CYS:N	2.70	0.64
6:7:50:ILE:O	6:7:139:LYS:N	2.31	0.64
2:3:388:LEU:HD21	6:7:249:ILE:HD12	1.79	0.64
5:6:26:GLN:NE2	5:6:94:ASP:OD2	2.31	0.64
5:6:387:VAL:HG22	5:6:495:ALA:HB3	1.80	0.64
6:7:361:GLY:O	6:7:618:ARG:NH2	2.31	0.64
5:6:147:SER:OG	5:6:163:GLU:OE2	2.10	0.64
11:L:145:LEU:HD12	11:L:148:LEU:HB3	1.80	0.64
4:5:356:GLY:O	4:5:624:LYS:NZ	2.24	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:202:ILE:HD12	5:6:220:ILE:HD13	1.81	0.63
6:7:261:VAL:HG21	6:7:301:HIS:O	1.98	0.63
3:4:266:PHE:HB3	3:4:394:THR:HG21	1.80	0.63
6:7:315:LYS:HE2	6:7:317:ALA:CA	2.27	0.63
9:A:524:GLU:O	9:A:528:ARG:NH1	2.31	0.63
11:L:26:LEU:HD21	13:N:80:LEU:HD13	1.80	0.63
1:2:541:LEU:CD1	5:6:479:ALA:CB	2.75	0.63
6:7:510:ALA:O	6:7:513:SER:OG	2.14	0.63
1:2:435:LYS:HD2	1:2:527:ARG:NE	2.12	0.63
1:2:579:ASP:O	1:2:583:THR:OG1	2.12	0.63
2:3:199:GLN:NE2	2:3:212:ARG:O	2.31	0.63
6:7:170:CYS:CA	6:7:235:VAL:HG13	2.29	0.63
6:7:554:LEU:CD2	6:7:558:LEU:HB2	2.29	0.63
6:7:631:ALA:HA	6:7:634:LEU:CD2	2.29	0.63
1:2:586:HIS:CD2	1:2:641:ARG:HH11	2.17	0.63
1:2:711:LYS:O	1:2:712:LEU:HD23	1.99	0.63
13:N:55:ILE:HD12	13:N:112:ILE:HD11	1.80	0.63
2:3:29:TYR:O	2:3:33:VAL:HG11	1.98	0.63
2:3:130:LYS:O	2:3:132:SER:OG	2.10	0.63
6:7:447:PHE:H	6:7:488:ALA:HB2	1.64	0.63
5:6:149:VAL:HG12	5:6:157:THR:HG22	1.81	0.62
5:6:498:ILE:HD11	5:6:511:ASN:C	2.19	0.62
3:4:523:GLN:O	3:4:527:ASN:ND2	2.32	0.62
6:7:414:LEU:HD11	6:7:450:MET:CE	2.28	0.62
11:L:78:GLU:OE1	11:L:81:SER:OG	2.11	0.62
4:5:519:ASP:N	4:5:519:ASP:OD1	2.32	0.62
6:7:174:LYS:HG2	6:7:423:LEU:HD11	1.80	0.62
10:H:23:SER:O	10:H:91:ARG:NH2	2.32	0.62
6:7:528:ASP:O	6:7:532:ARG:HG3	2.00	0.62
1:2:541:LEU:HD13	5:6:479:ALA:CB	2.25	0.62
14:3:901:ATP:H8	4:5:609:VAL:HG21	1.65	0.62
6:7:568:ARG:HH22	6:7:569:LYS:HD3	1.64	0.62
4:5:312:THR:HG22	12:M:141:GLN:HG2	1.81	0.62
5:6:612:GLN:O	5:6:615:SER:OG	2.12	0.62
6:7:181:THR:O	6:7:222:LEU:HD12	1.99	0.62
3:4:367:GLY:N	6:7:438:ASP:OD1	2.33	0.62
6:7:448:ASP:OD1	6:7:448:ASP:N	2.29	0.62
3:4:521:MET:O	3:4:525:VAL:HG23	2.00	0.62
1:2:627:THR:OG1	1:2:630:GLU:OE1	2.17	0.61
6:7:37:LEU:HA	6:7:40:LEU:HD12	1.82	0.61
6:7:167:VAL:HG11	6:7:266:GLN:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:411:GLY:O	6:7:415:THR:HG22	2.00	0.61
1:2:439:GLN:OE1	1:2:699:GLN:NE2	2.34	0.61
3:4:342:LEU:O	3:4:343:ILE:HD13	2.01	0.61
6:7:99:LEU:HD21	6:7:228:LYS:HE2	1.82	0.61
6:7:178:VAL:O	6:7:195:VAL:N	2.26	0.61
6:7:533:LEU:HA	6:7:536:HIS:HB2	1.82	0.61
5:6:364:GLN:O	5:6:572:ARG:NH2	2.33	0.61
5:6:505:SER:OG	5:6:506:LYS:NZ	2.32	0.61
12:M:43:SER:OG	12:M:45:ASP:O	2.17	0.61
4:5:94:PHE:HD2	4:5:121:ILE:HG21	1.64	0.61
6:7:372:ARG:HE	6:7:464:GLN:HB2	1.65	0.61
1:2:436:GLN:N	1:2:436:GLN:OE1	2.33	0.61
2:3:159:LEU:HD23	2:3:241:LEU:HD12	1.83	0.61
3:4:706:ASP:OD1	3:4:709:GLN:NE2	2.33	0.61
6:7:531:LEU:HB3	6:7:535:LYS:NZ	2.15	0.61
13:N:138:THR:O	13:N:142:GLN:NE2	2.34	0.61
1:2:541:LEU:HD21	5:6:479:ALA:C	2.20	0.61
6:7:420:LYS:HD3	6:7:427:MET:CE	2.31	0.61
6:7:587:GLU:HA	6:7:590:ARG:CG	2.31	0.61
4:5:563:HIS:O	4:5:567:THR:OG1	2.19	0.61
4:5:596:GLU:HG2	4:5:602:ARG:HA	1.82	0.61
5:6:548:HIS:O	5:6:550:ASN:ND2	2.34	0.61
6:7:537:ILE:HD12	15:7:801:ADP:C2	2.36	0.61
9:A:312:GLN:N	9:A:312:GLN:OE1	2.34	0.61
5:6:393:ALA:HA	15:6:901:ADP:H5'1	1.83	0.61
6:7:151:GLU:HA	6:7:153:LYS:CE	2.31	0.61
6:7:505:ILE:HD12	6:7:512:LEU:HD11	1.82	0.61
6:7:308:LYS:HZ2	6:7:560:ARG:HH12	1.49	0.60
6:7:372:ARG:O	6:7:611:ARG:NH2	2.34	0.60
5:6:116:LYS:NZ	5:6:205:THR:HG21	2.16	0.60
6:7:305:CYS:HB3	6:7:309:ASN:ND2	2.17	0.60
5:6:115:HIS:CG	5:6:129:ILE:HD11	2.36	0.60
6:7:315:LYS:HD2	6:7:319:LEU:HD23	1.82	0.60
6:7:417:ALA:N	6:7:430:GLU:O	2.34	0.60
9:A:59:LYS:NZ	9:A:86:LEU:O	2.34	0.60
1:2:539:VAL:HG13	1:2:544:TYR:HE2	1.64	0.60
4:5:53:THR:O	4:5:57:ASN:ND2	2.34	0.60
6:7:272:VAL:HB	6:7:304:ILE:O	2.01	0.60
6:7:524:LYS:HB3	6:7:525:PRO:HD2	1.82	0.60
9:A:563:LEU:O	9:A:567:LEU:N	2.34	0.60
3:4:270:LYS:NZ	3:4:363:ASP:OD2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:132:ILE:HD12	4:5:226:GLU:HB3	1.83	0.60
1:2:303:VAL:O	1:2:304:LEU:HD23	2.02	0.60
3:4:673:TYR:HE1	6:7:573:ILE:HB	1.67	0.60
4:5:442:ASP:OD1	4:5:443:GLU:N	2.35	0.60
5:6:205:THR:HG22	5:6:207:ALA:H	1.66	0.60
12:M:15:ASP:O	12:M:16:ILE:HD13	2.01	0.60
1:2:589:MET:SD	1:2:611:VAL:HG21	2.42	0.60
2:3:388:LEU:CD2	6:7:249:ILE:HD12	2.32	0.60
2:3:422:GLU:OE1	15:7:801:ADP:O3A	2.20	0.60
5:6:108:PHE:O	5:6:294:SER:OG	2.10	0.60
6:7:280:LEU:HB2	6:7:297:PHE:CD1	2.36	0.60
6:7:364:LYS:O	6:7:365:ARG:HD2	2.02	0.60
2:3:244:LYS:NZ	4:5:160:ALA:O	2.35	0.60
4:5:373:ASN:ND2	4:5:481:VAL:HG12	2.17	0.60
5:6:581:GLU:O	5:6:585:MET:N	2.35	0.60
6:7:455:ARG:HG2	6:7:508:PRO:HG3	1.82	0.60
11:L:64:GLU:N	11:L:64:GLU:OE1	2.35	0.60
1:2:297:VAL:HG23	1:2:397:LEU:HD11	1.84	0.60
1:2:487:GLY:O	1:2:756:ARG:NH1	2.35	0.59
1:2:518:LEU:O	1:2:521:THR:OG1	2.11	0.59
3:4:346:ARG:NH1	5:6:76:GLU:OE1	2.33	0.59
5:6:618:ARG:HA	5:6:621:GLU:HG2	1.84	0.59
13:N:123:GLU:O	13:N:127:GLU:N	2.35	0.59
1:2:667:SER:O	1:2:670:LYS:NZ	2.20	0.59
2:3:208:GLY:N	4:5:435:ASP:OD2	2.35	0.59
4:5:383:ALA:O	4:5:387:LEU:HD12	2.03	0.59
6:7:405:THR:HG22	6:7:406:GLY:H	1.66	0.59
12:M:89:THR:O	12:M:127:GLN:NE2	2.35	0.59
2:3:361:ILE:HG22	4:5:472:THR:HG21	1.83	0.59
4:5:132:ILE:HA	4:5:135:LEU:HD23	1.85	0.59
5:6:47:LEU:HD11	5:6:53:CYS:H	1.67	0.59
6:7:147:HIS:HB2	6:7:162:THR:O	2.02	0.59
6:7:287:GLN:HG2	6:7:288:MET:H	1.66	0.59
6:7:212:ARG:HH21	6:7:213:VAL:HG12	1.67	0.59
10:H:36:GLN:NE2	10:H:36:GLN:O	2.35	0.59
2:3:334:ILE:HD11	2:3:617:ARG:HB3	1.84	0.59
4:5:418:ASP:OD1	4:5:420:GLN:NE2	2.36	0.59
6:7:66:VAL:HG22	6:7:73:TYR:CD2	2.36	0.59
6:7:209:ASP:HA	6:7:212:ARG:HB2	1.84	0.59
6:7:386:ALA:CA	15:7:801:ADP:H5'1	2.29	0.59
13:N:37:LYS:O	13:N:41:ILE:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:299:ALA:HA	2:3:352:TYR:CE1	2.37	0.59
5:6:609:THR:HG23	5:6:610:VAL:H	1.67	0.59
6:7:479:ASN:HB3	6:7:481:ARG:HH21	1.68	0.59
5:6:69:LEU:O	5:6:73:ILE:N	2.35	0.59
5:6:70:ALA:O	5:6:74:ILE:N	2.35	0.59
5:6:342:LEU:O	5:6:345:SER:OG	2.21	0.59
5:6:423:ALA:N	5:6:438:ALA:O	2.35	0.59
5:6:427:ARG:HH22	7:F:13:DT:H4'	1.68	0.59
6:7:184:CYS:HA	6:7:220:LEU:HA	1.84	0.59
6:7:585:TYR:HE1	6:7:605:ASN:HB2	1.65	0.59
7:F:11:DT:H2"	7:F:12:DT:C7	2.33	0.59
4:5:89:GLU:OE2	4:5:89:GLU:N	2.36	0.59
6:7:381:GLY:HA2	6:7:490:PRO:CG	2.33	0.59
1:2:258:THR:O	1:2:261:ARG:NH1	2.36	0.58
6:7:612:LEU:HD11	6:7:633:ALA:CB	2.32	0.58
3:4:536:SER:O	3:4:539:GLY:N	2.36	0.58
6:7:607:LEU:O	6:7:611:ARG:HG3	2.03	0.58
12:M:102:TYR:CD1	12:M:125:LEU:HD11	2.38	0.58
14:2:902:ATP:O3'	4:5:386:GLN:NE2	2.35	0.58
6:7:171:THR:HB	6:7:423:LEU:HD22	1.85	0.58
6:7:317:ALA:O	6:7:565:LEU:HD22	2.03	0.58
6:7:574:PRO:O	6:7:578:THR:HG23	2.03	0.58
1:2:405:ASN:OD1	1:2:405:ASN:N	2.34	0.58
2:3:415:THR:HA	2:3:418:HIS:CD2	2.39	0.58
7:F:-6:DT:H1'	7:F:-5:DC:H5'	1.85	0.58
9:A:26:ASP:OD1	9:A:27:ILE:N	2.37	0.58
6:7:500:THR:HG22	6:7:503:GLN:NE2	2.17	0.58
11:L:78:GLU:O	11:L:81:SER:OG	2.21	0.58
1:2:724:TYR:HA	1:2:727:LEU:HD12	1.86	0.58
2:3:582:GLU:O	2:3:586:ASN:ND2	2.36	0.58
13:N:55:ILE:CD1	13:N:112:ILE:HD11	2.33	0.58
13:N:153:HIS:O	13:N:157:THR:OG1	2.20	0.58
1:2:565:ASP:OD1	1:2:608:ARG:N	2.36	0.58
6:7:421:ASP:HB2	6:7:425:GLY:N	2.17	0.58
11:L:21:PHE:O	11:L:38:ALA:N	2.36	0.58
9:A:23:VAL:HG22	9:A:75:VAL:O	2.04	0.58
9:A:321:GLU:O	9:A:325:HIS:ND1	2.34	0.58
2:3:335:ASN:OD1	2:3:443:VAL:N	2.36	0.58
5:6:442:MET:SD	5:6:485:LEU:HD13	2.44	0.58
1:2:370:ILE:HG22	1:2:371:PRO:HD2	1.87	0.57
1:2:434:SER:HB3	1:2:438:VAL:HG11	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:529:VAL:O	3:4:532:SER:OG	2.22	0.57
4:5:312:THR:HG22	12:M:141:GLN:CG	2.34	0.57
4:5:614:ALA:HA	4:5:617:ARG:NE	2.16	0.57
5:6:139:HIS:HB2	5:6:199:LYS:O	2.04	0.57
6:7:531:LEU:HD12	6:7:531:LEU:H	1.68	0.57
11:L:85:THR:OG1	11:L:86:LYS:N	2.37	0.57
6:7:178:VAL:HG22	6:7:228:LYS:HB3	1.86	0.57
2:3:260:ASN:OD1	2:3:260:ASN:N	2.37	0.57
6:7:357:LEU:HD11	6:7:483:SER:OG	2.04	0.57
14:2:902:ATP:O3G	4:5:380:PRO:HB3	2.04	0.57
4:5:505:PRO:O	4:5:509:SER:N	2.38	0.57
5:6:471:GLN:O	5:6:471:GLN:NE2	2.38	0.57
6:7:270:HIS:HB2	6:7:307:ASN:CB	2.34	0.57
6:7:387:LYS:HB3	15:7:801:ADP:O2B	2.05	0.57
2:3:53:ARG:NH1	12:M:87:ALA:HB2	2.20	0.57
2:3:299:ALA:HB1	2:3:302:ILE:HD11	1.86	0.57
2:3:320:VAL:HB	2:3:620:THR:HG21	1.87	0.57
5:6:385:CYS:HA	5:6:493:ALA:HB3	1.86	0.57
9:A:103:PRO:HD3	9:A:209:TYR:CE1	2.38	0.57
1:2:598:LYS:NZ	7:F:11:DT:OP2	2.27	0.57
5:6:148:GLY:N	5:6:163:GLU:OE2	2.38	0.57
6:7:280:LEU:HB2	6:7:297:PHE:HD1	1.70	0.57
9:A:395:ALA:O	9:A:431:GLN:NE2	2.36	0.57
12:M:150:ASP:OD1	12:M:152:ILE:N	2.38	0.57
2:3:378:THR:OG1	2:3:386:ARG:O	2.22	0.57
5:6:41:THR:O	5:6:45:ALA:N	2.37	0.57
6:7:561:ARG:O	6:7:565:LEU:HD23	2.04	0.57
6:7:575:ASP:HA	6:7:578:THR:CG2	2.34	0.57
1:2:541:LEU:HD22	5:6:479:ALA:CA	2.32	0.57
1:2:214:SER:OG	1:2:386:ASP:OD2	2.23	0.56
2:3:327:GLY:O	6:7:396:ARG:NE	2.38	0.56
9:A:124:GLU:HB3	9:A:127:ILE:HD11	1.86	0.56
2:3:422:GLU:CG	2:3:610:ARG:HH22	2.17	0.56
5:6:440:ALA:HA	5:6:443:LEU:HD12	1.86	0.56
6:7:319:LEU:CD1	6:7:322:GLU:HB3	2.36	0.56
6:7:575:ASP:HA	6:7:578:THR:HG23	1.87	0.56
2:3:443:VAL:O	2:3:444:LEU:HD23	2.05	0.56
4:5:128:ASN:ND2	9:A:340:GLN:OE1	2.38	0.56
6:7:566:CYS:HB2	6:7:618:ARG:O	2.05	0.56
9:A:21:ILE:HG23	9:A:52:ILE:HD11	1.87	0.56
9:A:299:VAL:O	9:A:302:SER:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:507:SER:O	5:6:511:ASN:N	2.38	0.56
12:M:104:PHE:CE2	12:M:108:LEU:HD13	2.41	0.56
5:6:531:GLU:N	5:6:531:GLU:OE1	2.39	0.56
9:A:82:ASP:O	9:A:85:GLU:N	2.37	0.56
9:A:253:ALA:O	9:A:257:GLU:N	2.39	0.56
9:A:411:LEU:HD11	10:H:200:HIS:NE2	2.19	0.56
6:7:334:GLU:HA	6:7:337:ALA:HB2	1.88	0.56
6:7:554:LEU:HD23	6:7:555:ASP:N	2.20	0.56
1:2:435:LYS:HD2	1:2:527:ARG:CZ	2.36	0.56
1:2:714:ASN:ND2	9:A:465:GLU:OE2	2.39	0.56
6:7:159:LYS:O	6:7:161:VAL:HG23	2.05	0.56
6:7:224:THR:HA	6:7:227:SER:HB3	1.88	0.56
6:7:233:GLN:HG3	6:7:262:THR:HG23	1.87	0.56
6:7:157:ILE:HD12	6:7:279:PRO:HG3	1.86	0.56
6:7:577:LEU:O	6:7:581:ILE:HG23	2.06	0.56
4:5:608:THR:OG1	4:5:611:GLN:OE1	2.17	0.55
5:6:429:GLU:N	5:6:429:GLU:OE1	2.39	0.55
6:7:183:THR:H	6:7:221:TYR:H	1.54	0.55
6:7:469:ILE:CD1	6:7:476:THR:HB	2.37	0.55
9:A:22:VAL:CG1	9:A:29:ALA:HB1	2.35	0.55
1:2:543:ALA:HA	1:2:557:GLU:H	1.72	0.55
2:3:470:LEU:O	2:3:473:ARG:N	2.40	0.55
3:4:389:ASP:OD1	3:4:390:ARG:N	2.39	0.55
9:A:81:VAL:HG21	9:A:86:LEU:HD13	1.88	0.55
12:M:104:PHE:CZ	12:M:108:LEU:HD13	2.41	0.55
6:7:149:ILE:O	6:7:152:VAL:HG22	2.07	0.55
1:2:532:THR:OG1	1:2:533:GLY:N	2.37	0.55
6:7:171:THR:CB	6:7:423:LEU:HD22	2.37	0.55
6:7:203:VAL:HG11	6:7:207:PRO:HG3	1.88	0.55
6:7:223:GLN:HE22	6:7:226:GLY:HA3	1.72	0.55
6:7:572:THR:HG22	6:7:623:ASP:OD1	2.06	0.55
2:3:299:ALA:HB1	2:3:302:ILE:CG1	2.37	0.55
2:3:470:LEU:O	2:3:474:PHE:N	2.36	0.55
6:7:157:ILE:CD1	6:7:279:PRO:HG3	2.37	0.55
6:7:437:ALA:HB3	6:7:442:CYS:HB2	1.88	0.55
2:3:6:GLU:OE1	2:3:6:GLU:N	2.39	0.55
4:5:253:VAL:HG12	4:5:307:ARG:HH11	1.72	0.55
5:6:147:SER:HG	5:6:163:GLU:CD	2.07	0.55
6:7:168:THR:HG21	6:7:238:GLN:HB2	1.89	0.55
6:7:212:ARG:HG2	6:7:213:VAL:H	1.72	0.55
6:7:459:HIS:CD2	6:7:511:LEU:HD13	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:470:ALA:HA	6:7:473:GLY:HA2	1.89	0.55
6:7:205:ASP:O	6:7:220:LEU:HG	2.06	0.55
6:7:555:ASP:O	6:7:559:MET:HG3	2.07	0.55
9:A:32:ALA:CB	9:A:215:ALA:HB2	2.36	0.55
2:3:480:MET:O	2:3:481:LEU:HD23	2.07	0.55
3:4:555:THR:O	3:4:557:GLN:NE2	2.40	0.55
6:7:231:LYS:HB2	6:7:259:GLY:O	2.07	0.55
8:G:9:DA:H1'	8:G:10:DT:H5'	1.89	0.55
1:2:605:LEU:HD12	1:2:606:GLN:H	1.72	0.55
3:4:594:GLU:OE1	3:4:595:GLN:NE2	2.40	0.55
6:7:334:GLU:HA	6:7:337:ALA:CB	2.36	0.55
6:7:424:THR:HB	6:7:426:GLU:HG3	1.89	0.55
6:7:458:ILE:HG23	6:7:511:LEU:HD11	1.87	0.55
6:7:469:ILE:N	6:7:476:THR:OG1	2.33	0.55
1:2:188:LEU:HD22	1:2:200:TYR:HB3	1.89	0.55
1:2:545:VAL:CG1	1:2:547:ARG:HH21	2.20	0.55
1:2:744:ILE:HA	1:2:747:VAL:HG13	1.89	0.55
6:7:164:ARG:HH21	6:7:243:GLN:HE22	1.55	0.55
6:7:173:VAL:O	6:7:174:LYS:HD2	2.07	0.55
6:7:324:LEU:HA	6:7:327:LEU:HD12	1.89	0.55
9:A:102:ARG:O	9:A:104:LEU:N	2.40	0.55
3:4:722:VAL:HG11	3:4:731:ALA:HB3	1.89	0.54
6:7:285:PHE:HB3	6:7:287:GLN:NE2	2.22	0.54
11:L:153:ILE:HG23	11:L:157:ARG:HH21	1.72	0.54
6:7:335:ARG:NH1	6:7:552:LYS:HB2	2.22	0.54
6:7:437:ALA:O	6:7:482:VAL:HG23	2.06	0.54
2:3:261:ASN:OD1	2:3:262:ILE:N	2.40	0.54
6:7:462:MET:HG2	6:7:514:ARG:CB	2.29	0.54
3:4:550:THR:OG1	3:4:551:LYS:N	2.40	0.54
5:6:498:ILE:HD11	5:6:511:ASN:O	2.02	0.54
12:M:103:GLU:N	12:M:103:GLU:OE1	2.40	0.54
4:5:616:ILE:O	4:5:619:SER:OG	2.21	0.54
5:6:163:GLU:OE1	5:6:163:GLU:N	2.40	0.54
6:7:37:LEU:HD21	6:7:86:PRO:HG2	1.90	0.54
6:7:615:ALA:CA	6:7:618:ARG:HG2	2.29	0.54
6:7:178:VAL:CG2	6:7:228:LYS:HD2	2.38	0.54
6:7:499:ARG:HG3	6:7:503:GLN:CG	2.36	0.54
9:A:201:MET:O	9:A:205:THR:OG1	2.15	0.54
6:7:323:GLU:OE2	6:7:561:ARG:HD2	2.07	0.54
7:F:1:DA:C2'	7:F:2:DT:H71	2.37	0.54
10:H:22:SER:OG	10:H:26:ILE:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:539:VAL:HG13	1:2:544:TYR:CE2	2.41	0.54
14:2:902:ATP:C2	4:5:533:ILE:HD11	2.42	0.54
3:4:712:LEU:HD13	3:4:719:MET:SD	2.48	0.54
6:7:166:ILE:HG13	6:7:240:HIS:HA	1.89	0.54
6:7:536:HIS:O	6:7:546:GLN:NE2	2.40	0.54
3:4:698:GLU:N	3:4:698:GLU:OE1	2.41	0.54
5:6:205:THR:HG22	5:6:207:ALA:N	2.23	0.54
5:6:534:GLU:OE1	5:6:534:GLU:N	2.41	0.54
6:7:395:SER:O	6:7:401:SER:HB3	2.08	0.54
1:2:641:ARG:NH2	14:2:902:ATP:O1B	2.41	0.54
6:7:37:LEU:HD21	6:7:86:PRO:CG	2.38	0.54
6:7:212:ARG:NH2	6:7:213:VAL:HG12	2.23	0.54
6:7:407:ARG:HA	6:7:407:ARG:NE	2.23	0.54
1:2:272:GLU:O	1:2:273:LEU:HD22	2.07	0.53
3:4:536:SER:OG	3:4:576:ASP:N	2.41	0.53
4:5:468:LYS:NZ	7:F:10:DT:OP1	2.41	0.53
1:2:207:MET:SD	1:2:215:PHE:N	2.81	0.53
3:4:459:ASP:OD2	3:4:463:ARG:NE	2.40	0.53
6:7:77:PHE:CE1	6:7:136:VAL:HG21	2.43	0.53
6:7:586:VAL:O	6:7:590:ARG:HG2	2.08	0.53
6:7:588:LEU:HD21	6:7:605:ASN:HD22	1.74	0.53
2:3:20:LEU:HD23	2:3:80:TYR:CD1	2.44	0.53
4:5:577:ALA:HA	4:5:633:ASP:HB2	1.90	0.53
6:7:437:ALA:CB	6:7:442:CYS:HB2	2.38	0.53
9:A:461:TYR:HE2	9:A:463:LEU:HD13	1.72	0.53
10:H:18:GLU:OE1	10:H:88:ARG:NH2	2.41	0.53
1:2:436:GLN:O	1:2:438:VAL:HG13	2.08	0.53
6:7:233:GLN:CG	6:7:262:THR:HG23	2.39	0.53
6:7:239:GLU:OE2	6:7:244:VAL:HG22	2.09	0.53
6:7:320:THR:OG1	6:7:321:PRO:HD3	2.08	0.53
6:7:462:MET:CE	6:7:514:ARG:HD2	2.39	0.53
2:3:361:ILE:CG2	4:5:472:THR:HG21	2.37	0.53
3:4:201:GLU:OE2	3:4:251:ARG:NE	2.41	0.53
6:7:147:HIS:HA	6:7:151:GLU:OE1	2.07	0.53
6:7:324:LEU:HA	6:7:327:LEU:HB2	1.89	0.53
13:N:153:HIS:HA	13:N:157:THR:HG21	1.91	0.53
6:7:153:LYS:HB2	6:7:155:GLN:NE2	2.24	0.53
6:7:244:VAL:HG12	6:7:245:PRO:HD2	1.91	0.53
6:7:141:LEU:HD23	6:7:142:SER:N	2.24	0.53
6:7:209:ASP:OD1	6:7:212:ARG:NE	2.40	0.53
6:7:233:GLN:HB2	6:7:262:THR:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:489:ASN:OD1	6:7:489:ASN:N	2.38	0.53
6:7:555:ASP:HB3	6:7:558:LEU:CD2	2.38	0.53
9:A:268:LEU:O	9:A:268:LEU:HD12	2.09	0.53
11:L:24:GLU:OE1	13:N:86:ARG:NH1	2.42	0.53
12:M:127:GLN:O	12:M:131:HIS:N	2.41	0.53
14:2:901:ATP:O3B	5:6:611:ARG:NH2	2.42	0.53
2:3:401:VAL:HB	2:3:443:VAL:HG23	1.89	0.53
5:6:404:PHE:CZ	5:6:565:LEU:HD21	2.44	0.53
6:7:412:VAL:HA	6:7:415:THR:HG22	1.91	0.53
12:M:34:MET:SD	12:M:34:MET:N	2.78	0.53
4:5:377:LEU:HD12	4:5:377:LEU:O	2.09	0.52
4:5:585:TYR:CZ	4:5:612:LEU:HD11	2.44	0.52
6:7:571:PRO:HD2	6:7:618:ARG:CZ	2.39	0.52
9:A:306:SER:O	9:A:310:SER:OG	2.17	0.52
4:5:355:PHE:CD2	4:5:625:ILE:HG12	2.44	0.52
6:7:459:HIS:HA	6:7:462:MET:HE2	1.92	0.52
6:7:459:HIS:HA	6:7:462:MET:CE	2.39	0.52
10:H:95:LEU:HD13	10:H:99:PHE:CZ	2.43	0.52
11:L:1:MET:SD	11:L:157:ARG:NH1	2.83	0.52
1:2:591:GLN:NE2	4:5:385:SER:OG	2.42	0.52
6:7:614:THR:HG1	6:7:618:ARG:HH11	1.54	0.52
9:A:27:ILE:HD12	9:A:393:LEU:HD13	1.90	0.52
6:7:102:TYR:CE2	6:7:225:ARG:HB3	2.45	0.52
6:7:326:GLU:OE1	6:7:326:GLU:N	2.39	0.52
9:A:452:VAL:HG11	9:A:487:HIS:CE1	2.44	0.52
15:4:901:ADP:H2'	15:4:901:ADP:N3	2.23	0.52
4:5:589:ARG:CB	4:5:607:ILE:HG21	2.40	0.52
10:H:184:LEU:HD23	10:H:189:VAL:CG1	2.40	0.52
10:H:196:GLY:C	10:H:197:ILE:HD12	2.30	0.52
2:3:138:VAL:HG11	6:7:292:LEU:HD22	1.90	0.52
3:4:172:ILE:HD12	3:4:247:MET:SD	2.50	0.52
3:4:351:ASP:OD1	5:6:122:THR:HG23	2.09	0.52
4:5:622:LEU:HB3	4:5:635:HIS:NE2	2.25	0.52
7:F:9:DT:H2"	7:F:10:DT:OP2	2.09	0.52
9:A:507:LEU:HD11	9:A:515:LEU:HB2	1.91	0.52
9:A:560:GLN:OE1	9:A:560:GLN:N	2.39	0.52
3:4:639:PRO:HG2	3:4:642:LEU:HD23	1.92	0.52
4:5:392:GLU:HG3	4:5:400:TYR:CD1	2.44	0.52
6:7:318:GLU:HA	6:7:565:LEU:HD13	1.92	0.52
10:H:97:TRP:O	10:H:144:THR:OG1	2.05	0.52
6:7:429:LEU:H	6:7:429:LEU:HD23	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:271:ILE:HA	6:7:305:CYS:SG	2.50	0.52
6:7:585:TYR:OH	6:7:603:ALA:HA	2.10	0.52
9:A:259:GLU:OE1	9:A:259:GLU:N	2.42	0.52
10:H:61:ARG:NH1	10:H:62:SER:OG	2.42	0.52
6:7:206:CYS:HB3	6:7:211:CYS:O	2.10	0.51
6:7:305:CYS:SG	6:7:309:ASN:HB2	2.50	0.51
6:7:438:ASP:HB2	6:7:481:ARG:HG2	1.92	0.51
1:2:605:LEU:HD12	1:2:606:GLN:N	2.25	0.51
6:7:378:CYS:HB2	6:7:486:ALA:HB3	1.92	0.51
13:N:114:THR:HG22	13:N:173:VAL:CG1	2.40	0.51
3:4:309:CYS:SG	3:4:310:ASN:N	2.84	0.51
3:4:605:ILE:CG1	5:6:232:ALA:HB1	2.39	0.51
6:7:496:ASN:HB2	6:7:499:ARG:HD3	1.92	0.51
1:2:513:ALA:HA	14:2:901:ATP:O1A	2.10	0.51
1:2:660:LEU:O	1:2:664:VAL:HG23	2.10	0.51
2:3:477:LEU:HD12	2:3:606:PRO:CG	2.39	0.51
4:5:382:THR:OG1	4:5:517:VAL:HG11	2.11	0.51
10:H:11:LYS:O	10:H:14:ASP:N	2.42	0.51
1:2:297:VAL:CG2	1:2:397:LEU:HD11	2.40	0.51
6:7:417:ALA:O	6:7:429:LEU:HA	2.11	0.51
10:H:54:SER:OG	10:H:56:ASN:OD1	2.25	0.51
1:2:360:LYS:NZ	1:2:382:ILE:HD11	2.26	0.51
3:4:767:HIS:HB3	3:4:771:LEU:HD12	1.91	0.51
4:5:369:ARG:HB3	4:5:613:GLU:OE2	2.10	0.51
1:2:542:THR:HG22	5:6:434:PHE:CE2	2.46	0.51
4:5:422:ARG:NH2	7:F:6:DT:O2	2.44	0.51
4:5:589:ARG:HG3	4:5:590:SER:N	2.24	0.51
5:6:151:MET:O	5:6:185:PHE:N	2.44	0.51
6:7:155:GLN:O	6:7:159:LYS:HD3	2.11	0.51
6:7:465:GLN:OE1	6:7:481:ARG:NH2	2.44	0.51
1:2:645:LEU:O	1:2:778:SER:OG	2.29	0.51
2:3:136:PRO:O	6:7:294:SER:OG	2.29	0.51
2:3:323:ILE:HG22	2:3:329:ARG:CB	2.41	0.51
14:3:901:ATP:C8	4:5:609:VAL:HG11	2.46	0.51
4:5:620:GLU:OE2	4:5:620:GLU:HA	2.10	0.51
6:7:264:MET:O	6:7:303:ILE:HG21	2.11	0.51
6:7:315:LYS:HG2	6:7:317:ALA:HA	1.93	0.51
9:A:23:VAL:HG21	9:A:77:CYS:HB2	1.91	0.51
2:3:29:TYR:C	2:3:33:VAL:HG11	2.31	0.51
2:3:127:ILE:N	2:3:199:GLN:O	2.38	0.51
6:7:315:LYS:HE3	6:7:319:LEU:HG	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:421:ASP:OD2	6:7:428:THR:HG23	2.11	0.51
1:2:482:LEU:HD23	1:2:750:MET:CG	2.41	0.51
6:7:174:LYS:HE3	6:7:174:LYS:HA	1.92	0.51
6:7:377:ILE:CG2	6:7:517:LEU:HB2	2.41	0.51
2:3:309:LYS:HA	2:3:312:ILE:HD12	1.93	0.50
3:4:279:PRO:HD2	6:7:231:LYS:HE3	1.93	0.50
3:4:316:THR:OG1	3:4:331:CYS:HB2	2.11	0.50
4:5:392:GLU:HG3	4:5:400:TYR:HD1	1.77	0.50
6:7:179:VAL:HA	6:7:194:PRO:HA	1.93	0.50
2:3:9:ILE:HA	2:3:12:ILE:HD12	1.93	0.50
13:N:57:PRO:O	13:N:59:GLN:NE2	2.44	0.50
4:5:586:VAL:HG22	4:5:589:ARG:NH1	2.27	0.50
4:5:643:PHE:O	4:5:647:THR:HG23	2.12	0.50
6:7:167:VAL:CG1	6:7:268:GLY:H	2.24	0.50
6:7:508:PRO:HG2	6:7:511:LEU:CB	2.42	0.50
1:2:314:CYS:N	1:2:319:TYR:O	2.42	0.50
1:2:622:TYR:OH	1:2:647:VAL:HG11	2.11	0.50
2:3:297:SER:O	2:3:300:PRO:HD3	2.11	0.50
3:4:566:VAL:HG13	3:4:611:ALA:HB2	1.93	0.50
4:5:622:LEU:HD22	4:5:635:HIS:HE2	1.74	0.50
5:6:188:ASP:OD1	5:6:192:SER:OG	2.30	0.50
6:7:556:MET:O	6:7:559:MET:HB2	2.11	0.50
6:7:587:GLU:HG3	6:7:590:ARG:NE	2.20	0.50
1:2:512:THR:HG21	1:2:648:VAL:HB	1.94	0.50
2:3:237:SER:O	2:3:257:LEU:HD12	2.12	0.50
5:6:594:ARG:O	5:6:598:THR:N	2.44	0.50
2:3:202:PRO:O	2:3:205:ALA:N	2.42	0.50
6:7:75:SER:O	6:7:78:SER:OG	2.12	0.50
6:7:241:SER:HA	6:7:244:VAL:CG2	2.42	0.50
6:7:587:GLU:CA	6:7:590:ARG:HG2	2.40	0.50
10:H:23:SER:OG	10:H:24:GLN:N	2.44	0.50
11:L:67:ASP:OD1	11:L:70:ILE:N	2.44	0.50
6:7:22:LYS:NZ	6:7:53:ASP:OD1	2.28	0.50
6:7:378:CYS:HA	6:7:486:ALA:O	2.10	0.50
8:G:9:DA:C8	8:G:10:DT:H72	2.45	0.50
1:2:581:ASP:OD1	1:2:581:ASP:N	2.44	0.50
2:3:415:THR:OG1	6:7:407:ARG:HB2	2.12	0.50
6:7:209:ASP:O	6:7:212:ARG:HB2	2.12	0.50
6:7:441:VAL:HG22	6:7:483:SER:CB	2.34	0.50
6:7:475:MET:SD	6:7:476:THR:N	2.82	0.50
6:7:614:THR:OG1	6:7:618:ARG:NH1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:642:ASP:OD1	6:7:645:ASN:HB3	2.12	0.50
3:4:348:GLU:N	3:4:348:GLU:OE2	2.45	0.50
5:6:430:GLU:HG2	5:6:431:SER:H	1.77	0.50
5:6:471:GLN:O	5:6:473:THR:N	2.43	0.50
6:7:182:TYR:CE1	6:7:222:LEU:HB2	2.46	0.50
6:7:344:ILE:HG22	6:7:345:TYR:N	2.27	0.50
1:2:546:ARG:NH2	7:F:10:DT:O3'	2.45	0.49
2:3:190:TYR:CZ	6:7:154:ALA:HA	2.47	0.49
3:4:759:ASP:OD1	3:4:760:VAL:N	2.45	0.49
4:5:589:ARG:CA	4:5:607:ILE:HG21	2.41	0.49
5:6:93:LYS:CA	5:6:98:LEU:HD13	2.41	0.49
6:7:67:VAL:O	6:7:159:LYS:HA	2.11	0.49
9:A:535:PHE:HD2	9:A:570:LEU:HD21	1.77	0.49
10:H:167:GLU:HG3	10:H:176:LEU:HD13	1.94	0.49
12:M:143:ALA:HB1	12:M:146:GLU:OE2	2.12	0.49
1:2:586:HIS:NE2	1:2:641:ARG:HD2	2.28	0.49
2:3:370:GLY:H	2:3:373:LEU:HD13	1.77	0.49
3:4:569:ASP:OD1	3:4:570:ASN:ND2	2.45	0.49
4:5:424:PHE:HZ	7:F:8:DT:H4'	1.77	0.49
6:7:377:ILE:HG21	6:7:517:LEU:HB2	1.93	0.49
6:7:634:LEU:HD12	6:7:635:ARG:N	2.26	0.49
2:3:436:SER:O	6:7:250:PRO:HG2	2.12	0.49
3:4:636:VAL:HG12	3:4:637:GLN:H	1.76	0.49
4:5:39:ARG:NH1	4:5:104:GLU:OE1	2.45	0.49
6:7:310:ASP:OD1	6:7:316:ASP:HB2	2.13	0.49
6:7:580:TYR:CE2	6:7:627:LYS:HE2	2.47	0.49
9:A:100:SER:O	9:A:211:GLY:N	2.45	0.49
9:A:260:GLN:OE1	9:A:264:HIS:NE2	2.46	0.49
1:2:541:LEU:HB2	5:6:478:ARG:CA	2.42	0.49
1:2:639:LEU:HD12	1:2:642:PHE:HB2	1.95	0.49
2:3:91:MET:O	2:3:93:GLU:N	2.45	0.49
3:4:462:ASP:OD1	3:4:462:ASP:N	2.43	0.49
6:7:345:TYR:HB3	6:7:536:HIS:CD2	2.47	0.49
6:7:382:ASP:OD2	6:7:387:LYS:HB2	2.08	0.49
6:7:516:ASP:OD1	6:7:517:LEU:N	2.44	0.49
9:A:221:LEU:HD23	9:A:222:ALA:N	2.28	0.49
1:2:572:ASP:OD1	1:2:615:ALA:HA	2.12	0.49
3:4:321:ASP:OD1	3:4:322:ARG:N	2.46	0.49
4:5:47:PHE:O	4:5:49:LYS:N	2.45	0.49
4:5:465:SER:HA	4:5:474:THR:HG23	1.93	0.49
5:6:585:MET:O	5:6:589:ASN:ND2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:546:GLN:O	6:7:548:PRO:HD3	2.12	0.49
11:L:113:LEU:HD23	11:L:114:ARG:H	1.78	0.49
11:L:151:LEU:O	11:L:154:HIS:NE2	2.45	0.49
3:4:416:LYS:NZ	6:7:424:THR:HG23	2.28	0.49
4:5:222:LEU:O	4:5:242:LEU:N	2.45	0.49
4:5:357:GLY:CA	4:5:620:GLU:HB3	2.42	0.49
4:5:376:LEU:HD23	4:5:483:ALA:O	2.13	0.49
6:7:165:GLY:HA3	6:7:237:MET:SD	2.53	0.49
6:7:168:THR:OG1	6:7:169:ARG:HG2	2.13	0.49
6:7:208:SER:OG	6:7:211:CYS:HB2	2.12	0.49
6:7:344:ILE:HG22	6:7:345:TYR:H	1.76	0.49
6:7:451:ALA:HB3	6:7:454:ASP:CG	2.33	0.49
7:F:-1:DC:H2'	7:F:0:DG:C8	2.47	0.49
1:2:370:ILE:HG22	1:2:371:PRO:CD	2.42	0.49
4:5:456:HIS:HD2	4:5:507:ILE:HD11	1.77	0.49
6:7:578:THR:HA	6:7:581:ILE:HG12	1.94	0.49
7:F:-8:DG:H2"	7:F:-7:DA:C8	2.48	0.49
8:G:12:DG:H2"	8:G:13:DA:O5'	2.11	0.49
1:2:470:ILE:HD12	1:2:513:ALA:HB3	1.95	0.49
1:2:512:THR:HG21	1:2:648:VAL:CB	2.43	0.49
3:4:524:TYR:CE2	3:4:528:LEU:HD11	2.48	0.49
5:6:26:GLN:O	5:6:30:GLU:N	2.42	0.49
5:6:340:GLN:HA	5:6:343:ILE:HD12	1.95	0.49
6:7:206:CYS:CB	6:7:211:CYS:HB3	2.42	0.49
2:3:308:VAL:HG12	2:3:312:ILE:HD11	1.94	0.49
5:6:521:ARG:HD3	5:6:611:ARG:NH1	2.28	0.49
6:7:179:VAL:HG22	6:7:194:PRO:HB3	1.93	0.49
6:7:239:GLU:HG2	6:7:240:HIS:H	1.78	0.49
6:7:372:ARG:NE	6:7:464:GLN:HB2	2.27	0.49
6:7:555:ASP:OD2	6:7:558:LEU:HD22	2.12	0.49
6:7:618:ARG:O	6:7:621:LEU:HG	2.13	0.49
9:A:369:ILE:HD12	9:A:369:ILE:H	1.78	0.49
2:3:190:TYR:CE2	6:7:154:ALA:HA	2.48	0.49
5:6:139:HIS:HB3	5:6:140:PRO:HD2	1.95	0.49
6:7:180:ALA:HB1	6:7:222:LEU:CD1	2.37	0.49
6:7:540:VAL:HG22	6:7:546:GLN:HE21	1.77	0.49
1:2:279:LEU:HD13	1:2:282:PHE:HE1	1.78	0.48
3:4:343:ILE:HG22	3:4:344:HIS:H	1.77	0.48
3:4:648:LEU:HD23	3:4:650:PHE:CE1	2.48	0.48
5:6:502:TYR:O	5:6:504:ARG:NE	2.45	0.48
6:7:234:GLU:OE2	6:7:256:MET:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:308:LYS:NZ	6:7:560:ARG:HH12	2.11	0.48
6:7:478:LEU:HD12	6:7:479:ASN:H	1.78	0.48
4:5:125:SER:OG	4:5:126:ASN:N	2.46	0.48
4:5:338:PRO:O	4:5:542:LYS:NZ	2.38	0.48
6:7:634:LEU:O	6:7:638:GLU:HB2	2.12	0.48
2:3:493:SER:OG	4:5:589:ARG:NH1	2.46	0.48
6:7:174:LYS:O	6:7:232:PHE:HB3	2.13	0.48
6:7:378:CYS:O	6:7:519:TRP:HB2	2.13	0.48
1:2:314:CYS:SG	1:2:343:THR:HG21	2.54	0.48
2:3:552:ARG:HD2	2:3:557:LEU:HD22	1.94	0.48
14:3:901:ATP:C8	4:5:609:VAL:HG21	2.47	0.48
4:5:585:TYR:CE2	4:5:612:LEU:HD11	2.49	0.48
6:7:176:MET:O	6:7:229:PHE:HA	2.12	0.48
6:7:438:ASP:HB2	6:7:481:ARG:N	2.17	0.48
6:7:501:VAL:CG2	6:7:505:ILE:HD11	2.42	0.48
6:7:571:PRO:CB	6:7:623:ASP:HA	2.38	0.48
1:2:474:ASP:OD1	1:2:475:TYR:N	2.46	0.48
3:4:718:ASP:OD1	3:4:721:LYS:NZ	2.46	0.48
7:F:-11:DA:H2"	7:F:-10:DT:C7	2.40	0.48
1:2:199:THR:O	1:2:203:ARG:N	2.40	0.48
1:2:541:LEU:HB2	5:6:478:ARG:C	2.34	0.48
6:7:566:CYS:HA	6:7:621:LEU:CD2	2.44	0.48
9:A:461:TYR:CE2	9:A:463:LEU:HD13	2.49	0.48
1:2:433:ASP:HB3	1:2:435:LYS:HE2	1.95	0.48
2:3:489:ASP:OD1	2:3:490:GLN:N	2.47	0.48
4:5:361:ARG:O	4:5:362:LEU:HD23	2.14	0.48
5:6:496:ASN:O	5:6:497:PRO:O	2.30	0.48
8:G:9:DA:H1'	8:G:10:DT:C5'	2.43	0.48
13:N:85:PHE:O	13:N:88:VAL:HG12	2.13	0.48
1:2:711:LYS:NZ	1:2:712:LEU:O	2.46	0.48
3:4:468:ILE:O	3:4:524:TYR:OH	2.16	0.48
7:F:11:DT:H2"	7:F:12:DT:H71	1.94	0.48
11:L:84:PHE:CE1	11:L:148:LEU:HD13	2.49	0.48
2:3:608:THR:HB	6:7:384:GLY:HA3	1.94	0.48
6:7:62:LEU:HA	6:7:66:VAL:HG23	1.95	0.48
9:A:262:GLN:O	9:A:266:SER:OG	2.26	0.48
9:A:538:ALA:HB1	9:A:569:SER:OG	2.13	0.48
14:2:902:ATP:O2B	4:5:384:LYS:HB2	2.14	0.48
3:4:524:TYR:CZ	3:4:528:LEU:HD11	2.49	0.48
3:4:598:LEU:HD12	3:4:599:SER:H	1.79	0.48
5:6:116:LYS:HZ3	5:6:205:THR:HG21	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:415:THR:OG1	6:7:469:ILE:HG12	2.14	0.48
7:F:9:DT:C2'	7:F:10:DT:H72	2.40	0.48
9:A:328:LEU:O	9:A:332:GLY:N	2.43	0.48
2:3:17:VAL:HG13	2:3:20:LEU:HD22	1.96	0.47
3:4:356:LYS:C	3:4:357:LEU:HD12	2.35	0.47
4:5:331:ARG:NE	4:5:550:GLU:OE2	2.43	0.47
4:5:439:VAL:CG1	4:5:481:VAL:HG23	2.44	0.47
6:7:203:VAL:CG1	6:7:207:PRO:HG3	2.44	0.47
6:7:626:GLU:O	6:7:629:ASP:HB3	2.14	0.47
11:L:5:ILE:HG23	11:L:6:ILE:HG23	1.96	0.47
2:3:112:SER:O	2:3:114:THR:HG22	2.13	0.47
5:6:368:VAL:HG13	5:6:369:ALA:H	1.78	0.47
6:7:431:GLY:HA3	6:7:435:VAL:CG1	2.39	0.47
10:H:160:MET:SD	10:H:199:HIS:NE2	2.86	0.47
6:7:269:ASP:O	6:7:271:ILE:HG23	2.15	0.47
6:7:378:CYS:HA	6:7:486:ALA:HB3	1.95	0.47
1:2:316:LYS:HG3	1:2:343:THR:HG23	1.97	0.47
2:3:138:VAL:CG1	6:7:292:LEU:HD13	2.45	0.47
2:3:592:ARG:HG3	2:3:607:ILE:HG21	1.97	0.47
3:4:331:CYS:O	3:4:332:THR:OG1	2.30	0.47
4:5:357:GLY:HA2	4:5:620:GLU:HB3	1.96	0.47
4:5:488:ILE:HD12	4:5:489:PHE:CE2	2.49	0.47
9:A:459:PHE:CE2	9:A:488:VAL:HG22	2.49	0.47
13:N:187:VAL:HG21	13:N:192:VAL:HG11	1.95	0.47
5:6:427:ARG:HB3	5:6:427:ARG:NH1	2.30	0.47
6:7:102:TYR:CD2	6:7:225:ARG:HB3	2.49	0.47
6:7:315:LYS:NZ	6:7:561:ARG:HG2	2.29	0.47
6:7:390:LEU:H	6:7:390:LEU:HD12	1.79	0.47
6:7:447:PHE:HZ	6:7:458:ILE:HG21	1.77	0.47
6:7:456:THR:HA	6:7:459:HIS:HB2	1.97	0.47
6:7:465:GLN:HG2	6:7:479:ASN:ND2	2.30	0.47
14:2:902:ATP:C8	14:2:902:ATP:H5'2	2.49	0.47
3:4:277:LEU:O	6:7:173:VAL:HG11	2.15	0.47
3:4:594:GLU:CD	3:4:594:GLU:O	2.52	0.47
4:5:622:LEU:HA	4:5:625:ILE:HG13	1.95	0.47
10:H:132:SER:O	13:N:63:LEU:HD11	2.15	0.47
1:2:306:GLN:OE1	1:2:356:ARG:NH2	2.42	0.47
1:2:512:THR:HB	1:2:648:VAL:HG21	1.96	0.47
2:3:476:LEU:HD13	2:3:478:PHE:CE2	2.50	0.47
3:4:542:ALA:N	3:4:585:THR:OG1	2.47	0.47
3:4:560:LEU:O	5:6:203:GLN:NE2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:120:GLN:HB3	4:5:246:ARG:HE	1.80	0.47
6:7:176:MET:HB2	6:7:232:PHE:HB2	1.95	0.47
6:7:639:MET:HA	6:7:639:MET:CE	2.45	0.47
11:L:163:SER:O	11:L:167:ILE:HD12	2.14	0.47
2:3:299:ALA:HB1	2:3:302:ILE:CD1	2.45	0.47
4:5:27:LEU:O	4:5:31:LYS:N	2.39	0.47
4:5:427:GLU:N	4:5:427:GLU:OE1	2.46	0.47
5:6:447:GLY:H	5:6:489:THR:HG21	1.79	0.47
6:7:205:ASP:HA	6:7:219:ARG:HD2	1.97	0.47
6:7:272:VAL:HG21	6:7:306:ILE:HD12	1.97	0.47
6:7:537:ILE:HA	6:7:540:VAL:HG23	1.97	0.47
14:2:902:ATP:C8	4:5:383:ALA:HB2	2.50	0.47
2:3:346:LYS:HZ1	2:3:346:LYS:CB	2.20	0.47
2:3:407:ASP:OD1	2:3:407:ASP:N	2.47	0.47
14:3:901:ATP:H8	4:5:609:VAL:HG11	1.79	0.47
4:5:424:PHE:CZ	7:F:8:DT:H4'	2.50	0.47
6:7:458:ILE:HG21	6:7:511:LEU:HD21	1.97	0.47
6:7:587:GLU:O	6:7:591:GLU:HG3	2.15	0.47
1:2:313:ASP:N	1:2:347:SER:O	2.46	0.47
2:3:459:THR:OG1	2:3:461:MET:O	2.33	0.47
3:4:177:ASP:CG	3:4:195:LEU:HD11	2.35	0.47
3:4:330:LEU:HD22	3:4:338:HIS:ND1	2.31	0.47
4:5:369:ARG:HG2	4:5:617:ARG:HH12	1.79	0.47
6:7:272:VAL:HG21	6:7:306:ILE:CD1	2.45	0.47
6:7:412:VAL:HG23	6:7:416:ALA:O	2.14	0.47
6:7:439:GLN:OE1	6:7:439:GLN:HA	2.14	0.47
6:7:577:LEU:HD11	6:7:627:LYS:HD3	1.96	0.47
7:F:6:DT:H2"	7:F:7:DT:OP2	2.15	0.47
1:2:545:VAL:O	1:2:545:VAL:HG12	2.14	0.46
5:6:93:LYS:HA	5:6:98:LEU:HD13	1.97	0.46
9:A:197:ARG:CG	9:A:200:ILE:HD12	2.45	0.46
9:A:288:ASP:OD2	9:A:295:ARG:NH2	2.40	0.46
1:2:279:LEU:O	1:2:281:THR:HG23	2.15	0.46
2:3:354:LEU:HD23	2:3:355:ASN:HB3	1.98	0.46
5:6:391:SER:HB3	15:6:901:ADP:H5'2	1.97	0.46
6:7:164:ARG:HD2	6:7:165:GLY:O	2.15	0.46
6:7:563:ILE:HG13	6:7:564:ASN:OD1	2.15	0.46
6:7:610:LEU:HD12	6:7:611:ARG:HG2	1.96	0.46
1:2:696:LEU:O	1:2:699:GLN:N	2.49	0.46
3:4:226:TYR:CZ	3:4:230:ILE:HD11	2.49	0.46
4:5:404:LYS:NZ	4:5:446:LYS:O	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:377:SER:O	5:6:379:ARG:NH2	2.48	0.46
5:6:502:TYR:OH	5:6:527:ILE:CG2	2.63	0.46
6:7:626:GLU:CD	6:7:629:ASP:HB2	2.36	0.46
7:F:12:DT:H2"	7:F:13:DT:H71	1.96	0.46
9:A:61:ALA:O	9:A:65:HIS:N	2.47	0.46
1:2:545:VAL:HG12	1:2:547:ARG:NH2	2.31	0.46
1:2:734:THR:OG1	1:2:735:GLY:N	2.48	0.46
2:3:219:ASP:OD1	2:3:220:ASP:N	2.48	0.46
4:5:123:LEU:HD21	4:5:293:VAL:HG12	1.98	0.46
5:6:623:MET:CE	5:6:636:HIS:HA	2.45	0.46
7:F:8:DT:H2"	7:F:9:DT:C6	2.50	0.46
2:3:264:LEU:HD12	2:3:265:LEU:H	1.81	0.46
2:3:357:ALA:HB1	2:3:358:PRO:HD2	1.97	0.46
3:4:200:LEU:HD12	3:4:247:MET:CE	2.44	0.46
3:4:360:SER:OG	3:4:390:ARG:NH2	2.49	0.46
3:4:594:GLU:O	3:4:594:GLU:CG	2.64	0.46
4:5:384:LYS:HE2	4:5:484:ALA:HB1	1.97	0.46
5:6:544:ILE:HA	5:6:547:LEU:HD12	1.97	0.46
6:7:306:ILE:HA	6:7:311:GLU:OE2	2.15	0.46
6:7:502:GLU:H	6:7:505:ILE:CG1	2.29	0.46
6:7:645:ASN:OD1	6:7:646:GLN:N	2.48	0.46
4:5:456:HIS:O	4:5:510:ARG:NH2	2.48	0.46
6:7:359:VAL:HG23	6:7:360:GLY:H	1.79	0.46
9:A:81:VAL:HG12	9:A:82:ASP:N	2.31	0.46
2:3:241:LEU:HD23	2:3:242:PRO:HA	1.98	0.46
6:7:166:ILE:N	6:7:237:MET:SD	2.89	0.46
6:7:167:VAL:HG13	6:7:268:GLY:H	1.81	0.46
6:7:175:PRO:HA	6:7:230:VAL:O	2.16	0.46
9:A:230:MET:CE	9:A:280:ALA:HB1	2.45	0.46
1:2:306:GLN:N	1:2:356:ARG:O	2.48	0.46
2:3:192:ASP:OD1	6:7:154:ALA:HB2	2.16	0.46
4:5:388:LEU:CD1	4:5:482:LEU:HD21	2.45	0.46
6:7:277:PHE:O	6:7:278:LEU:HD13	2.15	0.46
9:A:19:ILE:HG13	9:A:69:VAL:HG11	1.98	0.46
10:H:195:GLN:HB2	10:H:197:ILE:HD13	1.98	0.46
3:4:542:ALA:HB1	3:4:588:VAL:HG21	1.97	0.46
6:7:299:GLN:OE1	6:7:300:ALA:N	2.41	0.46
3:4:503:ARG:O	3:4:741:ARG:NH2	2.47	0.46
3:4:601:ALA:HB1	3:4:606:ILE:HG22	1.98	0.46
3:4:665:ALA:HB1	6:7:582:VAL:HG12	1.97	0.46
4:5:596:GLU:CG	4:5:602:ARG:HA	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:470:GLU:OE1	5:6:471:GLN:N	2.48	0.46
6:7:100:ASP:HA	6:7:103:ILE:HD12	1.97	0.46
1:2:348:ILE:HG22	1:2:349:ASN:O	2.16	0.45
1:2:566:GLN:N	1:2:608:ARG:O	2.37	0.45
2:3:62:LEU:HD21	2:3:99:PHE:CD1	2.51	0.45
2:3:133:LEU:HD21	2:3:135:ARG:CZ	2.46	0.45
6:7:364:LYS:HG2	6:7:365:ARG:H	1.81	0.45
6:7:382:ASP:N	6:7:383:PRO:HD3	2.31	0.45
6:7:577:LEU:HD22	6:7:627:LYS:HA	1.97	0.45
1:2:180:ILE:HD12	1:2:180:ILE:H	1.81	0.45
1:2:715:ILE:HG13	1:2:716:ASP:H	1.81	0.45
2:3:299:ALA:HB1	2:3:302:ILE:HG13	1.98	0.45
5:6:245:VAL:HG22	5:6:289:ALA:HB3	1.99	0.45
6:7:181:THR:HG23	6:7:223:GLN:HG3	1.97	0.45
6:7:457:ALA:O	6:7:460:GLU:HG2	2.16	0.45
6:7:499:ARG:HA	6:7:503:GLN:NE2	2.31	0.45
6:7:502:GLU:OE1	6:7:509:ALA:HB2	2.16	0.45
9:A:289:LEU:HD13	9:A:291:LEU:HB3	1.98	0.45
9:A:439:VAL:HG11	9:A:482:PHE:CE2	2.51	0.45
1:2:437:VAL:HB	1:2:706:GLU:CD	2.36	0.45
14:2:902:ATP:N7	4:5:383:ALA:HB2	2.31	0.45
3:4:378:HIS:O	3:4:382:VAL:HG13	2.16	0.45
5:6:152:CYS:SG	5:6:180:SER:N	2.89	0.45
6:7:160:LEU:HD12	6:7:276:VAL:HG23	1.98	0.45
9:A:138:GLU:OE2	9:A:190:ARG:N	2.50	0.45
9:A:163:ASP:OD1	9:A:164:GLN:N	2.47	0.45
2:3:301:SER:O	2:3:301:SER:OG	2.33	0.45
3:4:613:THR:OG1	3:4:614:SER:N	2.49	0.45
5:6:92:VAL:HG21	5:6:102:LYS:HE3	1.99	0.45
6:7:106:ARG:HH21	6:7:190:GLU:HG3	1.80	0.45
6:7:193:GLN:OE1	6:7:202:PRO:HA	2.16	0.45
6:7:578:THR:O	6:7:581:ILE:HG12	2.17	0.45
9:A:187:GLN:OE1	9:A:191:ARG:NH2	2.46	0.45
9:A:262:GLN:O	9:A:266:SER:N	2.44	0.45
2:3:138:VAL:HG13	6:7:292:LEU:HD13	1.99	0.45
2:3:477:LEU:HD12	2:3:606:PRO:CD	2.47	0.45
3:4:299:ILE:HG22	3:4:300:PRO:O	2.17	0.45
3:4:464:LEU:CB	3:4:483:LEU:HD21	2.47	0.45
5:6:139:HIS:HB3	5:6:140:PRO:CD	2.46	0.45
5:6:508:LEU:HD13	5:6:651:VAL:HG13	1.98	0.45
6:7:212:ARG:CZ	6:7:212:ARG:HB3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:321:PRO:O	6:7:324:LEU:HG	2.17	0.45
6:7:474:ILE:HB	6:7:475:MET:CE	2.47	0.45
6:7:517:LEU:CD2	6:7:636:LEU:HD21	2.46	0.45
11:L:71:LEU:HA	11:L:74:ILE:HG22	1.97	0.45
2:3:159:LEU:HD23	2:3:241:LEU:CG	2.45	0.45
6:7:141:LEU:HD23	6:7:142:SER:HB3	1.98	0.45
6:7:447:PHE:CZ	6:7:458:ILE:HG21	2.51	0.45
12:M:65:ASN:OD1	12:M:66:ASN:N	2.50	0.45
3:4:176:ILE:HD11	3:4:182:GLN:CG	2.47	0.45
3:4:211:LEU:O	3:4:262:GLN:NE2	2.43	0.45
6:7:164:ARG:HG2	6:7:271:ILE:O	2.17	0.45
6:7:235:VAL:HG12	6:7:236:LYS:H	1.81	0.45
6:7:261:VAL:HG12	6:7:261:VAL:O	2.17	0.45
10:H:20:GLU:OE2	10:H:20:GLU:N	2.45	0.45
14:2:902:ATP:H5'2	4:5:383:ALA:HA	1.99	0.45
6:7:386:ALA:HA	15:7:801:ADP:H3'	1.99	0.45
6:7:434:LEU:HD12	6:7:442:CYS:SG	2.57	0.45
9:A:23:VAL:HA	9:A:52:ILE:HD13	1.99	0.45
9:A:484:LEU:HD22	9:A:501:LEU:HD22	1.99	0.45
1:2:743:HIS:O	1:2:746:SER:OG	2.35	0.45
3:4:234:GLN:HG3	3:4:396:ILE:HD13	1.98	0.45
4:5:623:ALA:HB2	4:5:631:ALA:HB2	1.98	0.45
6:7:415:THR:O	6:7:432:GLY:N	2.50	0.45
6:7:569:LYS:NZ	6:7:623:ASP:HB2	2.31	0.45
1:2:218:SER:OG	1:2:272:GLU:OE1	2.26	0.44
1:2:277:GLU:OE2	1:2:286:HIS:NE2	2.49	0.44
3:4:374:LEU:C	3:4:375:LEU:HD12	2.37	0.44
3:4:581:MET:SD	3:4:582:ASN:ND2	2.90	0.44
5:6:574:PHE:HZ	5:6:628:CYS:HG	1.66	0.44
6:7:182:TYR:HD2	6:7:220:LEU:HD12	1.82	0.44
6:7:334:GLU:O	6:7:337:ALA:HB3	2.17	0.44
8:G:13:DA:H2'	8:G:14:DT:H72	1.99	0.44
9:A:27:ILE:HD12	9:A:393:LEU:CD1	2.48	0.44
11:L:93:MET:HB2	11:L:151:LEU:HD22	1.98	0.44
4:5:250:GLU:O	4:5:308:TYR:OH	2.34	0.44
5:6:430:GLU:HG2	5:6:431:SER:N	2.33	0.44
6:7:182:TYR:HA	6:7:221:TYR:O	2.17	0.44
6:7:344:ILE:CG2	6:7:345:TYR:H	2.31	0.44
6:7:508:PRO:HG2	6:7:511:LEU:HB2	1.99	0.44
10:H:184:LEU:HD23	10:H:189:VAL:HG11	2.00	0.44
7:F:-4:DG:H2"	7:F:-3:DA:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:97:VAL:O	13:N:100:ILE:HG22	2.16	0.44
13:N:122:GLN:O	13:N:125:SER:OG	2.11	0.44
3:4:274:MET:O	3:4:277:LEU:HD23	2.18	0.44
4:5:622:LEU:HD22	4:5:635:HIS:NE2	2.33	0.44
6:7:52:LEU:HD12	6:7:141:LEU:H	1.82	0.44
6:7:569:LYS:HZ2	6:7:623:ASP:HB2	1.83	0.44
3:4:294:ARG:NE	3:4:296:SER:OG	2.50	0.44
5:6:574:PHE:HE2	5:6:628:CYS:HA	1.82	0.44
6:7:183:THR:HA	6:7:189:SER:O	2.17	0.44
6:7:326:GLU:HA	6:7:329:GLN:CB	2.45	0.44
12:M:121:ILE:O	12:M:124:THR:OG1	2.33	0.44
2:3:343:SER:O	2:3:343:SER:OG	2.34	0.44
2:3:426:VAL:HG12	2:3:428:ILE:HG12	1.99	0.44
3:4:160:VAL:HG12	3:4:162:SER:H	1.83	0.44
3:4:374:LEU:N	3:4:374:LEU:HD23	2.33	0.44
3:4:648:LEU:HD23	3:4:650:PHE:HE1	1.82	0.44
5:6:145:LEU:HD13	5:6:189:VAL:HG12	2.00	0.44
5:6:223:ARG:H	5:6:226:LEU:HD22	1.83	0.44
6:7:160:LEU:HD11	6:7:301:HIS:HE2	1.82	0.44
6:7:266:GLN:N	6:7:269:ASP:OD2	2.45	0.44
6:7:585:TYR:CE1	6:7:605:ASN:HB2	2.49	0.44
6:7:595:GLN:OE1	6:7:598:MET:HG3	2.18	0.44
3:4:276:SER:C	3:4:277:LEU:HD22	2.37	0.44
6:7:235:VAL:HG12	6:7:236:LYS:N	2.32	0.44
6:7:465:GLN:HA	6:7:480:ALA:O	2.17	0.44
10:H:98:GLU:O	10:H:145:ASN:ND2	2.50	0.44
1:2:717:GLU:OE1	1:2:720:ILE:HD12	2.18	0.44
2:3:34:LYS:O	2:3:39:GLU:N	2.50	0.44
4:5:150:ILE:HD13	4:5:252:VAL:HG11	2.00	0.44
4:5:156:ILE:HG23	4:5:218:ASP:OD1	2.17	0.44
5:6:38:ILE:O	5:6:42:ARG:NE	2.50	0.44
5:6:84:LEU:O	5:6:87:SER:OG	2.22	0.44
5:6:151:MET:HG3	5:6:157:THR:HG23	2.00	0.44
15:6:901:ADP:N3	15:6:901:ADP:H2'	2.33	0.44
6:7:156:HIS:ND1	6:7:161:VAL:HG21	2.32	0.44
6:7:212:ARG:HB3	6:7:214:ASN:OD1	2.18	0.44
12:M:143:ALA:HB1	12:M:146:GLU:CD	2.39	0.44
2:3:159:LEU:HD23	2:3:241:LEU:CD1	2.45	0.44
3:4:177:ASP:OD1	3:4:195:LEU:HD11	2.18	0.44
6:7:171:THR:OG1	6:7:423:LEU:HD22	2.18	0.44
6:7:193:GLN:NE2	6:7:203:VAL:HG23	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:379:LEU:H	6:7:487:ALA:HA	1.83	0.44
7:F:11:DT:H2"	7:F:12:DT:C5	2.53	0.44
9:A:243:GLN:NE2	9:A:249:ILE:HD12	2.33	0.44
13:N:55:ILE:HD13	13:N:133:LEU:HD11	2.00	0.44
14:2:902:ATP:O2A	4:5:384:LYS:N	2.51	0.43
3:4:269:ASP:OD1	3:4:269:ASP:N	2.50	0.43
3:4:308:SER:OG	3:4:309:CYS:N	2.51	0.43
3:4:661:ASP:OD1	3:4:661:ASP:N	2.51	0.43
4:5:586:VAL:HG13	4:5:589:ARG:HH11	1.83	0.43
6:7:315:LYS:HE3	6:7:319:LEU:CG	2.48	0.43
9:A:279:SER:OG	9:A:419:ARG:NH2	2.51	0.43
3:4:345:ASN:HA	5:6:244:VAL:HG21	1.98	0.43
5:6:93:LYS:N	5:6:98:LEU:HD13	2.33	0.43
5:6:516:ALA:HB1	5:6:607:ARG:HH22	1.81	0.43
6:7:148:SER:O	6:7:151:GLU:HG2	2.18	0.43
6:7:277:PHE:C	6:7:278:LEU:HD22	2.38	0.43
9:A:197:ARG:HG3	9:A:200:ILE:HD12	2.01	0.43
10:H:95:LEU:HD13	10:H:99:PHE:HZ	1.83	0.43
12:M:16:ILE:O	12:M:16:ILE:HG22	2.18	0.43
3:4:354:LEU:HD11	3:4:374:LEU:HB2	2.00	0.43
6:7:164:ARG:CG	6:7:272:VAL:HG22	2.48	0.43
6:7:359:VAL:HG23	6:7:360:GLY:N	2.34	0.43
6:7:465:GLN:HG2	6:7:479:ASN:HA	2.00	0.43
6:7:612:LEU:HD12	6:7:613:SER:N	2.32	0.43
1:2:467:ALA:O	1:2:469:SER:N	2.51	0.43
1:2:545:VAL:CG1	1:2:547:ARG:NH2	2.80	0.43
2:3:333:ASP:OD1	2:3:333:ASP:N	2.51	0.43
3:4:171:PHE:HZ	3:4:217:HIS:HB3	1.83	0.43
3:4:545:LEU:O	3:4:564:ALA:N	2.48	0.43
4:5:614:ALA:O	4:5:617:ARG:HB2	2.18	0.43
6:7:174:LYS:CG	6:7:423:LEU:HD11	2.48	0.43
6:7:314:ASP:HB3	6:7:315:LYS:HD2	2.01	0.43
2:3:177:ASP:N	2:3:177:ASP:OD1	2.52	0.43
2:3:190:TYR:O	6:7:154:ALA:HB1	2.18	0.43
3:4:639:PRO:O	3:4:643:LEU:HD12	2.18	0.43
4:5:574:SER:OG	4:5:575:GLU:N	2.49	0.43
4:5:593:GLY:O	4:5:596:GLU:HB3	2.18	0.43
5:6:313:THR:OG1	5:6:328:LYS:NZ	2.52	0.43
6:7:446:GLU:HA	6:7:488:ALA:HA	2.00	0.43
6:7:465:GLN:HG2	6:7:479:ASN:HD22	1.83	0.43
7:F:1:DA:C8	7:F:2:DT:H73	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:92:ILE:O	10:H:95:LEU:HD12	2.19	0.43
2:3:323:ILE:HG22	2:3:329:ARG:HB2	2.00	0.43
5:6:384:VAL:HG12	5:6:385:CYS:H	1.82	0.43
6:7:178:VAL:HG23	6:7:179:VAL:HG23	1.99	0.43
6:7:362:VAL:HB	6:7:614:THR:HG21	2.00	0.43
9:A:566:PHE:CZ	9:A:570:LEU:HD22	2.54	0.43
1:2:485:PHE:CE2	1:2:701:ILE:HG22	2.53	0.43
3:4:298:VAL:O	3:4:299:ILE:HD13	2.18	0.43
5:6:243:ILE:HG21	5:6:291:LEU:HD23	2.00	0.43
5:6:623:MET:HE1	5:6:636:HIS:HA	2.01	0.43
6:7:60:GLU:HA	6:7:63:ALA:HB3	2.01	0.43
6:7:157:ILE:HD13	6:7:157:ILE:HA	1.86	0.43
6:7:168:THR:O	6:7:236:LYS:HB2	2.18	0.43
6:7:203:VAL:HG12	6:7:204:HIS:H	1.83	0.43
6:7:358:LEU:CD1	6:7:394:ILE:HD11	2.37	0.43
6:7:381:GLY:HA2	6:7:490:PRO:HG2	2.01	0.43
6:7:469:ILE:HB	6:7:476:THR:HB	2.01	0.43
9:A:32:ALA:HB2	9:A:215:ALA:HB2	2.00	0.43
9:A:230:MET:HE3	9:A:280:ALA:HB1	1.99	0.43
1:2:513:ALA:HA	14:2:901:ATP:O2A	2.18	0.43
4:5:460:GLU:OE2	4:5:610:ARG:NE	2.49	0.43
6:7:326:GLU:O	6:7:329:GLN:HB3	2.19	0.43
6:7:460:GLU:CD	6:7:467:ILE:HA	2.39	0.43
11:L:136:ILE:HG22	12:M:126:ARG:HH12	1.84	0.43
12:M:88:GLU:OE2	12:M:91:HIS:N	2.51	0.43
1:2:181:ALA:HB1	1:2:247:VAL:HG22	2.00	0.43
1:2:541:LEU:HD11	5:6:479:ALA:CB	2.44	0.43
1:2:543:ALA:O	1:2:556:LEU:CD1	2.57	0.43
2:3:290:ILE:O	2:3:294:LEU:HD12	2.19	0.43
3:4:598:LEU:HD12	3:4:599:SER:N	2.34	0.43
6:7:390:LEU:O	6:7:394:ILE:HG22	2.19	0.43
6:7:438:ASP:OD2	6:7:481:ARG:HG2	2.19	0.43
1:2:296:VAL:N	1:2:364:GLN:O	2.46	0.43
2:3:428:ILE:HG22	2:3:429:SER:H	1.84	0.43
2:3:628:SER:O	2:3:630:SER:N	2.50	0.43
3:4:705:SER:OG	3:4:706:ASP:N	2.52	0.43
6:7:610:LEU:CD1	6:7:611:ARG:HG2	2.49	0.43
2:3:151:VAL:HG23	2:3:151:VAL:O	2.19	0.42
3:4:279:PRO:HD3	6:7:231:LYS:HD3	2.01	0.42
4:5:365:GLY:O	4:5:367:CYS:N	2.52	0.42
6:7:172:GLU:H	6:7:423:LEU:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:226:SER:O	9:A:226:SER:OG	2.34	0.42
3:4:479:LYS:HA	3:4:482:ILE:HD12	2.01	0.42
3:4:601:ALA:CB	3:4:606:ILE:HG22	2.49	0.42
6:7:145:LYS:O	6:7:162:THR:OG1	2.38	0.42
6:7:330:ASP:OD2	6:7:335:ARG:NE	2.52	0.42
6:7:364:LYS:HG2	6:7:365:ARG:N	2.33	0.42
13:N:177:LEU:HD12	13:N:214:GLN:NE2	2.35	0.42
2:3:138:VAL:CG1	6:7:292:LEU:HB3	2.49	0.42
3:4:354:LEU:HD12	3:4:375:LEU:O	2.19	0.42
4:5:70:GLU:OE2	4:5:70:GLU:N	2.52	0.42
6:7:78:SER:OG	6:7:79:ASP:N	2.52	0.42
6:7:215:LYS:O	6:7:217:GLY:N	2.51	0.42
6:7:269:ASP:OD1	6:7:269:ASP:N	2.52	0.42
7:F:7:DT:C1'	7:F:8:DT:H5'	2.49	0.42
9:A:240:ILE:O	9:A:244:LEU:N	2.48	0.42
9:A:459:PHE:HE2	9:A:488:VAL:HG22	1.83	0.42
9:A:542:SER:OG	9:A:543:GLY:N	2.52	0.42
1:2:420:PHE:O	5:6:142:HIS:NE2	2.52	0.42
1:2:755:ALA:HB1	1:2:760:ARG:HB3	2.01	0.42
2:3:192:ASP:CG	6:7:154:ALA:HB2	2.39	0.42
5:6:383:ASN:OD1	5:6:491:ILE:HG22	2.20	0.42
6:7:171:THR:OG1	6:7:423:LEU:HD13	2.19	0.42
6:7:233:GLN:OE1	6:7:235:VAL:HG23	2.20	0.42
6:7:469:ILE:HD12	6:7:476:THR:O	2.20	0.42
11:L:138:GLY:O	11:L:140:GLY:N	2.52	0.42
13:N:187:VAL:HG21	13:N:192:VAL:CG1	2.49	0.42
2:3:34:LYS:O	2:3:38:ALA:N	2.53	0.42
5:6:582:ALA:HB2	5:6:634:GLU:CB	2.49	0.42
6:7:132:LYS:HB3	6:7:228:LYS:HZ3	1.84	0.42
6:7:462:MET:HE3	6:7:514:ARG:HB2	2.01	0.42
10:H:129:TYR:O	10:H:133:ALA:HB3	2.19	0.42
2:3:475:ASP:HB3	2:3:614:THR:HG21	2.02	0.42
3:4:518:LYS:HB2	3:4:518:LYS:NZ	2.35	0.42
4:5:621:SER:O	4:5:625:ILE:HG13	2.20	0.42
6:7:107:LEU:HD12	6:7:110:GLU:HB2	2.02	0.42
6:7:237:MET:HE2	6:7:253:MET:HG2	2.02	0.42
6:7:354:LEU:HD21	6:7:394:ILE:CD1	2.37	0.42
6:7:575:ASP:O	6:7:578:THR:OG1	2.31	0.42
9:A:259:GLU:O	9:A:263:SER:OG	2.20	0.42
2:3:264:LEU:HD11	2:3:266:SER:OG	2.20	0.42
2:3:345:ALA:HB2	14:3:901:ATP:C5	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:482:ASP:O	2:3:483:VAL:HG22	2.20	0.42
2:3:552:ARG:HD2	2:3:557:LEU:HD13	2.02	0.42
3:4:475:ASN:O	3:4:478:ILE:HG22	2.20	0.42
6:7:458:ILE:CG2	6:7:511:LEU:HD21	2.50	0.42
6:7:463:GLU:N	6:7:463:GLU:OE1	2.52	0.42
11:L:134:ALA:O	11:L:136:ILE:HG23	2.19	0.42
1:2:542:THR:O	1:2:542:THR:OG1	2.29	0.42
3:4:154:VAL:HG12	3:4:155:TRP:H	1.84	0.42
3:4:548:TYR:N	3:4:562:THR:O	2.44	0.42
5:6:447:GLY:O	5:6:489:THR:HG21	2.20	0.42
6:7:236:LYS:HE2	6:7:236:LYS:HA	2.00	0.42
6:7:447:PHE:N	6:7:488:ALA:HB2	2.32	0.42
6:7:583:GLY:O	6:7:586:VAL:HB	2.20	0.42
9:A:114:GLN:O	9:A:115:VAL:HG13	2.18	0.42
13:N:34:THR:HG22	13:N:36:GLN:H	1.85	0.42
1:2:574:PHE:H	1:2:615:ALA:HB2	1.85	0.42
2:3:33:VAL:O	2:3:37:ILE:HD11	2.20	0.42
2:3:226:CYS:SG	2:3:227:LYS:N	2.92	0.42
2:3:347:SER:HB3	4:5:461:GLN:NE2	2.35	0.42
6:7:280:LEU:HD12	6:7:297:PHE:CD1	2.55	0.42
6:7:469:ILE:HD12	6:7:476:THR:HB	2.00	0.42
6:7:571:PRO:HD2	6:7:618:ARG:NE	2.35	0.42
6:7:571:PRO:HA	6:7:623:ASP:OD2	2.20	0.42
7:F:13:DT:H2'	7:F:13:DT:OP2	2.20	0.42
9:A:418:SER:O	9:A:422:LYS:NZ	2.53	0.42
9:A:516:LEU:HD21	9:A:535:PHE:CE2	2.55	0.42
9:A:535:PHE:CD2	9:A:570:LEU:HD21	2.54	0.42
13:N:114:THR:HG22	13:N:173:VAL:HG12	2.02	0.42
2:3:469:SER:OG	2:3:473:ARG:NH1	2.53	0.42
4:5:614:ALA:HA	4:5:617:ARG:HH21	1.85	0.42
4:5:617:ARG:HA	4:5:620:GLU:HB2	2.02	0.42
5:6:253:GLY:O	5:6:285:ASN:ND2	2.53	0.42
6:7:458:ILE:HD11	6:7:484:ILE:HG13	2.01	0.42
6:7:484:ILE:HA	6:7:484:ILE:HD13	1.73	0.42
6:7:499:ARG:HA	6:7:503:GLN:CD	2.40	0.42
6:7:617:ALA:HB2	6:7:625:VAL:HG22	2.01	0.42
2:3:464:ILE:HG22	2:3:466:LEU:HD21	2.03	0.41
3:4:330:LEU:HD21	3:4:336:THR:HA	2.02	0.41
3:4:551:LYS:HD3	3:4:558:LEU:HD23	2.02	0.41
5:6:64:LYS:O	5:6:67:GLN:NE2	2.52	0.41
6:7:287:GLN:HG2	6:7:288:MET:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:315:LYS:CD	6:7:319:LEU:HD23	2.49	0.41
9:A:295:ARG:HH11	9:A:385:ALA:HB2	1.85	0.41
10:H:175:HIS:O	10:H:177:LYS:N	2.52	0.41
13:N:33:ILE:HG22	13:N:38:VAL:HG23	2.02	0.41
13:N:196:VAL:HG23	13:N:215:LEU:HB3	2.02	0.41
2:3:138:VAL:HG12	6:7:292:LEU:HB3	2.02	0.41
2:3:337:LEU:HD12	2:3:338:LEU:H	1.85	0.41
6:7:165:GLY:O	6:7:166:ILE:HD13	2.20	0.41
6:7:176:MET:O	6:7:230:VAL:N	2.53	0.41
6:7:364:LYS:C	6:7:365:ARG:HD2	2.40	0.41
6:7:421:ASP:O	6:7:425:GLY:N	2.53	0.41
6:7:439:GLN:HG2	6:7:481:ARG:HD2	2.00	0.41
7:F:7:DT:H2"	7:F:8:DT:OP2	2.20	0.41
10:H:47:GLU:OE1	10:H:47:GLU:N	2.48	0.41
13:N:108:ARG:NH2	13:N:137:GLU:OE2	2.52	0.41
14:2:901:ATP:O3A	5:6:611:ARG:NH2	2.51	0.41
3:4:487:PHE:O	3:4:489:GLY:N	2.50	0.41
6:7:406:GLY:CA	6:7:450:MET:HA	2.47	0.41
6:7:482:VAL:HG22	6:7:483:SER:O	2.21	0.41
7:F:9:DT:H2"	7:F:10:DT:C7	2.43	0.41
9:A:111:SER:O	9:A:111:SER:OG	2.38	0.41
5:6:179:CYS:SG	5:6:180:SER:N	2.92	0.41
5:6:435:VAL:C	5:6:436:ILE:HD12	2.40	0.41
5:6:498:ILE:HD12	5:6:511:ASN:C	2.19	0.41
6:7:354:LEU:O	6:7:357:LEU:HB3	2.20	0.41
6:7:400:ARG:NE	6:7:400:ARG:HA	2.36	0.41
7:F:8:DT:C6	7:F:9:DT:H73	2.54	0.41
11:L:48:MET:O	11:L:51:HIS:N	2.53	0.41
2:3:159:LEU:HB3	2:3:241:LEU:HD12	2.02	0.41
2:3:428:ILE:O	2:3:435:ALA:HB3	2.21	0.41
2:3:608:THR:HG22	6:7:383:PRO:O	2.21	0.41
3:4:395:GLY:HA3	3:4:419:VAL:HG12	2.02	0.41
4:5:583:SER:O	4:5:587:LEU:HD23	2.21	0.41
6:7:260:GLU:N	6:7:260:GLU:OE1	2.52	0.41
6:7:377:ILE:HG21	6:7:517:LEU:HD13	2.02	0.41
6:7:412:VAL:HA	6:7:415:THR:CG2	2.50	0.41
6:7:524:LYS:NZ	6:7:646:GLN:O	2.53	0.41
6:7:537:ILE:HD12	15:7:801:ADP:N3	2.35	0.41
9:A:23:VAL:HG21	9:A:77:CYS:CB	2.50	0.41
1:2:300:THR:HG21	1:2:360:LYS:O	2.21	0.41
3:4:169:LYS:HD3	3:4:172:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:91:LEU:HD22	4:5:121:ILE:HD11	2.02	0.41
9:A:21:ILE:CG2	9:A:52:ILE:HD11	2.49	0.41
9:A:60:ARG:O	9:A:64:GLU:N	2.48	0.41
1:2:404:THR:OG1	1:2:423:VAL:O	2.38	0.41
2:3:62:LEU:HD21	2:3:99:PHE:HD1	1.85	0.41
6:7:206:CYS:SG	6:7:211:CYS:HB3	2.60	0.41
6:7:644:LEU:O	6:7:644:LEU:HD12	2.20	0.41
12:M:45:ASP:OD1	12:M:45:ASP:N	2.54	0.41
12:M:80:VAL:HG23	12:M:81:HIS:H	1.86	0.41
3:4:496:THR:OG1	3:4:497:LEU:N	2.53	0.41
4:5:119:ILE:HG22	4:5:120:GLN:N	2.36	0.41
5:6:103:ASP:OD1	5:6:104:CYS:N	2.49	0.41
5:6:458:ASP:OD1	5:6:459:GLN:N	2.53	0.41
6:7:46:VAL:HG12	6:7:46:VAL:O	2.20	0.41
6:7:166:ILE:HB	6:7:238:GLN:O	2.21	0.41
1:2:312:TYR:HD1	1:2:348:ILE:HG12	1.85	0.41
1:2:573:GLU:OE1	1:2:616:ASN:ND2	2.50	0.41
14:2:901:ATP:O3'	5:6:379:ARG:NH1	2.53	0.41
2:3:592:ARG:CG	2:3:607:ILE:HG21	2.51	0.41
4:5:442:ASP:CG	4:5:484:ALA:HB3	2.41	0.41
5:6:92:VAL:HG21	5:6:102:LYS:CE	2.50	0.41
6:7:60:GLU:O	6:7:63:ALA:HB3	2.21	0.41
6:7:98:ALA:HA	6:7:101:VAL:HG12	2.02	0.41
6:7:172:GLU:O	6:7:423:LEU:HD21	2.21	0.41
6:7:182:TYR:CE1	6:7:222:LEU:HD13	2.56	0.41
6:7:182:TYR:CB	6:7:220:LEU:HB2	2.24	0.41
6:7:204:HIS:O	6:7:220:LEU:HD11	2.21	0.41
6:7:566:CYS:HB2	6:7:619:LEU:HA	2.03	0.41
9:A:403:HIS:O	9:A:403:HIS:ND1	2.52	0.41
13:N:157:THR:HG22	13:N:160:MET:CE	2.51	0.41
2:3:158:ASP:OD1	2:3:159:LEU:N	2.48	0.41
3:4:201:GLU:O	3:4:205:THR:OG1	2.18	0.41
4:5:130:THR:HG22	4:5:131:ASN:H	1.86	0.41
5:6:66:ASP:HB3	5:6:69:LEU:HD13	2.02	0.41
6:7:166:ILE:O	6:7:238:GLN:N	2.43	0.41
6:7:280:LEU:HD12	6:7:297:PHE:CG	2.56	0.41
6:7:620:ARG:C	6:7:621:LEU:HD12	2.41	0.41
1:2:574:PHE:HD1	1:2:574:PHE:HA	1.76	0.40
2:3:165:VAL:CG1	2:3:166:PRO:HD2	2.50	0.40
2:3:325:PRO:HD3	6:7:544:SER:HB3	2.02	0.40
4:5:488:ILE:HD12	4:5:489:PHE:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:115:HIS:ND1	5:6:129:ILE:HD11	2.35	0.40
6:7:184:CYS:HA	6:7:220:LEU:CA	2.49	0.40
6:7:233:GLN:OE1	6:7:234:GLU:N	2.54	0.40
6:7:293:LEU:O	6:7:293:LEU:HG	2.20	0.40
2:3:479:VAL:HG21	2:3:603:ARG:HH11	1.86	0.40
3:4:416:LYS:HE2	6:7:424:THR:HG23	2.03	0.40
5:6:157:THR:HG21	5:6:185:PHE:CG	2.56	0.40
11:L:122:ASP:OD1	11:L:123:ILE:N	2.53	0.40
11:L:128:LEU:HD21	11:L:148:LEU:HD11	2.02	0.40
1:2:367:PRO:O	1:2:370:ILE:HD11	2.22	0.40
1:2:597:SER:OG	1:2:598:LYS:N	2.54	0.40
2:3:370:GLY:N	2:3:373:LEU:HD13	2.36	0.40
3:4:377:ALA:HA	3:4:421:VAL:HG11	2.04	0.40
3:4:763:ALA:O	3:4:767:HIS:ND1	2.49	0.40
5:6:316:ASP:OD1	5:6:317:MET:N	2.55	0.40
6:7:233:GLN:CB	6:7:262:THR:HG23	2.51	0.40
6:7:245:PRO:HB2	6:7:248:HIS:HB2	2.02	0.40
6:7:569:LYS:HE3	6:7:622:SER:CA	2.51	0.40
6:7:626:GLU:OE1	6:7:629:ASP:HB2	2.21	0.40
9:A:341:THR:HG22	9:A:343:GLY:N	2.37	0.40
1:2:244:PHE:CD1	1:2:268:VAL:HG21	2.57	0.40
2:3:10:LYS:O	2:3:14:ARG:NE	2.45	0.40
2:3:44:LEU:HD22	2:3:77:LEU:CD1	2.51	0.40
4:5:586:VAL:O	4:5:589:ARG:HG3	2.21	0.40
5:6:586:LEU:HD21	5:6:637:VAL:HG22	2.03	0.40
6:7:144:GLU:CB	6:7:162:THR:HG21	2.52	0.40
6:7:172:GLU:OE1	6:7:263:ARG:NH2	2.54	0.40
6:7:223:GLN:OE1	6:7:226:GLY:N	2.45	0.40
6:7:380:MET:O	6:7:520:LEU:HA	2.21	0.40
6:7:418:VAL:HG23	6:7:428:THR:O	2.22	0.40
2:3:608:THR:OG1	2:3:610:ARG:HB2	2.20	0.40
3:4:468:ILE:HD11	3:4:483:LEU:CD1	2.52	0.40
4:5:120:GLN:NE2	4:5:247:SER:OG	2.54	0.40
6:7:381:GLY:HA2	6:7:490:PRO:CD	2.52	0.40
9:A:244:LEU:O	9:A:246:LEU:N	2.55	0.40
11:L:113:LEU:HD23	11:L:114:ARG:N	2.36	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	597/887 (67%)	471 (79%)	124 (21%)	2 (0%)	41	74
2	3	567/819 (69%)	452 (80%)	114 (20%)	1 (0%)	47	78
3	4	602/866 (70%)	502 (83%)	99 (16%)	1 (0%)	47	78
4	5	560/733 (76%)	433 (77%)	124 (22%)	3 (0%)	29	66
5	6	591/817 (72%)	474 (80%)	112 (19%)	5 (1%)	19	56
6	7	618/720 (86%)	530 (86%)	88 (14%)	0	100	100
9	A	536/575 (93%)	441 (82%)	94 (18%)	1 (0%)	47	78
10	H	193/202 (96%)	149 (77%)	44 (23%)	0	100	100
11	L	169/203 (83%)	135 (80%)	34 (20%)	0	100	100
12	M	158/212 (74%)	119 (75%)	38 (24%)	1 (1%)	25	62
13	N	199/228 (87%)	163 (82%)	35 (18%)	1 (0%)	29	66
All	All	4790/6262 (76%)	3869 (81%)	906 (19%)	15 (0%)	44	74

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	6	497	PRO
5	6	617	ILE
4	5	303	GLY
12	M	142	ALA
1	2	473	HIS
1	2	625	SER
4	5	366	LEU
13	N	131	LYS
2	3	348	GLN
5	6	362	LEU
5	6	417	SER
9	A	245	LEU
3	4	209	PRO

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Mol	Chain	Res	Type
5	6	608	ILE
4	5	206	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	531/781 (68%)	490 (92%)	41 (8%)	13	43
2	3	502/699 (72%)	472 (94%)	30 (6%)	19	50
3	4	545/759 (72%)	526 (96%)	19 (4%)	36	63
4	5	497/630 (79%)	474 (95%)	23 (5%)	27	57
5	6	526/718 (73%)	494 (94%)	32 (6%)	18	50
6	7	541/630 (86%)	514 (95%)	27 (5%)	24	55
9	A	469/501 (94%)	439 (94%)	30 (6%)	17	48
10	H	170/176 (97%)	157 (92%)	13 (8%)	13	43
11	L	158/184 (86%)	148 (94%)	10 (6%)	18	49
12	M	146/188 (78%)	138 (94%)	8 (6%)	21	53
13	N	184/205 (90%)	176 (96%)	8 (4%)	29	58
All	All	4269/5471 (78%)	4028 (94%)	241 (6%)	25	53

All (241) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	244	PHE
1	2	245	ASP
1	2	258	THR
1	2	271	SER
1	2	284	LYS
1	2	307	LEU
1	2	314	CYS
1	2	337	CYS
1	2	374	ARG

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Mol	Chain	Res	Type
1	2	381	VAL
1	2	420	PHE
1	2	423	VAL
1	2	438	VAL
1	2	442	THR
1	2	484	LEU
1	2	506	ILE
1	2	520	TYR
1	2	522	GLU
1	2	524	VAL
1	2	532	THR
1	2	547	ARG
1	2	552	ARG
1	2	553	GLU
1	2	570	LEU
1	2	574	PHE
1	2	581	ASP
1	2	584	SER
1	2	590	GLU
1	2	610	THR
1	2	621	ARG
1	2	643	ASP
1	2	645	LEU
1	2	660	LEU
1	2	670	LYS
1	2	697	LEU
1	2	737	LEU
1	2	742	ARG
1	2	749	ARG
1	2	778	SER
1	2	792	ARG
1	2	798	TYR
2	3	20	LEU
2	3	63	LEU
2	3	77	LEU
2	3	106	ARG
2	3	125	GLU
2	3	153	GLU
2	3	190	TYR
2	3	196	LEU
2	3	214	VAL
2	3	231	ARG

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Mol	Chain	Res	Type
2	3	254	ARG
2	3	275	ARG
2	3	283	LYS
2	3	302	ILE
2	3	308	VAL
2	3	341	ASP
2	3	346	LYS
2	3	347	SER
2	3	363	THR
2	3	402	CYS
2	3	466	LEU
2	3	473	ARG
2	3	478	PHE
2	3	481	LEU
2	3	483	VAL
2	3	497	VAL
2	3	544	LEU
2	3	597	VAL
2	3	603	ARG
2	3	617	ARG
3	4	157	THR
3	4	200	LEU
3	4	221	PHE
3	4	231	CYS
3	4	296	SER
3	4	316	THR
3	4	338	HIS
3	4	411	VAL
3	4	419	VAL
3	4	462	ASP
3	4	500	GLN
3	4	510	LEU
3	4	550	THR
3	4	608	GLN
3	4	613	THR
3	4	653	LEU
3	4	676	ARG
3	4	689	LEU
3	4	726	ARG
4	5	27	LEU
4	5	63	TYR
4	5	94	PHE

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Mol	Chain	Res	Type
4	5	130	THR
4	5	137	SER
4	5	151	VAL
4	5	202	CYS
4	5	244	CYS
4	5	258	VAL
4	5	376	LEU
4	5	384	LYS
4	5	439	VAL
4	5	448	ARG
4	5	504	MET
4	5	505	PRO
4	5	555	LEU
4	5	567	THR
4	5	574	SER
4	5	582	LYS
4	5	602	ARG
4	5	617	ARG
4	5	636	VAL
4	5	652	MET
5	6	54	THR
5	6	55	LEU
5	6	56	GLU
5	6	57	VAL
5	6	114	ARG
5	6	152	CYS
5	6	167	LYS
5	6	182	ARG
5	6	194	PHE
5	6	195	LEU
5	6	199	LYS
5	6	227	VAL
5	6	239	THR
5	6	299	THR
5	6	301	ARG
5	6	346	LEU
5	6	365	PHE
5	6	379	ARG
5	6	398	LEU
5	6	405	SER
5	6	410	TYR
5	6	425	VAL

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Mol	Chain	Res	Type
5	6	451	ILE
5	6	471	GLN
5	6	476	ILE
5	6	478	ARG
5	6	521	ARG
5	6	533	ASN
5	6	579	SER
5	6	609	THR
5	6	611	ARG
5	6	644	LEU
6	7	25	ASP
6	7	149	ILE
6	7	155	GLN
6	7	160	LEU
6	7	162	THR
6	7	173	VAL
6	7	198	LEU
6	7	212	ARG
6	7	220	LEU
6	7	238	GLN
6	7	269	ASP
6	7	295	GLU
6	7	307	ASN
6	7	308	LYS
6	7	336	LEU
6	7	387	LYS
6	7	438	ASP
6	7	448	ASP
6	7	461	VAL
6	7	466	THR
6	7	475	MET
6	7	484	ILE
6	7	489	ASN
6	7	531	LEU
6	7	546	GLN
6	7	568	ARG
6	7	636	LEU
9	A	12	ARG
9	A	18	ARG
9	A	68	ASP
9	A	74	LEU
9	A	77	CYS

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Mol	Chain	Res	Type
9	A	115	VAL
9	A	132	THR
9	A	166	ASP
9	A	183	ARG
9	A	188	ARG
9	A	205	THR
9	A	207	PHE
9	A	221	LEU
9	A	255	THR
9	A	256	LEU
9	A	258	LEU
9	A	285	PHE
9	A	295	ARG
9	A	296	HIS
9	A	311	CYS
9	A	324	LEU
9	A	369	ILE
9	A	405	THR
9	A	409	CYS
9	A	441	ARG
9	A	471	SER
9	A	507	LEU
9	A	514	CYS
9	A	551	PHE
9	A	564	THR
10	H	14	ASP
10	H	15	LEU
10	H	16	LEU
10	H	34	VAL
10	H	37	VAL
10	H	61	ARG
10	H	70	ARG
10	H	80	CYS
10	H	86	TYR
10	H	89	CYS
10	H	95	LEU
10	H	112	CYS
10	H	155	ILE
11	L	2	ASP
11	L	27	HIS
11	L	29	ILE
11	L	75	LYS

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Mol	Chain	Res	Type
11	L	85	THR
11	L	113	LEU
11	L	114	ARG
11	L	141	THR
11	L	160	LEU
11	L	169	ARG
12	M	30	LYS
12	M	47	GLU
12	M	70	THR
12	M	85	CYS
12	M	109	THR
12	M	126	ARG
12	M	163	THR
12	M	174	THR
13	N	29	ASP
13	N	39	LEU
13	N	107	CYS
13	N	133	LEU
13	N	154	LYS
13	N	171	ARG
13	N	207	SER
13	N	228	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	289	GLN
1	2	439	GLN
1	2	586	HIS
1	2	591	GLN
1	2	671	HIS
1	2	694	GLN
1	2	699	GLN
1	2	714	ASN
2	3	7	GLN
2	3	55	ASN
2	3	233	GLN
2	3	551	GLN
2	3	586	ASN
3	4	204	HIS
3	4	344	HIS
3	4	353	GLN

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Mol	Chain	Res	Type
3	4	368	GLN
3	4	378	HIS
3	4	520	GLN
3	4	557	GLN
3	4	570	ASN
3	4	699	HIS
4	5	120	GLN
4	5	126	ASN
4	5	134	GLN
4	5	233	GLN
4	5	373	ASN
4	5	420	GLN
4	5	541	ASN
5	6	400	GLN
5	6	471	GLN
5	6	496	ASN
5	6	612	GLN
6	7	479	ASN
6	7	496	ASN
6	7	503	GLN
6	7	546	GLN
9	A	276	ASN
9	A	467	HIS
9	A	540	GLN
10	H	109	GLN
10	H	175	HIS
11	L	55	GLN
12	M	20	GLN
13	N	36	GLN
13	N	69	GLN
13	N	147	ASN
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	$\#\|Z\| > 2$
15	ADP	7	801	-	24,29,29	0.98	2 (8%)	29,45,45	1.65	5 (17%)
15	ADP	6	901	-	24,29,29	0.96	1 (4%)	29,45,45	1.52	4 (13%)
15	ADP	4	901	-	24,29,29	0.96	1 (4%)	29,45,45	1.45	5 (17%)
14	ATP	2	902	-	26,33,33	0.91	1 (3%)	31,52,52	2.00	6 (19%)
14	ATP	3	901	-	26,33,33	0.92	1 (3%)	31,52,52	1.61	5 (16%)
14	ATP	2	901	-	26,33,33	1.00	2 (7%)	31,52,52	1.76	5 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	ADP	7	801	-	-	3/12/32/32	0/3/3/3
15	ADP	6	901	-	-	3/12/32/32	0/3/3/3
15	ADP	4	901	-	-	2/12/32/32	0/3/3/3
14	ATP	2	902	-	-	3/18/38/38	0/3/3/3
14	ATP	3	901	-	-	3/18/38/38	0/3/3/3
14	ATP	2	901	-	-	2/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	7	801	ADP	C5-C4	2.60	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	6	901	ADP	C5-C4	2.59	1.47	1.40
15	4	901	ADP	C5-C4	2.58	1.47	1.40
14	2	902	ATP	C5-C4	2.52	1.47	1.40
14	3	901	ATP	C5-C4	2.51	1.47	1.40
14	2	901	ATP	C5-C4	2.44	1.47	1.40
15	7	801	ADP	C2-N3	2.10	1.35	1.32
14	2	901	ATP	C2'-C1'	-2.08	1.50	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	902	ATP	PA-O3A-PB	-5.95	112.42	132.83
14	2	901	ATP	PB-O3B-PG	-5.13	115.22	132.83
14	2	901	ATP	PA-O3A-PB	-5.03	115.56	132.83
14	2	902	ATP	PB-O3B-PG	-4.76	116.50	132.83
15	7	801	ADP	PA-O3A-PB	-4.39	117.76	132.83
14	2	902	ATP	C3'-C2'-C1'	4.06	107.10	100.98
15	6	901	ADP	PA-O3A-PB	-3.96	119.23	132.83
14	3	901	ATP	PB-O3B-PG	-3.91	119.39	132.83
15	7	801	ADP	N3-C2-N1	-3.91	122.57	128.68
14	3	901	ATP	PA-O3A-PB	-3.85	119.60	132.83
15	4	901	ADP	C3'-C2'-C1'	3.54	106.30	100.98
15	4	901	ADP	PA-O3A-PB	-3.32	121.44	132.83
15	6	901	ADP	C3'-C2'-C1'	3.25	105.88	100.98
15	6	901	ADP	N3-C2-N1	-3.18	123.71	128.68
15	4	901	ADP	N3-C2-N1	-3.16	123.74	128.68
14	3	901	ATP	N3-C2-N1	-3.14	123.77	128.68
14	2	901	ATP	N3-C2-N1	-3.09	123.86	128.68
14	2	902	ATP	N3-C2-N1	-2.98	124.03	128.68
15	7	801	ADP	C2-N1-C6	2.79	123.53	118.75
14	3	901	ATP	C4-C5-N7	-2.71	106.58	109.40
15	6	901	ADP	C4-C5-N7	-2.68	106.61	109.40
14	3	901	ATP	C3'-C2'-C1'	2.60	104.89	100.98
15	4	901	ADP	C4-C5-N7	-2.34	106.96	109.40
14	2	902	ATP	C4-C5-N7	-2.30	107.00	109.40
15	7	801	ADP	C1'-N9-C4	2.29	130.66	126.64
14	2	901	ATP	C4-C5-N7	-2.22	107.08	109.40
14	2	901	ATP	C2'-C3'-C4'	2.22	106.96	102.64
14	2	902	ATP	O4'-C4'-C3'	2.12	109.31	105.11
15	4	901	ADP	O3B-PB-O2B	2.08	115.60	107.64
15	7	801	ADP	O3B-PB-O2B	2.05	115.46	107.64

There are no chirality outliers.

All (16) torsion outliers are listed below:

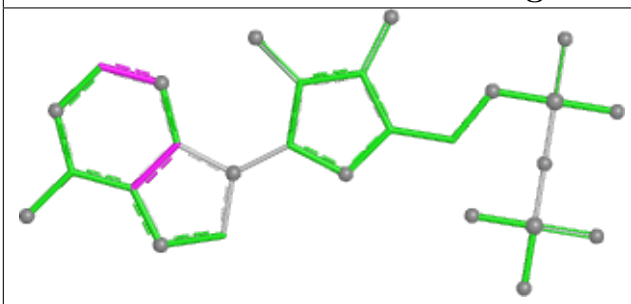
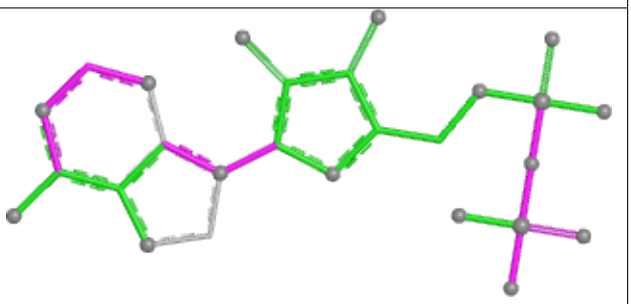
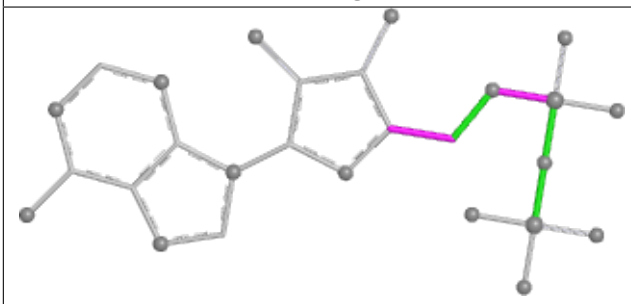
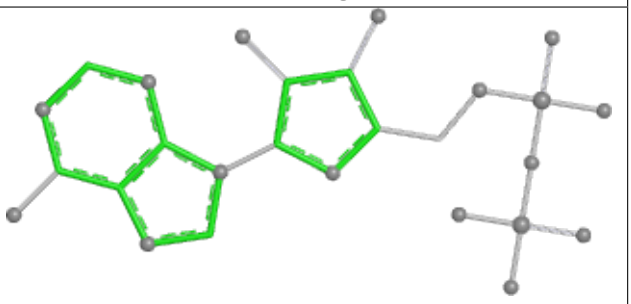
Mol	Chain	Res	Type	Atoms
14	2	902	ATP	C5'-O5'-PA-O1A
14	3	901	ATP	C5'-O5'-PA-O3A
15	4	901	ADP	C5'-O5'-PA-O1A
15	6	901	ADP	C5'-O5'-PA-O3A
15	7	801	ADP	C5'-O5'-PA-O3A
14	2	901	ATP	C3'-C4'-C5'-O5'
14	2	901	ATP	O4'-C4'-C5'-O5'
14	2	902	ATP	C3'-C4'-C5'-O5'
14	2	902	ATP	C5'-O5'-PA-O3A
14	3	901	ATP	C5'-O5'-PA-O1A
15	6	901	ADP	C5'-O5'-PA-O1A
15	7	801	ADP	C5'-O5'-PA-O1A
15	6	901	ADP	O4'-C4'-C5'-O5'
15	7	801	ADP	O4'-C4'-C5'-O5'
15	4	901	ADP	C5'-O5'-PA-O3A
14	3	901	ATP	O4'-C4'-C5'-O5'

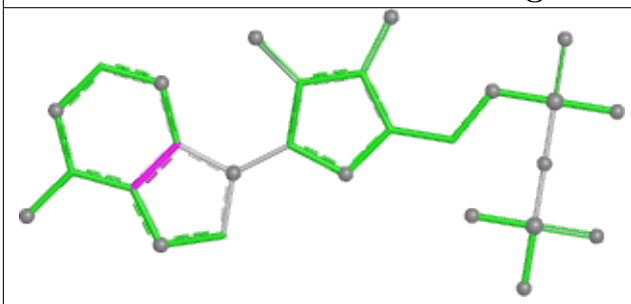
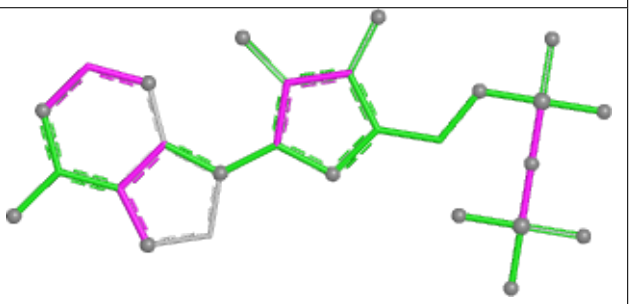
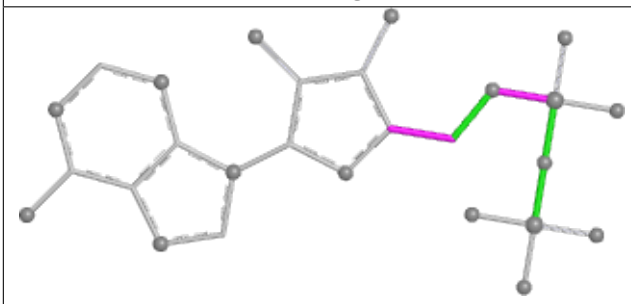
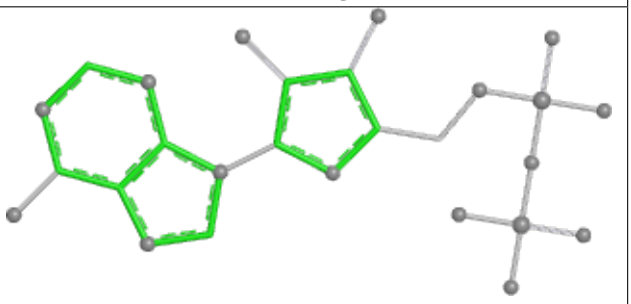
There are no ring outliers.

6 monomers are involved in 36 short contacts:

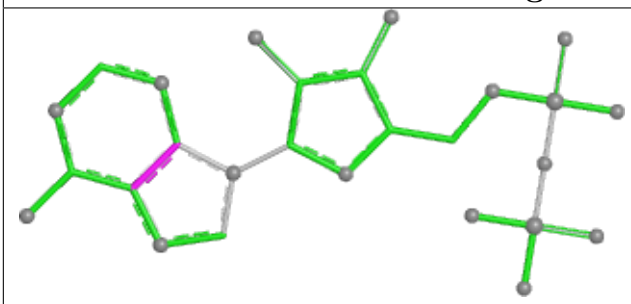
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	7	801	ADP	9	0
15	6	901	ADP	3	0
15	4	901	ADP	1	0
14	2	902	ATP	11	0
14	3	901	ATP	5	0
14	2	901	ATP	7	0

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.

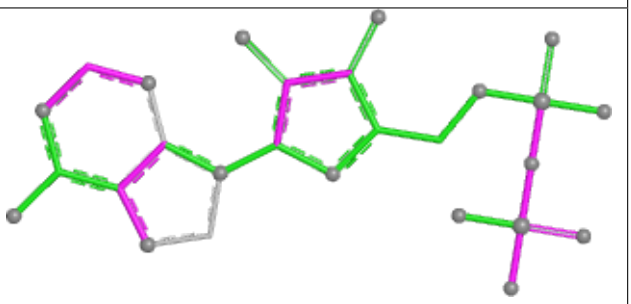
Ligand ADP 7 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP 6 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

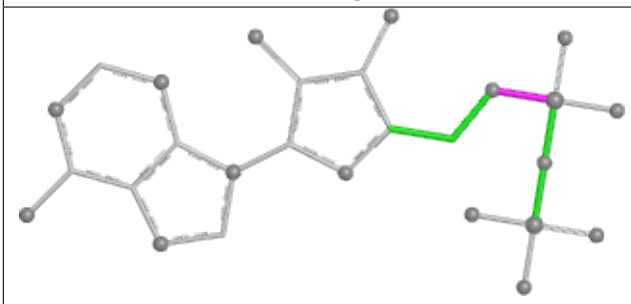
Ligand ADP 4 901



Bond lengths



Bond angles



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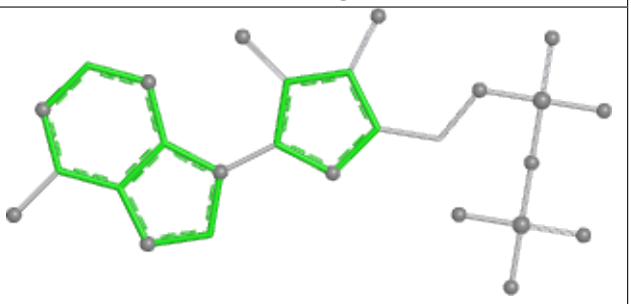
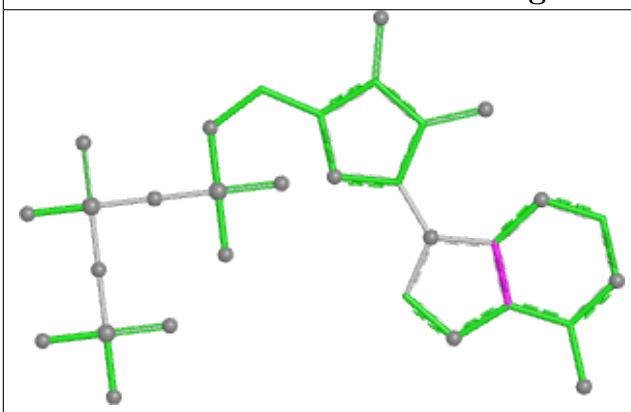
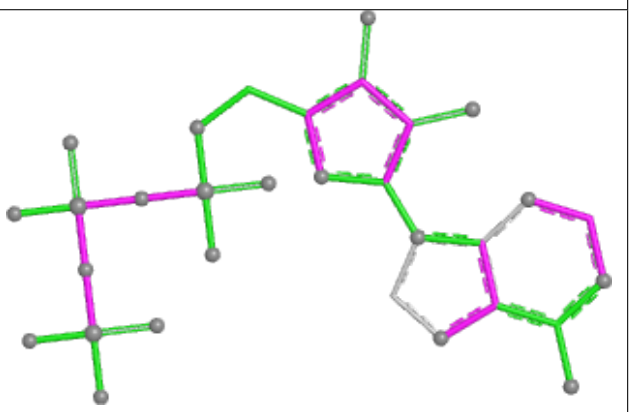


Rings

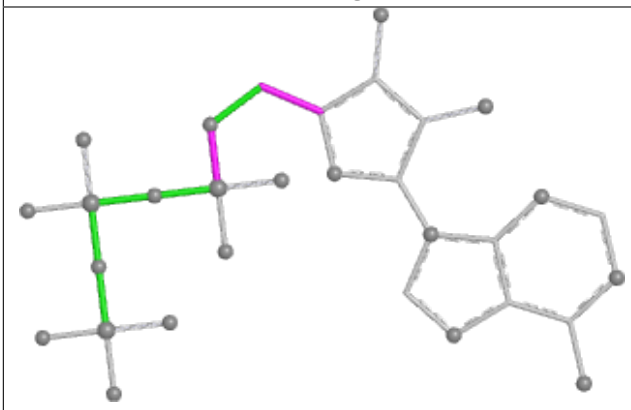
Ligand ATP 2 902



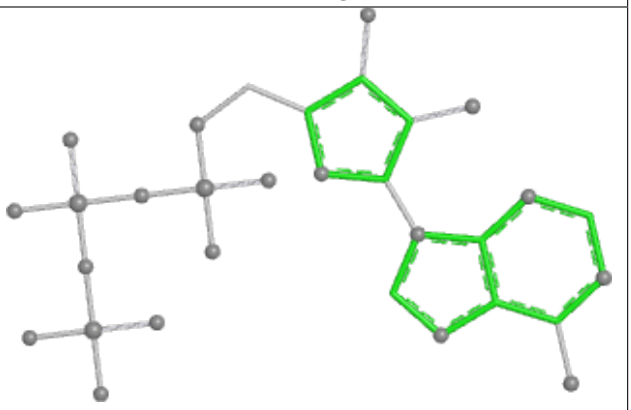
Bond lengths



Bond angles

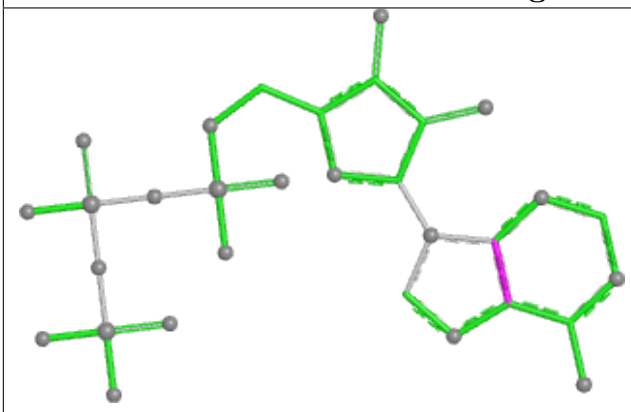


Torsions

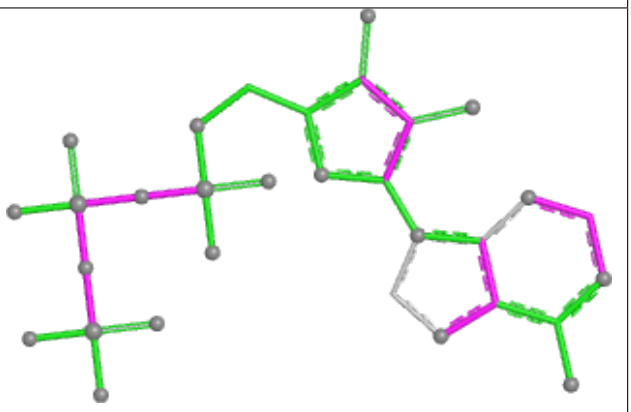


Rings

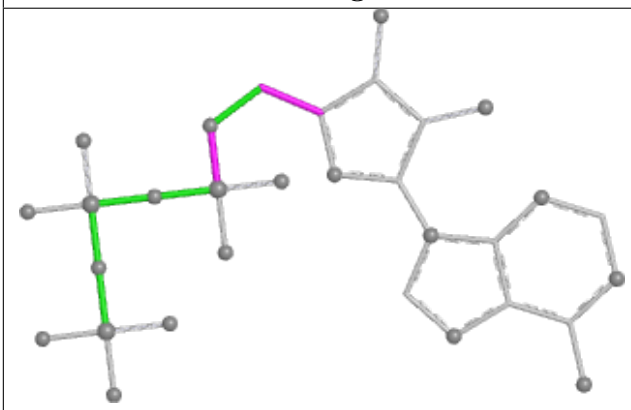
Ligand ATP 3 901



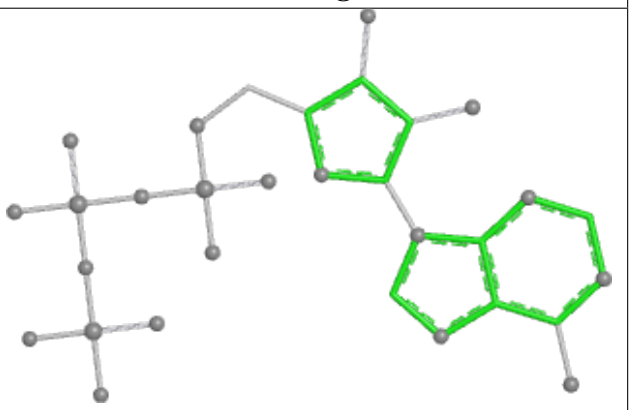
Bond lengths



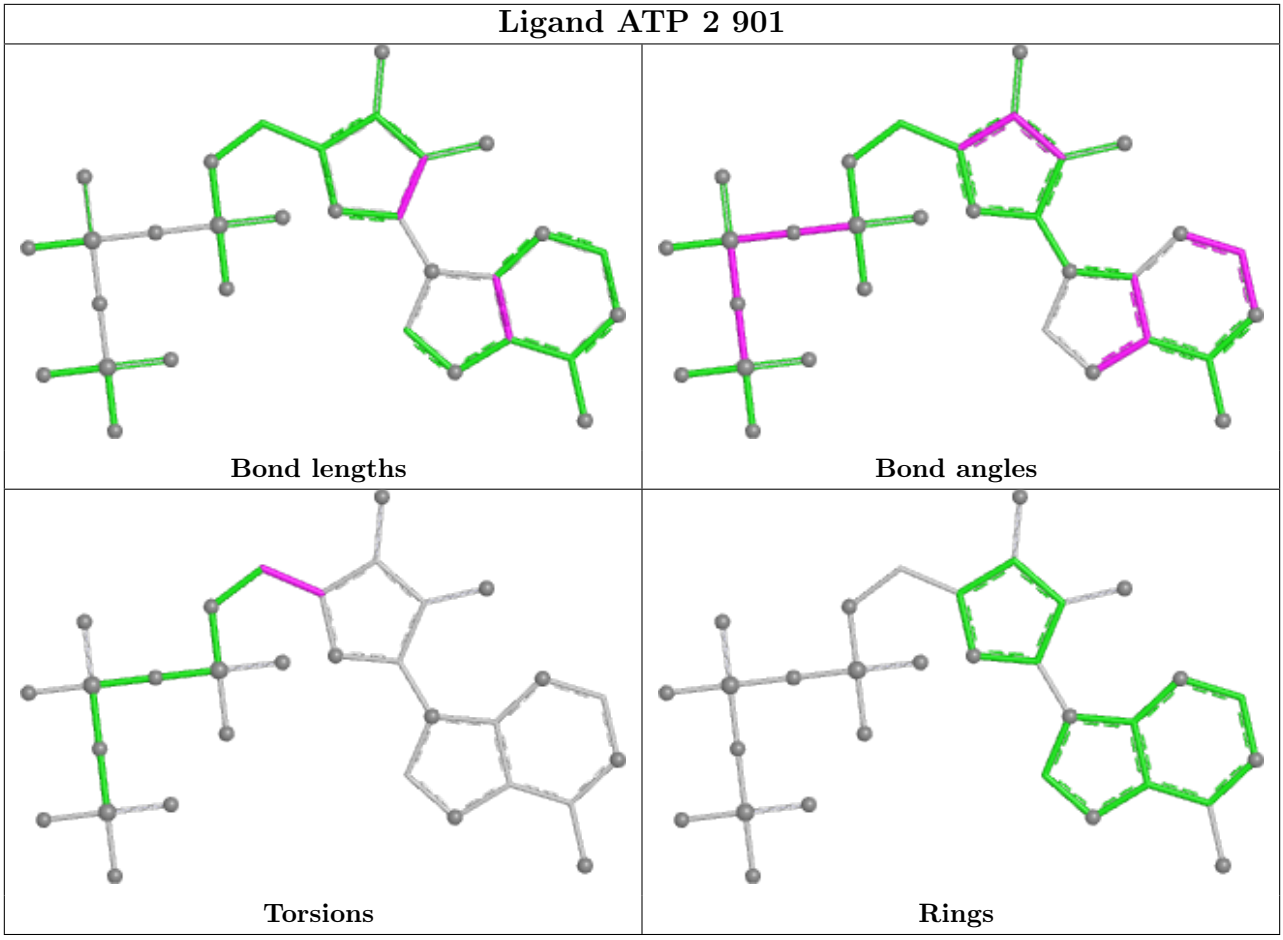
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	7	2

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	10.45
1	7	142:SER	C	143:THR	N	6.25

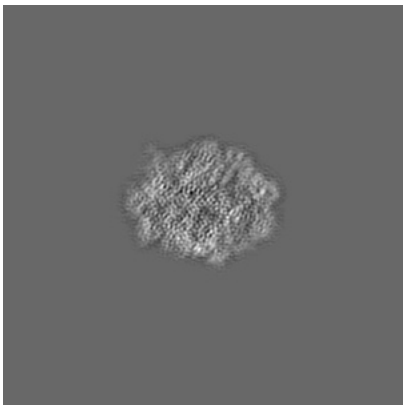
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4785. These allow visual inspection of the internal detail of the map and identification of artifacts.

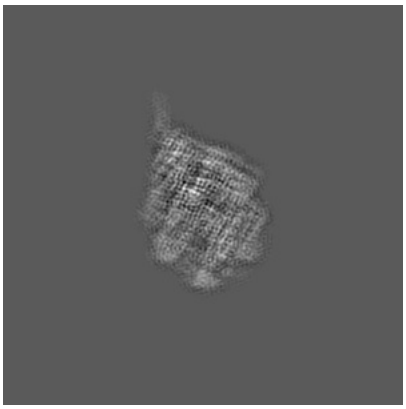
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

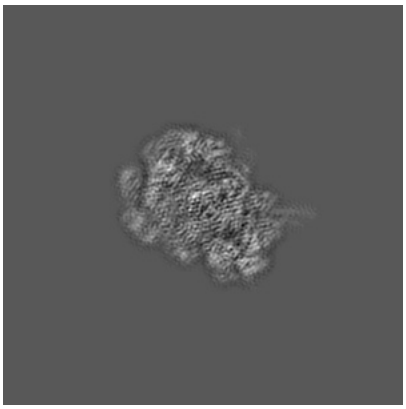
6.1.1 Primary map



X

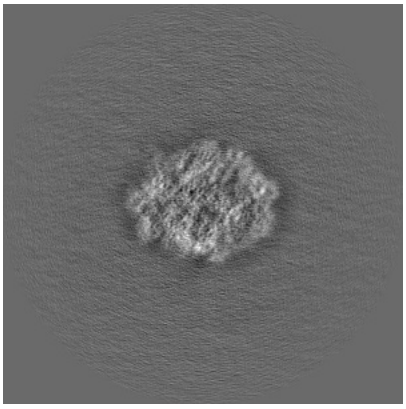


Y

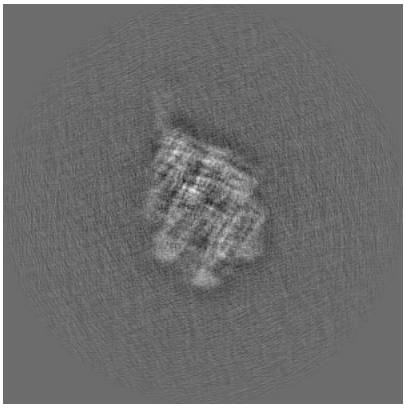


Z

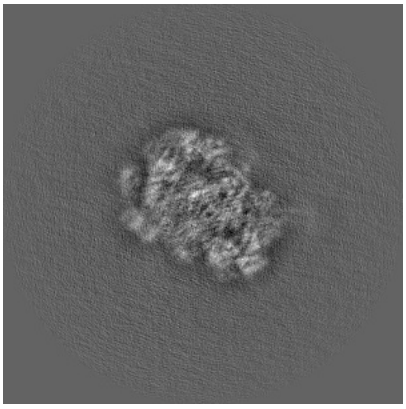
6.1.2 Raw map



X



Y

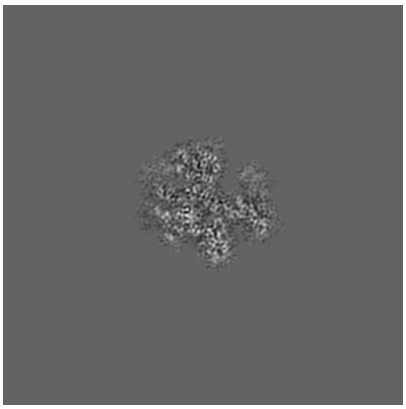


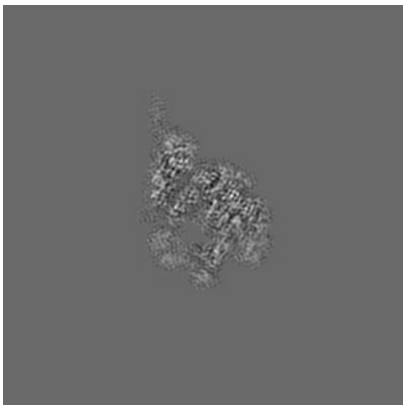
Z

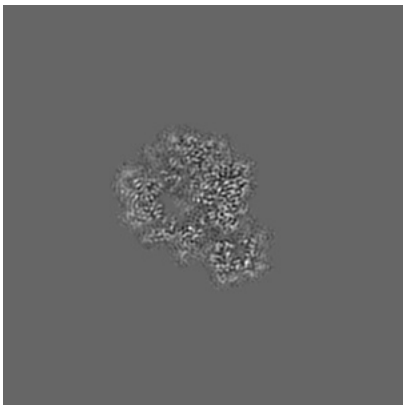
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

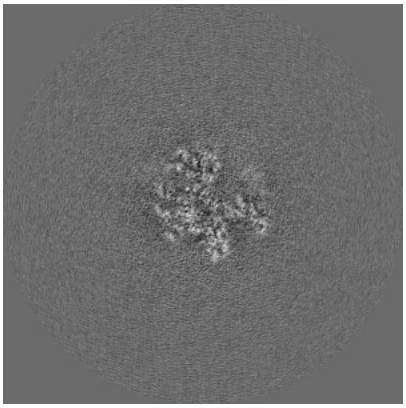
6.2.1 Primary map

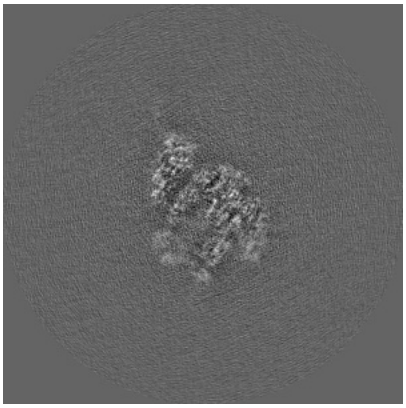

X Index: 192

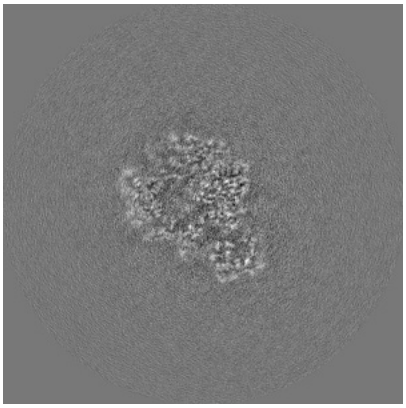

Y Index: 192


Z Index: 192

6.2.2 Raw map


X Index: 192

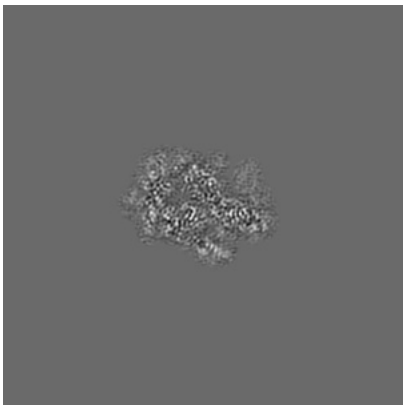

Y Index: 192

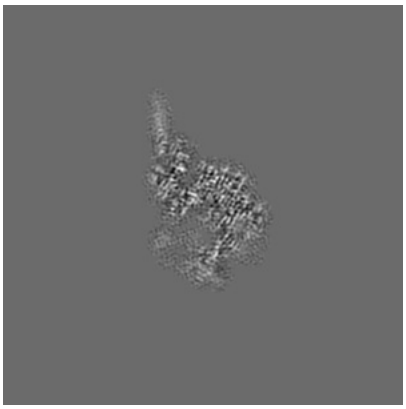

Z Index: 192

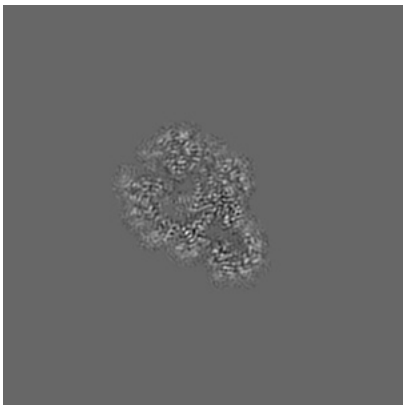
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

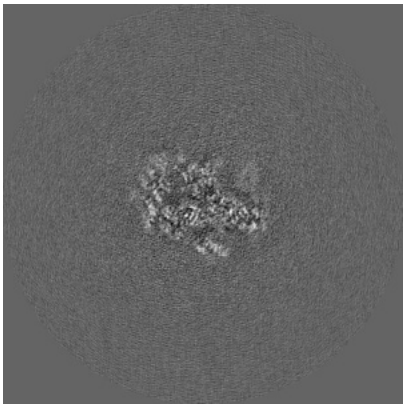
6.3.1 Primary map

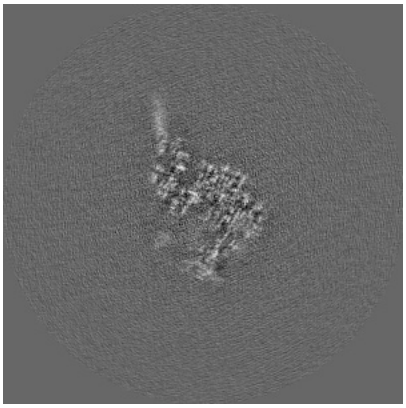

X Index: 204

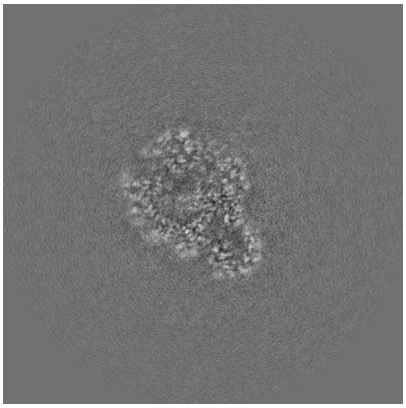

Y Index: 186


Z Index: 198

6.3.2 Raw map


X Index: 203

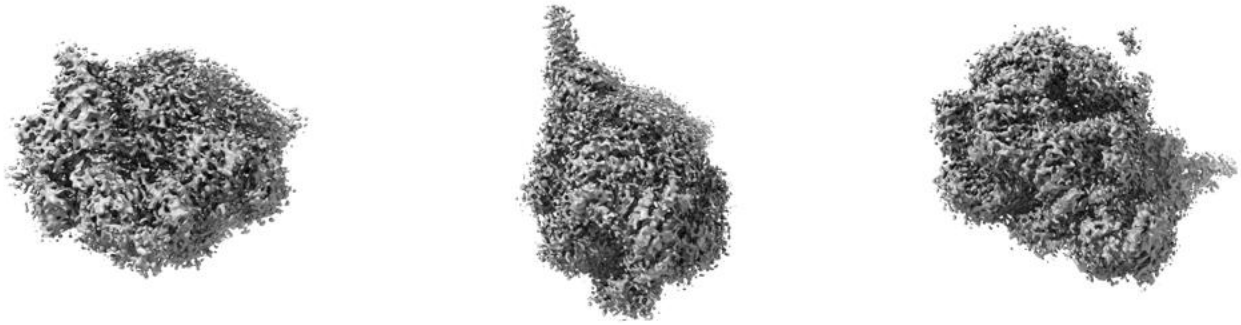

Y Index: 186


Z Index: 198

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 0.007. 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.

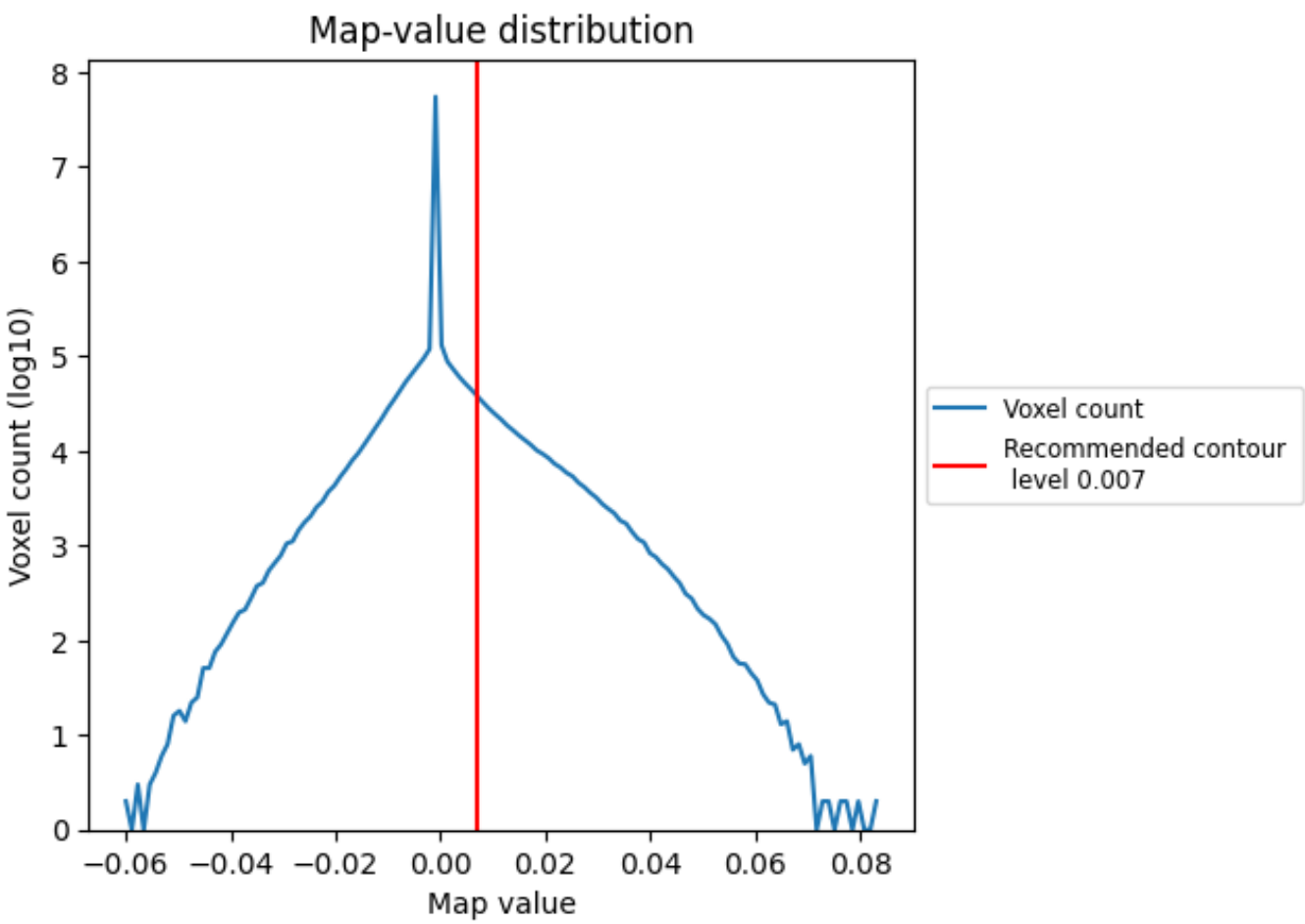
6.5 Mask visualisation (i)

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

7 Map analysis (i)

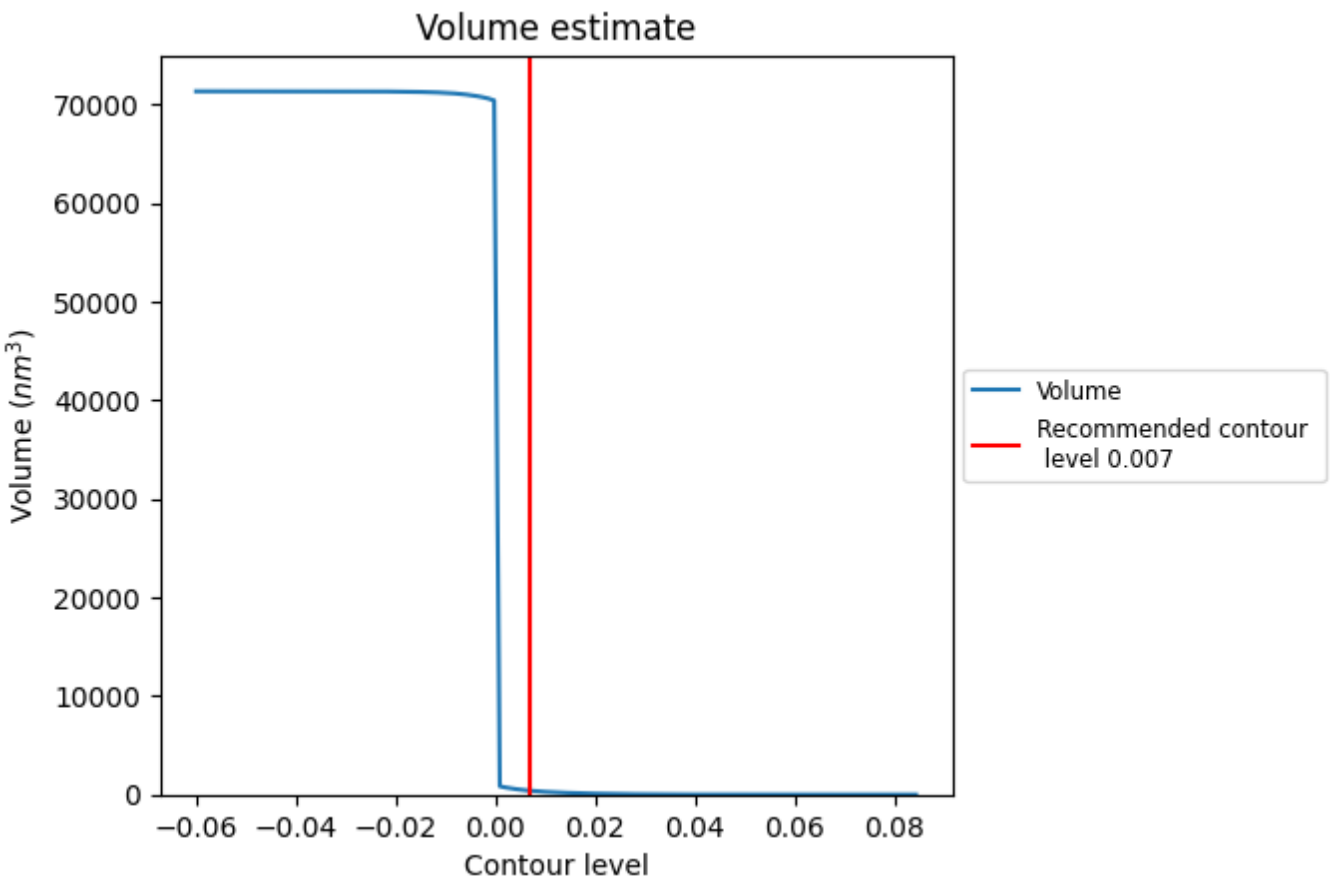
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

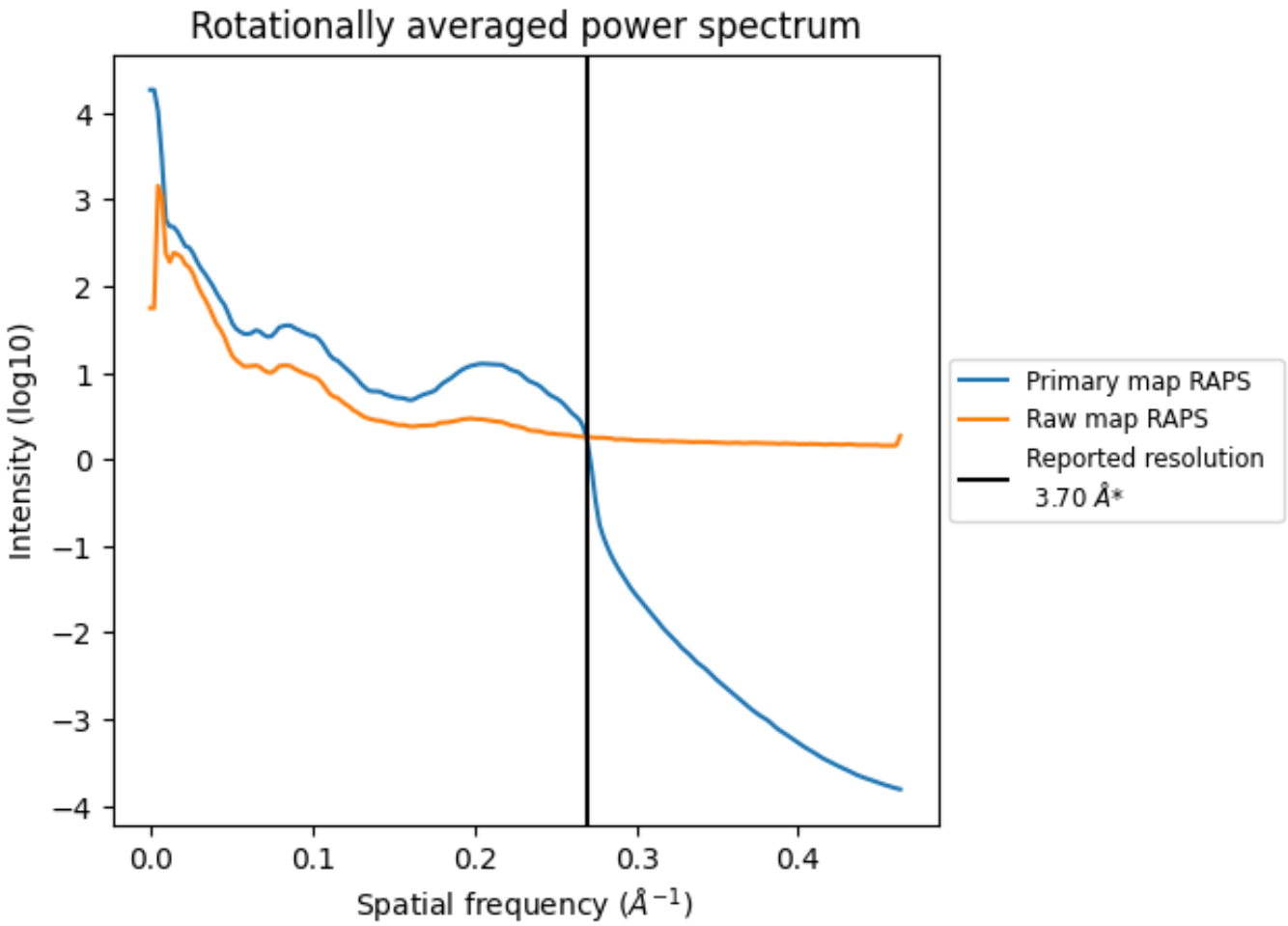
7.2 Volume estimate (i)



The volume at the recommended contour level is 389 nm^3; this corresponds to an approximate mass of 351 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)

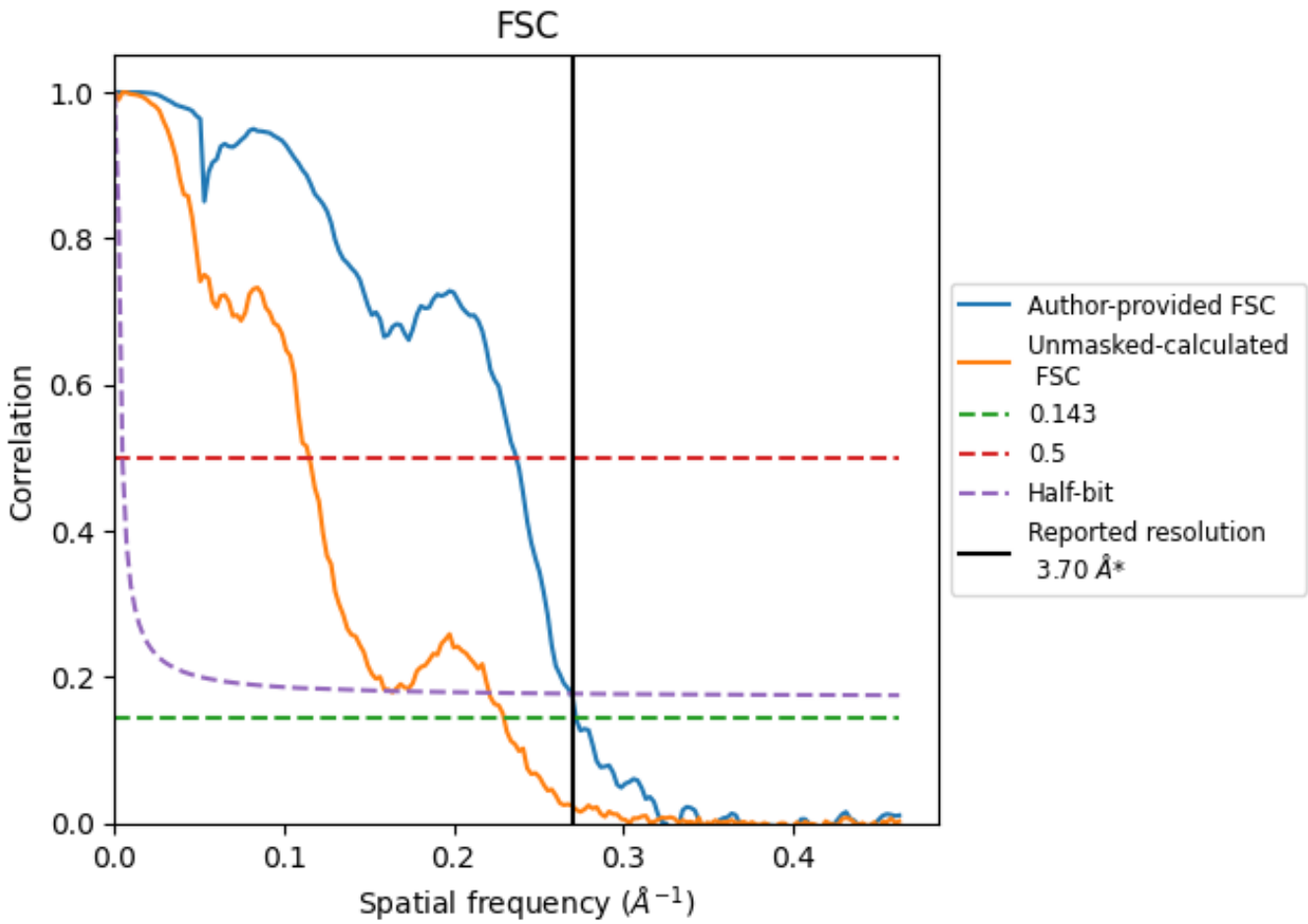


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

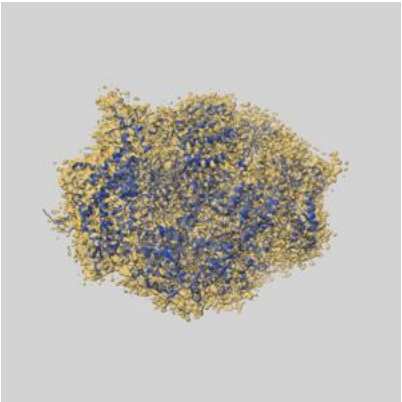
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.67	4.22	3.71
Unmasked-calculated*	4.35	8.70	6.13

*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 4.35 differs from the reported value 3.7 by more than 10 %

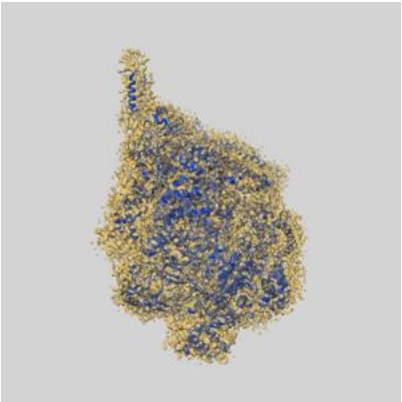
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4785 and PDB model 6RAW. Per-residue inclusion information can be found in section 3 on page 8.

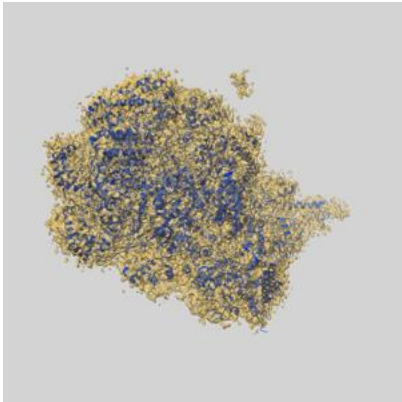
9.1 Map-model overlay (i)



X



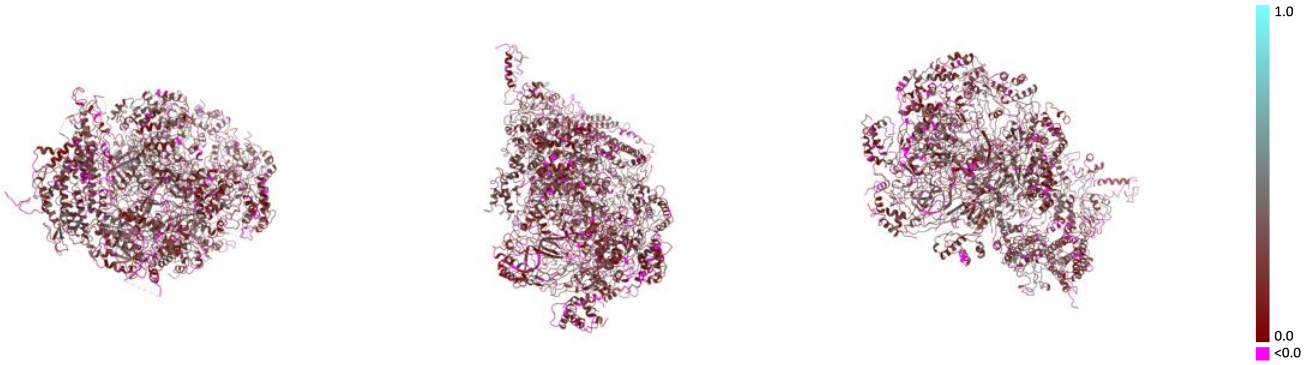
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007 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.

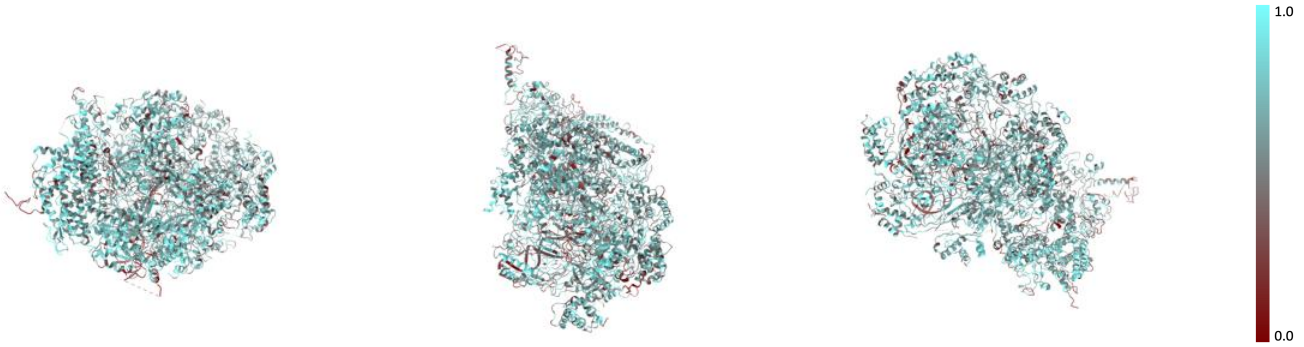
9.2 Q-score mapped to coordinate model (i)



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.

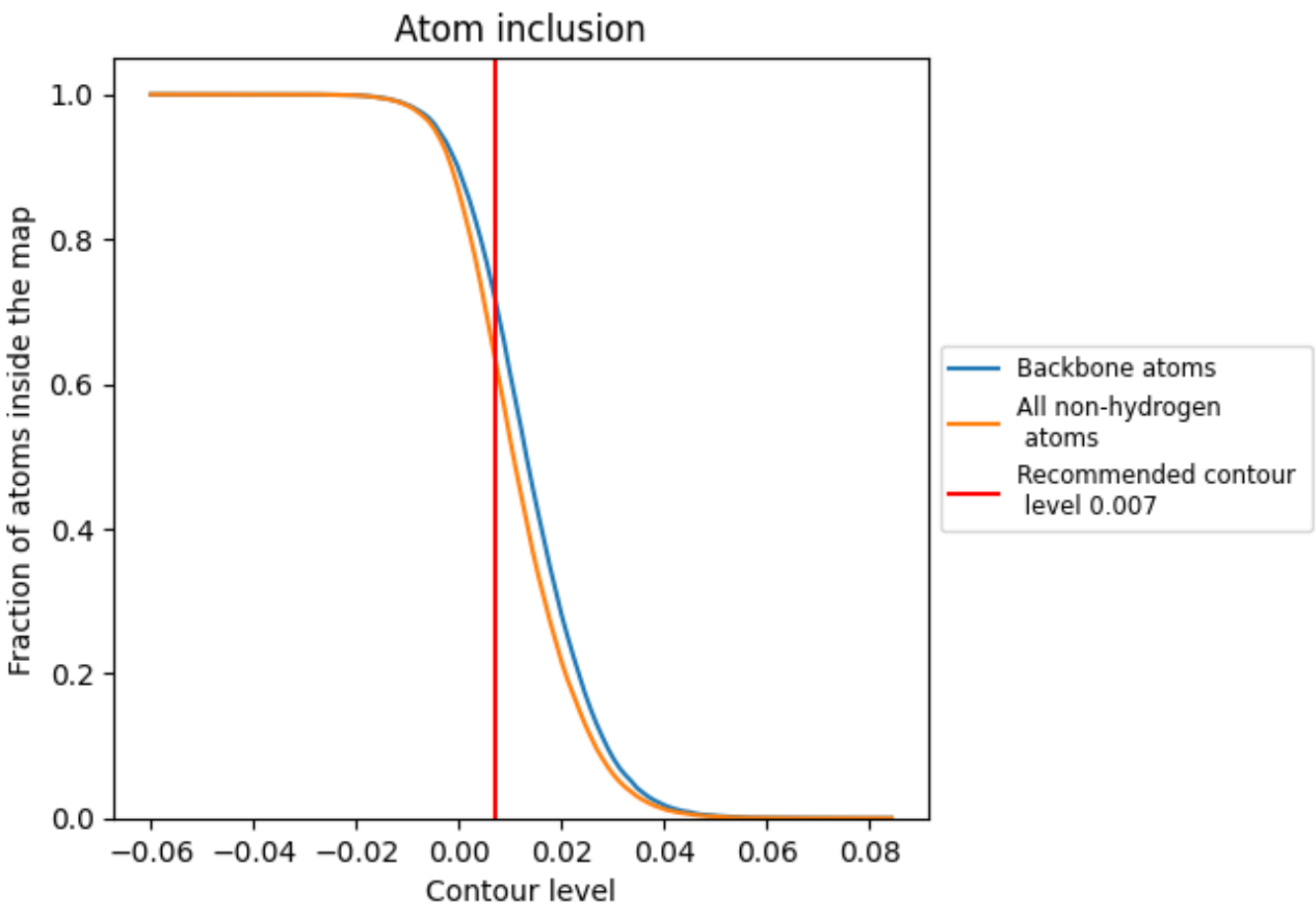
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.007).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6360	0.2150
2	0.6616	0.2350
3	0.6590	0.2350
4	0.6092	0.1810
5	0.6713	0.2520
6	0.6043	0.1870
7	0.6409	0.2290
A	0.6505	0.2160
F	0.3643	0.0840
G	0.2932	0.0700
H	0.5667	0.1460
L	0.7427	0.2770
M	0.6171	0.2070
N	0.6551	0.2090